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ARTICLE

Hydration of Linear Alkanes Is Governed by the Small Length-Scale Hydrophobic Effect

Harshita Singh and Jaeger Srinivas*

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ABSTRACT: Longstanding questions of the hydrophobic effect is well understood for small spherical solutes, for which contact diameter of 2–3 nm and the hydration free energy is either negligibly driven, zero for larger sizes (2–3 nm), or is enthalpically driven. The subtle entropic effect in the case of molecular molecules such as linear alkanes is not understood very clearly now, we have simulated the hydration free energy of linear alkanes using free surface to calculate one of a spherical droplet model of $d = 2$ nm using molecular simulation. We show that the hydration free energy of alkanes, independent of their size, are governed by the small length scale hydrophobic effect. That is, unlike the case of large spherical solutes, the hydration free energies of linear alkanes are enthalpically driven.



1 INTRODUCTION

Molecular interactions in water are ubiquitous in living systems (protein-protein including protein folding, lipid binding, formation of biological membranes) and industrial settings,^{1–4} and self-assembly of surfaces of metal-water interfaces.^{5–7} Many processes are strongly influenced by the size and shape of hydrophobic solutes. For instance, solubility with respect to the size (the number of methylene groups) varies by a factor of 1000 between $n = 1$ and $n = 10$, and a stronger dependence between n of metal-water interface is compared to the case with smaller solute.^{8–10} Contact surface between an aliphatic and water hydrophobic that the ΔG of cavity-shaped ones,¹¹ hydrophobicity varies in a systematic way in length scale-dependent hydration

of small spherical solutes of 1–3 nm and is enthalpically driven, entropically driven, and formation of a hydrogen-bonded network of water molecules around the solute, which results in the loss of their configurational freedom.¹² The hydration free energy of small hydrophobic solutes is characterized by the nature of density fluctuations in the volume of bulk water equivalent to the volume occupied by the solute.^{13–15} Above a critical size of a spherical solute of $d = 2$ nm, water molecules act to form a network through hydrogen bonds around the solute. The water surface fluctuation and associated entropy,¹⁶ hydration of large hydrophobic solutes is thus driven by the entropic loss.¹⁷

Upon freezing, the water-water interface becomes also an air-water interface, therefore the hydration free energy of large alkanes is well captured by the air-water hydrophobic energy.¹⁸

Entropy and enthalpy contributions to the hydration free energy are well understood for spherical solutes, however, lack of understanding is lacking for nonspherical solutes, such

as linear alkanes. Whether or not the gas-liquid-like character of contactless or semienclosed air-water walls at $n = 10$ the underlying mechanism playing a critical role in the hydrophobic hydration of hydrocarbon chains. Therefore, deciphering the hydration behavior of linear alkanes is key to understanding these so-called proteins.¹⁹

Hydration of linear alkanes has been previously studied using both molecular simulation and experiments. Hydration free energies of linear alkanes, with heptane and decane, have been simulated via free energy perturbation (FEP)²⁰ and scaled particle theory (SPT),²¹ respectively. Ferguson et al. utilized the conventional Gibbs ensemble (GE) method to study exchange interaction dynamical (DSE) simulation to study hydration of long linear alkanes up to decane, but did not discuss the enthalpy and entropy contributions.²² Other works have focused on only a few alkanes,²³ in experiments, natural free energies and enthalpies of alkanes, ranging from methane to octane have been determined.^{24–26} Because of the difficulty, systematic determination of the hydration free energy of larger alkanes is unrealistic.²⁷ Along with their hydration, aggregation of alkanes in air-water interface has been studied in both experiments²⁸ and simulations²⁹ because of its importance in understanding biogenesis³⁰ and behavior of amphiphilic polymers³¹ and proteins at various interfaces.³² In this work, we have used umbrella sampling to find

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Determination of Equilibrium Adsorbed Morphologies of Surfactants at Metal-Water Interfaces Using a Modified Umbrella Sampling-Based Methodology

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ABSTRACT: Surfactants adsorb to metal-water interfaces in varied morphologies, including self-assembled monolayers (SAMs), cylindrical and spherical vesicles, or hemispheres. Current molecular simulation methods are unable to efficiently sample the formation of these morphologies because of the large diffusion/energy barriers. We introduce a modified umbrella sampling-based methodology that allows sampling of these morphologies from any initial configuration and avoids long energy differences between them. Using this methodology, we first find energy differences between three lying-down configurations of a model amphiphilic bilayer of sodium dodecylsulfate (SDS) at a gold-water interface (two alkyl tails, unchanged orientation), and another bilayer perpendicular to the surface and then compare it to a gold-water interface. We find that while SDS tails remain between the charged head groups of just a few, their orientation is a quasi-free, strongly hydrophobic interaction between the alkyl tails of just 11 amphiphilic molecules leading to a morphology with adsorbed hemispherical vesicles lying atop a monolayer. Adsorbed molecules adsorb in a densely packed bilayer with the molecules standing up on the surface in the top layer and lying parallel to the surface in the second layer. Cations and anions surfactant moieties display a complex structure between. These results illustrate the use of molecular simulations in studying the nature of adsorbed morphologies of surfactants at metal-water interfaces.

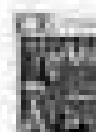


1. INTRODUCTION

Understanding surfactant-metal interactions is important for numerous applications, including corrosion inhibition,¹ membrane fabrication of chemical reactions in heterogeneous catalysis,² synthesis of functional porous composites,³ and regulating electrocatalytic reactions.⁴ Surfactants have a strong affinity to adsorb at metal-water interfaces and display a rich adsorption behavior as a function of their molecular properties. As an example, varying the alkyl tail length of sodium dodecylsulfate (SDS) during the SDS-mediated synthesis of gold nanowires increases the aspect ratio of the nanowires, presumably because longer alkyl tails cause stronger oriented packing in the adsorbed SAM layer,⁵ in the synthesis of gold nanowires, increasing the use of the outer head of surfactants has been shown to enhance the aspect ratio of the nanowires.⁶ Instead, most studies of morphologies of adsorbed surfactants on metal and/or carbon has revealed the formation of plane,⁷ spherical,⁸ and cylindrical vesicles.⁹⁻¹² The formation of these morphologies is assumed to be dictated by molecular geometry,¹³⁻¹⁵ lateral hydrophobic interactions,¹⁶⁻¹⁸ as well as energetic interactions between the adsorbate, surface, and the surrounding.¹⁹⁻²¹ For instance, based on the differences in the electric field magnitude (EFM) images, Kozlov et al. propose that the adsorption of C_{12} TAO molecules on gold is induced by

$h\nu$ interactions resulting in cylindrical vesicles, while C_{12} TAO and sodium dodecyl sulfate (SDS) adsorb as hemispherical vesicles due to the interactions between the alkyl tails and the surface.²² Using ion frequency generation (IFG) microscopy, Khan et al. show that the various alkyl diethyl hexyl ammonium bromide surfactants with four carbon long (C_4) alkyl tails adsorb in random orientations on a gold surface, whereas the ones with C_{12} alkyl tails adsorb in a linear SAM, thereby highlighting the importance of lateral hydrophobic interactions between the alkyl tails in the adsorption.²³ It should be noted that in these studies, the AFM and IFG microscopy have resolutions of, at best, tens of nanometers and therefore are unable to resolve the morphologies at the atomic scale.

While it is recognized that multiple factors influence the adsorption morphology of surfactants at metal-water interfaces, by utilizing existing insights to predict the various morphologies, [Benson, September 21, 2020](#)
[Mishra, December 14, 2020](#)



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A Comparative Study of Supervised and Unsupervised Machine Learning Algorithms on Consumer Reviews

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Abstract—For any organization handling consumers, reviews and feedbacks are quite important. For this purpose, the bulk of data is generated from various social networking sites in form of reviews and feedbacks. In order to understand consumer's perception about its firm, this research evaluates various supervised and unsupervised machine learning algorithms on two data sets. A comparative analysis is made for determining the efficiency of these algorithms on dataset datasets for text classification. This research is an attempt to find the best fit classifier for consumer's perception using sentiment analysis. So, in order to accomplish this objective, built text preprocessing techniques are applied on datasets that feature various techniques are applied on the provided data. Thereafter, classification and clustering are applied using supervised and unsupervised machine learning algorithms respectively. Further, these algorithms are evaluated and the result reveals that supervised machine learning algorithms especially Support Vector Machine (SVM) outperforms unsupervised machine learning algorithms for genuine dataset. And Naive Bayes (NB), Logistic Regression (LR) outperforms unsupervised machine learning algorithm for consumer dataset.

Index Terms—Support Vector Machine (SVM), K-Means Clustering (KMC), Decision Tree (DT), Random Forest (RF), Logistic Regression (LR), Natural Language Toolkit (NLTK), K-Means clustering(KMC), Hierarchical clustering (HC), neural language processing (NLP)

I. INTRODUCTION

In recent times, social comments and social networking sites like Twitter, Facebook, LinkedIn, Amazon etc. have become a prominent source to express and dispense reviews, and also to get opinions regarding products, services, business, health, resources etc [1]. All of this processed information flows as organization to its enhancement in their product quality, sales, services and profits [2]. It is really difficult to reach out directly to its consumers by an organization or business. Therefore, sentiment analysis on reviews and feedbacks serves as means with its consumers. For this purpose, text classification is recommended. Text classification is the mechanism of categorizing text into different organized groups. In text classification process, NLP and various classification algorithms assigns predefined labels to text according to its content [3]. In text classification, data is

classified in distinct categories (positive, negative and neutral) based on the polarity of text data. Text clustering generates the clusters based up on the similarity of data and it is one of the applications of cluster analysis. It uses MLP and machine learning to understand and categorize clusters of text data. As per our literature study there is very little discussion about comparison between supervised and unsupervised machine learning algorithms. So, in this research text classification and text clustering of consumer's reviews has been performed on two data sets using supervised and unsupervised machine learning algorithms by using the motivation from [4]. For this purpose, a comparison of various supervised (SVM, DT, RF, LR, NB) and unsupervised (KMC, KMC) machine learning algorithms has been attempted to find the best fit algorithm for sentiment analysis using consumer's reviews. Thus, only two unsupervised machine learning algorithms (KMC, KMC) are used among all unsupervised algorithms. Hence clustering, Hierarchical clustering, Principle Component Analysis, independent component analysis, Apriori algorithm, Singular value decomposition) none being most of these algorithms are used to work with dimensionality reduction, matrix decomposition and association rule mining [5], [6], [7], [8].

The structure of this research includes a related work in section II. Section III demonstrates the research methodology followed by supervised and unsupervised machine learning algorithms. Experimental setup and results are discussed in section IV. Finally, section V describes the conclusion and future scope of this research.

II. RELATED WORK

To extract fruitful knowledge from data there is a need to convert this data to structured form and NLP plays crucial role in it. NLP is very useful in classification, extraction, speech tagging, etc. [9]. NLP algorithms mainly depend on machine learning algorithms for learning various rules [10]. In literature [11] the analysis of various supervised and unsupervised algorithms was performed on the basis of consumer's feelings, opinions, interests and experiences about a specific product. The result depicts that LR outperforms NB.

Improvisation in opinion mining using data preprocessing techniques based on consumer's review

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Abstract

In today's digital age, an enormous volume of data is generated daily from various internet sources, including social media sites, emails, and customer reviews. With competition on the rise, it has become essential for organizations to understand their customer needs and preferences. To gain meaningful insights from business language data, such as reviews, and understand customer perceptions, sentiment analysis is an effective method. This research article presents a new preprocessing approach consisting of three stages: data collection, cleaning, and transformation. The approach was applied to three datasets - restaurant, cell phone, and purchase - and evaluated using various machine learning classifiers for sentiment prediction. A comparison was made between two sets of techniques: set1 employed data cleaning and transformation with stemming, while set2 used data cleaning and transformation with lemmatization. The results indicated that set1 data cleaning, transformation with lemmatization performed better during preprocessing when evaluated using various machine learning classifiers, such as support vector machine (SVM), logistic regression (LR), decision tree (DT), random forest (RF), and Naive Bayes (NB). Specifically, SVM LR, DT, and NB performed better for the restaurant dataset, while DT, LR, and RF outperformed for the cell phone dataset. In the purchase dataset, LR, DT, and NB outperformed for set1 compared to set2. Working with the best preprocessing techniques for subsequent comparison. Additionally, another comparison was made between two sets of techniques: set1 included data cleaning, transformation with lemmatization, and synonym phrases, while set2 either included text cleaning, transformation with lemmatization, and synonym phrases. The sets were evaluated using machine learning classifiers, and the results revealed that set1 performed better with most classifiers.

Keywords

Support vector machine (SVM), Random forest (RF), Decision tree (DT), Logistic regression (LR), Naive Bayes (NB).

1. Introduction

The consumer is one of the assets of every organization. In order to survive in this competitive marketplace, it is mandatory for every organization to assess the sentiments, expectations, and feedback of consumers. For this assessment, it is required to perform the sentiment analysis of data collected from various internet sources. The data collected from various internet sources consists various types of attributes such as tags, hashtags, directions, language (HTML) tags, timestamps, distributions, special characters, and text spacing factor (TRF), etc. Due to this, it becomes difficult for both business and customer to get the exact meaning of the reviews.

Moreover, the presence of this unwanted noise in data increases the dissimilarity between each word in the text. It is considered a serious threat and it becomes challenging for classifiers to classify this noisy data. So, to get accurate sentiments it is mandatory to remove this unwanted noise from the data. In previous studies, various preprocessing techniques were used for different types of datasets and all these techniques were evaluated to find the best preprocessing techniques using various classifiers such as support vector machine (SVM), logistic regression (LR), decision tree (DT), random forest (RF), Naive Bayes (NB).

Some of the basic preprocessing approaches like removal of stop words, punctuation, abbreviation, spell correction [1-3] stemming/lemmatization were used in various pieces of research. Similarly, various

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QUALITY OF LIFE AND PSYCHOLOGICAL DISTRESS AMONG SELF-HELP GROUP AFFILIATED AND HOSPITALIZED AIDS PATIENTS

Hardeep Lal Joshi¹, Rahnaf² and Kaldeep³

ABSTRACT

Background: The disease that is feared in terms of the twenty-first century is AIDS. Mental health professionals are currently looking for some psychosocial approaches for these patients to cut alongside pharmacological treatment for AIDS victims to lessen their distress. **Objective:** The current study intends to examine the effects of AIDS patients' affiliation with the self-help groups on their psychological distress and quality of life. **Participants:** A group of 137 AIDS patients participated in the investigation (71 affiliated with a self-help group and 66 hospitalized). The 50 age range from 22 to 57 years. **Measuring Tools:** WHO Quality of Life-Brief and General Health Questionnaire-12 were administered on all the participants of the study. **Data Analysis:** Collected data was subjected to T-test and Discriminant Functional Analysis. **Findings:** The study revealed that AIDS patients who are a part of a self-help group have a better quality of life and suffer less psychological distress than hospitalized patients. The findings of the discriminant analysis concluded that both groups showed discrimination in not distress (i.e., Physical health, of quality of life).

Key Words: Quality of Life, Psychological Distress, AIDS patients, Self-Help Group

INTRODUCTION

Human immunodeficiency virus (HIV) is one of the most devastating diseases of the 21st century. Professionals and health practitioners have tried various strategies and pharmacological treatments for HIV patients. Although they achieved great success but a complete solution is yet to be seen. Now, mental health professionals are trying psychological treatment along with pharmacotherapy to treat these patients. The trained psychological interventions used till date are support groups and peer-to-peer interventions. The former focuses on professionally facilitated groups (1, 14, 12 participants), whereas the latter arranges reducing the stress and have among AIDS patients (18-14 participants). Some studies used peer approaches with a co-facilitator alongside a trained therapist (12, 25 participants). Professionals and healthcare personnel have the chance to deal with HIV/AIDS patient's difficulties effectively through support groups. The World Health Organization (WHO) recommended using support groups as interventional groups to increase patient literacy, promote ART adherence, and address their psychosocial needs. As a result, stigma and discrimination associated with the disease are reduced, self-esteem is increased, coping skills are strengthened, and psychosocial functioning is improved. These groups also assist and motivate people to share their experiences.

HIV drastically impacts a person's physical, social, and psychological health (Langer-Saunders et al., 2016). More HIV/AIDS patients than the general population

suffer mental health issues like depression and anxiety. Psychological distress has been shown to have a detrimental effect on the quality of life in several pieces of research (Samitar et al., 2016; Niu et al., 2016; Ye et al., 2016). Higher degrees of psychological distress and functional impairment were linked to a lower life quality (Adebo et al., 2013). Compared to the general people, the quality of life is lower and psychological discomfort is higher among HIV-positive women (Yvarek & Gull, 2015).

Self-help support group supports people living with HIV who cannot engage in daily life activities in the presence of others. HIV-positive individuals, their caregivers, families, and stress receive psychosocial help for their persistent psychological and social issues. The focus of previously published literature on psychological aid has been on (a) clinical arrangements or services related to care (Dargatzis et al., 2015; Gebrey et al., 2008) (b) certain group-supporting interventions (Dargatzis et al., 2015; Moked et al., 2011; Pardo & Bard, 2017), or (c) conclusions for patient groups (Cripps et al., 2009; Scott-Strauss et al., 2008). More studies are needed to explore and conceptualize psychological support strategies for patients with HIV, taking gender into account (Dargatzis et al., 2015; Cripps et al., 2009; Pardo & Bard, 2017). Numerous psychological support services can be provided by non-specialist hospital personnel or by practitioners, which is crucial in settings with limited resources. Kaye et al. (2011) and Moked et al. (2011) suggested that numerous psychological support services can be provided by

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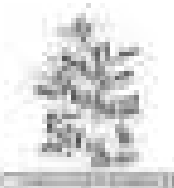
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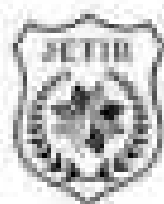
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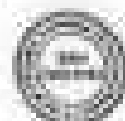
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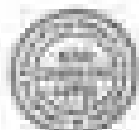
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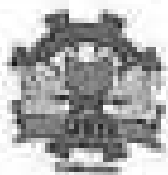


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A POST-COLONIAL READING OF SALMAN RUSHDIE'S *MIDNIGHT'S CHILDREN: A PERSPECTIVE*

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ABSTRACT

Literature transcends everyday world because its producers are above political motivations. Literature reflects the ideological and cultural forces in which the literary text is infused with the cultural and historical context. Salman Rushdie is an Indian-born British writer whose works reflecting cultural values with historical forces, is primarily concerned with the uneasy connections, disruptions, and negotiations between Eastern and Western civilisations, with much of his fiction being set in the Indian subcontinent. History of the nation in Rushdie's novels is narrated and unfolded through the life of the individual. For Rushdie, Indian history is like a morning tea which connects India with the past as well as the contemporary scenes. The present paper discusses the idea that like other postcolonial theorists, Rushdie seems to search for new moral order and justice. In *Midnight's Children*, he presents that the world is hybrid and complex, and its complex relations are intermingled. To break with the traditional concepts of national identity is that of cultural identity needs to break away with the determining factors of religion, race/caste and nation.

Keywords: Post-colonial, hybridity, nation, state, ideological situation, cultural differences, National identity, Identity crisis, Magic Realism, Migration.

Postcolonial theory is a method of interpreting, reading, and critiquing the cultural processes of colonialism, where it proposes that the exercise of colonial power is also the exercise of culturally determined powers of representation. Postcolonial literature is a body of literary writings that reacts to the discourse of colonialism. Post-colonial literature often involves writings that deal with issues of decolonisation or the political and cultural independence of people formerly subjected to colonial rule. It is the critical analysis of history, culture, literature and the studies of discourse that are specific to the former colonies of England, France, Spain, and other European imperial Powers. Postcolonial literature has focused specially on the Third World countries.

Salman Rushdie is one of the world's most important writers of postmodern fiction. It is not hard to establish Salman Rushdie's fame as his novels have sold in millions and been translated into multiple languages. Perhaps most revealing, the name of Salman Rushdie has become so familiar internationally that even those who do not generally read literary fiction have heard of him and know something about his subject concerning which he writes. He is an eminent writer, however, it is harder to establish what it is precisely that he is famous for: his works in the 1980s *Fury* caused controversy. Moreover, *Midnight's Children* (1981) has been greeted not only as a work of startling originality but as one that was destined to become a landmark text in the subsequent canonisation of postcolonial fiction. Postcolonial literary theory opens by ideas and concepts developed in the anti-colonial struggle.

RUPTURED NATURE OF FREEDOM: AN EXISTENTIAL READING OF SALMAN RUSHDIE'S *MIDNIGHT'S CHILDREN*

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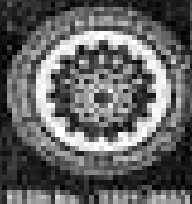
ABSTRACT

Postcolonial literature generally refers to literature written both during the colonial and decolonized period. Strictly speaking, the term is more relevant to those texts which come from erstwhile colonies. But unfortunately, this literature particularly the fiction produced shortly before the onset of freedom or after such events as Nadine Gordimer's *Johannesburg*, or J. M. Coetzee's *Disgrace* or Chinua Achebe's *Arrow of God* and more recent, postcolonial fiction, more particularly Salman Rushdie's *Midnight's Children* project ruptured nature of freedom. It is in so far, man is immersed in historical situation, he does not even succeed in conceiving of his fathers in a political organization; this is not as simply said, that he is accustomed to these fathers, but because he apprehends freedom in its plenitude, in its fulfils and because he cannot even imagine that he can exist otherwise, in its vicinity, in its lack.

Keywords: Freedom, negation, mobilization, being-in-itself, being-for-itself, determinative, nihilism, existentialism, Sartre.

Postcolonial literature generally refers to literature written both during the colonial and decolonized period. Strictly speaking, the term is more relevant to those texts which come from erstwhile colonies. But unfortunately, this literature particularly the fiction produced shortly before the onset of freedom or after such events as Nadine Gordimer's *Johannesburg*, or J. M. Coetzee's *Disgrace* or Chinua Achebe's *Arrow of God* and more recent, postcolonial fiction, more particularly Salman Rushdie's *Midnight's Children* project ruptured nature of freedom. It is in so far, man is immersed in historical situation, he does not even succeed in conceiving of his fathers in a political organization; this is not as simply said, that he is accustomed to these fathers, but because he apprehends freedom in its plenitude, in its fulfils and because he cannot even imagine that he can exist otherwise, in its vicinity, in its lack. The present paper is an attempt to understand the postcolonial-era colonial, and nature of determinative role of freedom. Freedom is identical with existence. Hence, it has no meaning unless it precedes oneself. Human nature is free because it is not enough. It is free because, as Jean-Paul Sartre, put it, is perpetually wrenches away from itself and because it has been separated by a split-second from what it is to what it will be. Indian struggle for freedom is all its manifestations and their failures and successes—raised from nothingness which is nothing-to-be at the heart of Indian individuals or masses—and which forced reality to make itself instead to be, i.e. to change itself.

Freedom is free in existential necessity. One may disagree it is that fact, but it is not a



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By 

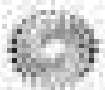
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A chemosensing approach for the colorimetric and spectroscopic detection of Cr³⁺, Cu²⁺, Fe³⁺, and Cd²⁺ metal ions

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Highlights

- A new molecular probe 5-(carbazoyl-β-phenylethynyl)hydrazonyl-densomethyl-2,3,6,7-tetrahydro-1H-imidazo[1,1-b]pyridin-8-yl (AMHMPO) is designed.
- Colorimetric and spectroscopic detection of Cr³⁺, Cu²⁺, Fe³⁺, and Cd²⁺ ions by AMHMPO is studied.
- Three-dimensional excitation-emission (3D-EEM) intensity studies are described.
- The recyclability and quantitative analytical parameters such as detection limits, quantification limits, linear ranges, Stern-Volmer constants, and acidic basic medium effects are analyzed and described.

Abstract

Metals cations are pervasive in domestic and industrial wastewaters and have adverse effects on human and aquatic life. The present study describes the development of the molecular probe 5-(carbazoyl-β-phenylethynyl)hydrazonyl-densomethyl-2,3,6,7-tetrahydro-1H-imidazo[1,1-b]pyridin-8-yl (AMHMPO) to detect Cr³⁺, Cu²⁺, Fe³⁺, and Cd²⁺ ions by using UV-visible, fluorescence, colorimetric and excitation-emission matrix (EEM) spectroscopy techniques. The interaction of Cr³⁺, Cu²⁺, Fe³⁺, and Cd²⁺ can be observed by the absorption maxima shift, turn-off, colour changes, and EEM shifts. In addition, fluorescence limits of detection (7.66 × 10⁻⁷ M, 5.44 × 10⁻⁸ M, 26.87 × 10⁻⁷ M, and 12.49 × 10⁻⁷ M in wide linear ranges, low limits of quantification, high values of Stern-Volmer constant, Job's plot and Benesi-Hildebrand plot justify the 1:1 association affinity with association constants of 1.46 × 10⁴ M⁻¹, 1.89 × 10⁴ M⁻¹, 2.89 × 10⁴ M⁻¹, 3.13 × 10⁴ M⁻¹ for AMHMPO-metal ions (Cr³⁺, Cu²⁺, Fe³⁺, and Cd²⁺ ions), respectively. Paper- and mask-based kits are developed to explore the utility of the designed chemosensor.

Sparks



Development of heterocyclic 2,7-diamino-3-phenylazo-6-phenylpyrazolo [1,5-a]pyrimidine as antimicrobial agent and selective probe for UV-visible and colorimetric detection of Hg²⁺ ions

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Keywords:
Pyrazolo [1,5-a]pyrimidine
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ABSTRACT

Mercury is considered as a highly toxic metal ion due to its lethal effects on humans and the ecological system. The increasing level of environmental mercury ion threatening to the ecosystem, public health and economy. The development of new environmentally safe agents molecules can be a potential cure for both of the above mentioned problems. Hence, we have synthesized 2,7-diamino-3-phenylazo-6-phenylpyrazolo [1,5-a]pyrimidine (PPI) as a new heterocyclic ligand, and its selective Hg²⁺ ion detection. The developed sensing probe PPI exhibited limit of detection (LOD) 1.26×10^{-8} M, and limit of quantification (LOQ) 4.38×10^{-7} M in the linear range 1.4100×10^{-7} M with good selectivity affinity of 1.4446×10^4 M⁻¹ for Hg²⁺ ions. Interestingly, the synthesized heterocyclic metal (PPI) provided a significant colorimetric change from colorless to yellow upon binding with Hg²⁺ ions. Moreover, the developed probe exhibited excellent selectivity sensitivity affinity against other harmful metals and non-hazardous metal. Cytotoxic studies on normal cell lines were also carried out for the compound which proved that compound is non-toxic (LD₅₀ 500 to cell survival) and can be applied as being probe for mercury poisoning detection.

1. Introduction

Heavy metal ions are important for various biological and environmental processes [1,2]. The ingestion of heavy metal ions shows a certain level of highly poisonous and can lead to the development of diverse complications in humans [3]. In several environmental systems, the level of heavy metals is increasing above the drinking levels due to diverse anthropogenic and natural activities [4,5]. Out of all the heavy metals, mercury is considered as one of the most harmful heavy metals due to its toxicity in both as well as combined forms [6]. A number of reports has been limited to mining, petroleum refining and coal burning are responsible for increased levels of mercury in the environment [7,8].

Mercury can be present in various forms in the environment such as

Hg²⁺, Hg⁰, Hg⁺ and alkyl or aryl mercury compounds [9]. It could be responsible for various diseases such as, vomiting, diarrhea, blood excretion of the gums, general paralysis, tremors, dysarthria and visual field restrictions [10,11]. The detection of mercury will be helpful in diagnosis, treatment and prevention of such health issues. Looking at the serious side effects of increased mercury pollution it has become a big concern to develop novel non-toxic methods that are rapid and can be applicable to the environment and biological system [12]. Specifically, the development of receptor molecules that can give optical feedback in response release or retention of existing agents can be handy in therapeutic applications [13,14].

In the past, it was reported that the presence of amino functionalized molecules can show good mercury binding affinity [15]. Moreover,

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Obtaining Water from Air Using Porous Metal–Organic Frameworks (MOFs)

Binj Mohan¹ , Sarish Kumar² · Qianzhong Chen¹

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Abstract

Water collection from moisture in air, i.e., atmospheric water harvesting, is an urgent future need for society. It can be used for water production everywhere and anytime as an alternative water source in remote areas. However, water harvesting and collection usually relies on desalination, fog, and dewing harvesting, which are energy intensive. In this context, metal–organic frameworks (MOFs) have broad applicability for water harvesting in water-scarce areas. Therefore, the current discussion focuses on this approach. Furthermore, recent progress on MOFs for moisture harvesting is critically discussed. In addition, the design, operation, and water harvesting mechanism of MOFs are studied. Finally, we discuss critical points for future research for the design of new MOFs as moisture harvesters for use in practical applications.

Graphical Abstract

MOF adsorbents offer excellent operating capacity in various temperatures and pressure ranges. Rational water harvesters can thus be developed by adjusting structural

 Detailed publication information available on the last page of the article.



Sarish

CRITICAL REVIEW

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Nanomaterials for miRNA detection: the hybridization chain reaction strategy

Dr. Mohan, ¹ Sandeep Kumar, ² Sunil Kumar, ³ Kunal Mehta, ⁴ Deependra Tyagi, ⁵ Omkar Pankajasthai, ⁶ Nitesh Renukashahi ⁷ and Amanda J. L. Pomato ⁸

MicroRNAs (miRNAs) are a class of endogenous small RNA and can play crucial functions in biological processes. In particular, the group of miRNAs is responsible for information coded in the cell and disease. Among various techniques for miRNA detection, the hybridization chain reaction (HCR) strategy shows potential and efficiency. This review summarizes and studies the most efficient HCR strategy for detecting miRNA using nanomaterials due to their characteristic detection and excellent performance. In addition, signal amplification for the sensitive detection of miRNA due to the chain reaction has been studied. The key factors, such as kind of detection (DNA), linear length, the importance of the strategy (limitations or challenges), and future perspectives are described. Finally, the study will provide new insights for developing a miRNA detection strategy applicable to disease diagnosis.

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1. Introduction

miRNA is a novel global molecule, but with the increasing health issues, different types of diseases, such as cancer, heart and kidney failure, HIV, and liver damage, have become a serious issue for millions of people.^{1–3} Also, it is difficult to monitor health coverage in many countries due to their high population and lack of resources. However, it can be achieved by developing simple strategies to detect overexpression or underexpression of miRNAs in various cell samples.^{4–6} There are numerous microRNAs (miRNAs) that are helpful in the expression of a gene. Upon hybridization with messenger RNA, miRNAs cause a negative regulation of gene translation. The expression of miRNAs is responsible for various diseases, most importantly cancer.^{7–9} Therefore, miRNAs can be used for early detection in disease diagnosis. miRNAs can be found in serum or plasma, and by circulating miRNAs in the form of extracellular vesicle-derived miRNA. Spreading miRNAs on the test substrates or biosensors, as extracellular vesicles increase the miRNA amount, making detection more accessible and reliable.¹⁰ Extracellular vesicles also protect

miRNAs from DNA degradation and increase its stability.¹¹ It was also to prove that miRNAs is an essential biomolecule and can reveal important biological and biochemical information. Hence, there is a great need to develop new techniques for detecting miRNAs to save the disease diagnosis and public health needs.^{12–14}

1.1 Importance of miRNAs

miRNAs are short primary transcripts (genetically), then can be controlled at the transcriptional and post-transcriptional levels. It is, however, challenging to follow the exact mechanism for the regulation at multiple levels. Any changes in miRNA levels can contribute a disorder in the body. The low amount of mature and pre-miRNAs in production, their dynamic changes, and degradation can reduce a disorder. Also, nucleotide sequence influences the stability of mature miRNAs, and their degradation can provide information about genes.¹⁵ In addition, miRNA is associated with oncogene signaling in the immune system and is essential for cellular cancer, stem lymphoblastoid leukemia, osteosarcoma, multiple myeloma, prostate, and ovarian cancers, etc. It can be discovered by the expression level of miRNA in cells.¹⁶ In addition, miRNAs and circulating DNA help verify the biomarkers present in tissues and some cells. Hence, miRNAs can act as a biomarker for diagnosis, prognosis, and therapeutic application for various diseases.^{17–19}

1.2 Importance of the HCR strategy

The hybridization chain reaction (HCR) provides a promising way to detect miRNAs compared to other signal amplification

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RESEARCH ARTICLE

Nonlinear interaction of quadruple Gaussian laser beams with narrow band gap semiconductors

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Sanjeev Kumar^{4*}, Anam Chaudhary^{5*}

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Abstract This paper presents an investigation on nonlinear propagation of quadruple Gaussian (QG) laser beam in narrowband semiconductor (e.g., n-type InGaAs) plasma. In the presence of laser beam, the electron field in the conduction band becomes relativistic that makes the medium highly nonlinear. As a result the laser beam gets self-focused. Following variational theory approach in W.K.B approximation the variational solution of the nonlinear Schrödinger wave equation (NLSE) for the field of quadruple laser beam has been obtained. Particular emphasis is put on dispersive nonlinearities of beam spot size and longitudinal phase (Gouy phase) shift arising of the laser beam resulting from the dispersive balance between diffraction, focusing, and nonlinear refraction due to free electron plasma.

Introduction

The advent of laser [1] in the early 1960s led to extend a class of systems that led to a revolution in the field of light-matter interactions. The past few years have seen the immense advances. One was the proposal of emitting laser resonators [2] for visible energy production that multi-junction heterostructure's nonlinear theory for energy without involving the global electron charge transfer nonlinearly obtained via the laser-driven parametric amplification [3]

Field's acceleration by laser-driven plasma wave is an extremely interesting and fascinating idea that can bring high parametric amplification to laser light. The efforts to translate these concepts into reality, however, have to overcome two primary problems: (i) The creation of relativistic plasma requires ultrahigh laser intensities in the range of 10^{18} – 10^{20} W/cm², and (ii) the plasma has to be extremely homogeneous. These laser driving requirements have made it difficult even to carry out preliminary experiments to test the proposed idea.

Therefore, there have been ongoing efforts to the observation in excited plasma environments, where these wave interactions could be mitigated. One route that includes the theoretical framework and shed light on the potential feasibility of these ideas. Primarily, such an alternative route is provided by carbon-based plasma-based in the narrow band semiconductor [4, 5] (Fig. 1). Plasma current (negative and positive carriers under conditions in which free electron carriers, in Fig. 1 a and b) is produced, as negative charge, either the conduction band edge is a positive charge, and neutral atoms are shown given. In a gap there are two kinds of charge carrier, electrons and positive ions (atoms lacking electrons). In a crystal metal the only mobile carriers are electrons, positive ions are not mobile in the crystal lattice. A semiconductor has two kinds of mobile carrier electrons and positive "holes" or missing electrons. All these plasma are shown in present paper.

Interaction of narrow laser beams with semiconductor plasmas is rich in various nonlinear effects. This opens a great free parametric interaction to several nonlinear effects like self-focusing, self-collapsing, self phase modulation etc. All these nonlinear effects are extremely complex but still in physics to provide a necessary and full the

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Stimulated Raman scattering of self focused elliptical q-Gaussian laser beam in plasma with axial temperature ramp: effect of ponderomotive force

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ABSTRACT

The phenomenon of stimulated Raman scattering (SRS) of elliptical q-Gaussian laser beams interacting nonlinearly with underdense plasma has been investigated theoretically. Using variational theory semi-analytical solutions of the coupled nonlinear wave equations for the three waves (pump, SPW and scattered) have been obtained under WKB approximation technique. The equations so obtained have been solved numerically to analyze the effects of laser as well as plasma parameters on the dynamics of pump beam and further its effect on the power of scattered wave. It has been observed that power of the scattered wave is significantly affected by the self focusing effect of pump beam.

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Self-focusing of Gaussian
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1. Introduction

Laser [1] is one of the most successful pieces of apparatus gifted by twentieth century science. When laser made its debut in 1960 people considered it to be solution which is searching for its problems. Since its invention the impact of laser on our lives has changed with time and still is changing. Now laser is ubiquitous in every aspect of life: from super market barcode scanners, security checkpoints, CD writers to high end applications like medical diagnosis and surgery, inertial confinement fusion. The extent of diversity in the applications of laser can be estimated from the fact that same instrument is being used to produce highest [2] as well as lowest temperature [3] on earth i.e. the instrument can heat as well as can cool down.

Laser has played an important role in revealing true beauty of interaction of light with matter through the appearance of several new phenomena. This includes a gainst from parametric instabilities [4-6] to several self action effects like self-focusing [7], self-channeling [8], self-phase modulation [9] etc. Being extremely complex and rich in physics, these nonlinear phenomena have potential to engage researchers for several upcoming years. Therefore, for the better understanding of light-matter interactions several researchers are making conscious efforts to improve upon the understanding of these

COMPLEX INVARIANTS FOR SOME TIME-INDEPENDENT AND TIME-DEPENDENT CLASSICAL SYSTEMS

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We present a construction of quadratic, cubic and quartic complex invariants for one-dimensional time-independent and time-dependent classical systems within the framework of canonical method. The concerned Hamiltonians are scaled on an extended complex phase space characterized by $(z = x + iy, p = p_x + ip_y)$. The results of this work may be useful for understanding complex trajectories of both classical and quantum systems.

MSC: 81.90.18

Keywords: complex invariants, canonical method, PT-symmetric Hamiltonian, 3DPS approach

1. Introduction

The invariant theory, an important branch of nonlinear dynamics, has played an important role to get a better insight into some properties of dynamical systems [1–11]. Since invariants are analytic functions, therefore, one can learn a lot about



Relativistic effects on electron acceleration by elliptical q -gaussian laser beam driven electron plasma wave

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Abstract

Theoretical investigation on propagation dynamics of an elliptical q -Gaussian laser beam in a plasma by considering the relativistic mass nonlinearity of plasma electrons has been presented. The study is then extended to investigate the electron plasma wave (EPW) excitation by the laser beam. Following variational theory the nonlinear wave equations governing the evolution of laser beam and plasma wave have been reduced to a set of coupled ordinary differential equations for the beam widths of pump beam and EPW. Further the acceleration of electrons by the EPW excited by the laser beam has been investigated. The results obtained from numerical analysis reveal a stronger self-focusing of the q -Gaussian laser beam, which is desirable to excite a large amplitude electron plasma wave (EPW) for electron acceleration by extending the interaction length.

Keywords Self-focusing · q -Gaussian · Electron acceleration · Plasma wave

1 Introduction

For the past few decades, the high power laser community has been pursuing to bring the huge particle accelerators off the shelf (Dineen (2006); Gupta et al. (2020); Malik (2012)). Limitations of conventional technology mean that kilometer-sized accelerators are required for high-energy physics research. Similarly, major installations are required for medical applications such as particle beam treatment of tumors, which includes all but the largest research hospitals. By contrast, laser-plasma-based techniques can support accelerating electric fields of least four orders of magnitude larger than those of conventional techniques (Esarey et al. (2009); Joshi (2006)), leading to the hope that particle accelerators could one day become a commonplace tool.

Plasma particle accelerators are based on the principle that particles can be accelerated by the electric fields generated within a plasma (a state of matter heated to a temperature at which electrons are stripped from their atoms, ions Tajima and Dawson (1978)). Because the plasma has already been ionized, plasma particle accelerators are not susceptible to

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Analytical solutions in the Schrödinger equation for a generalized Cornell potential and its applications to diatomic molecules and heavy nucleus

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Here, analytical expressions of energy eigenvalues and eigen functions for a generalized Cornell potential are obtained by solving the two-dimensional Schrödinger equation using the Nikiforov-Uvarov functional method along with Green's function approximation. Energy spectra of three physically important potentials viz. the parabolic oscillator, the Kratzer and the Coulomb potential potentials are derived from the general results. Further, within the framework of the Kratzer potential, energy eigenvalues spectra of diatomic molecules Cl_2 , NH_3 , O_2 , LiH and HCl are compared. The energy spectra of two bound neutrons are also investigated using the Coulomb potential potential in form of the generalized Cornell potential. The obtained results are in good agreement with the numerical energy studies. The study is further extended to calculate and study the partition function and other associated thermodynamic quantities for heavy nucleus.

Keywords: Schrödinger equation; generalized Cornell potential; Nikiforov-Uvarov functional method; Green's function approximation; energy spectra; wave spectra

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Stimulated Raman scattering of self-focused elliptical q -Gaussian laser beam in plasma with axial density ramp: effect of ponderomotive force

Sarvesh Gupta¹, Sanjeev Kumar^{1*} & S. B. Bhattachaj²

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Abstract: The phenomenon of stimulated Raman scattering (SRS) of elliptical q -Gaussian laser beam interacting nonlinearly with resonant plasma has been investigated theoretically. When an intense laser beam with frequency ω_0 propagates through plasma, due to the resonant interaction with its counter-propagating component of ponderomotive force, resonant wave. Due to this ponderomotive scattering of plasma, the laser beam gets coupled with a scattering plasma wave (SPW) at frequency $\omega_s = \omega_0 - \omega_{pe}$. Using numerical theory and analytical relation of the set of coupled nonlinear wave equations for the three wave system SPW and counter-propagating laser beam under WKB approximation technique, it has been observed that growth of the scattered wave is significantly affected by the self-focusing effect of pump beam.

Introduction

After successful laser [1] is considered to be the most successful piece of apparatus from 1960 onwards. When laser beam is added to 1960 simply considered it to be a device which is emitting the light problem. Since it, describe the impact of laser on the skin, the changed with time, and still is changing. Now, laser is

dispersed in every aspect of life. From upper market, but with various security checkpoints, CD-ROMs to high end applications like medical diagnosis and surgery, aerial communication system. The extent of diversity in the application of laser can be estimated from the fact that total investment is being used to produce higher [2] as well as lower temperatures [3] or rather, the temperature can be as well as can cool down. Laser has played an important role in creating new frontiers of interaction of light with matter through the appearance of various new phenomena. This opens a whole new parameter modulation [4-6] to several well known effects like self-focusing [7], self-bleeding [8], self-phase modulation [9] etc. Being extremely complex and rich in physics, these nonlinear phenomena have attracted a large number of researches in several operating areas. Therefore, the detailed understanding of light-matter interaction, aerial interaction, or making connection efforts to improve upon the understanding of these nonlinear phenomena. These efforts have collectively led the foundation of an entirely new branch of science known as laser-plasma interaction.

Raman scattering occurs due to interaction of light with optical phonons. Equivalently, we can say that it is the scattering of light due to quantized molecular vibrations of the medium (Fig. 1). Usually, Raman scattering is an inelastic scattering in which an incident photon with energy $h\nu_0$ produces a scattered photon with energy $h\nu_s$ while the remaining energy $h(\nu_0 - \nu_s)$ results in the vibrational excitation of the molecule. Thus, Stokes component of the Raman scattering corresponds to creation of an optical phonon. The frequency ω_s corresponding to the scattered photon is called Stokes frequency and is smaller than the incident light frequency by an amount equal to that of generated phonon.

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Nonlinear interaction of Bessel–Gauss laser beams with plasmas with axial temperature ramp

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Abstract Theoretical investigation on nonlinear interaction of intense Bessel–Gauss laser beams with plasmas with axial temperature ramp has been presented. Explicit report on investigation of self-action effects of the laser beam like self-focusing, self-channelling and axial phase shift of the laser beam. Optical nonlinearity of the plasmas has been modelled by the ponderomotive force acting on the plasma electrons due to the intensity gradient over the axial section of the laser beam. Using variational theory based on Lagrangian formalism, nonlinear partial differential equation (PDE) governing the evolution of beam envelope has been reduced to a ordinary differential equation for the beam width of the laser beam along the propagation direction. The evolution equation for the axial phase of the laser beam has been obtained by the Fourier transform of the amplitude structure of the laser beam into coordinate space in (R, k_z) space. The differential equations so obtained have been solved numerically to analyse the effect of laser-plasma interaction on the propagation behaviour of the laser beam.

Keywords Self-focusing · Bessel–Gauss laser · Ponderomotive force · Variational theory · Self-trapping

Introduction

Laser systems in the tera-petawatt regime find the applications that include many plasma-based [1–7]. However, light's interaction with plasmas, in different, the laser power has given rise to interest at the onset of new processes. Initially, it was believed that diffraction of the laser beam can not be avoided during its propagation whether through vacuum or through material media as it occurs at a fundamental level from process momentum conservation of photons. However, in 1964, Chirva *et al.* [4] showed that in media whose index of refraction depends on the intensity of light, the spreading of an optical beam is prevented and be observed. Hence, the expansion of optical beam due to diffraction is neither inevitable nor unchangeable.

Self-focusing and self-trapping are two examples of nonlinear optical effects which require balancing of many physical mechanisms. Self-focusing describes the contraction of a light induced channel in an elongated medium when carries the optical beam [8]. The channel occurs in a fibre. Self-trapping occurs when self-focusing counteracts exactly counteracts beam spreading due to diffraction. When this happens, the cross-section of the light induced channel remains indefinitely constant with propagation distance over the distance of the self-trapping [9]. Other similar mechanisms also exist. For example, a modified self-trapping effect occurs when self-focusing is countered by jet flow beam spreading due to refraction. In that case, the cross-section of the beam beam is not necessarily tiny, i.e., it remains constant as long as it general, the diameter of a trapped beam may be slightly modulated along the propagation direction, as it varies owing to the method used due to a periodic expansion of optical beam [11]. This results in a channel with constant

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PAPER

Energy eigenvalue spectra and applications of the sextic and the Coulomb perturbed potentials

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Keywords: Schrödinger equation, exact potential, Coulomb-perturbed potential, exact solutions, exact eigenvalues, Bethe-ansatz, spectrum**Abstract**

Keeping in view the importance of the anharmonic potentials, closed-form solutions to the N -dimensional Schrödinger equation, for the Coulomb-perturbed and the sextic potentials using the Nikiforov-Uvarov functional analysis and power series methods respectively, are investigated. Complete energy spectrum is obtained for both the potentials by evaluating some restriction on wave function parameters of the sextic potential and the Green's function approximation for overlapped term of the Coulomb-perturbed potential. A relationship between energy eigenvalues of the two potentials is verified in higher dimensions. This study is further extended to find physical applications of both the potentials. The energy eigenvalues of the Coulomb-perturbed potential are used to compute the mass spectra of the mesons via σ , M_1 , M_2 , ρ and ω (where $\rho = \omega, \rho$). Within the framework of the sextic potential, B and Λ baryons chains are analysed and M_1^* and M_2^* baryons have been identified as critical point nuclei. The results of this study are consistent with other similar studies.

1. Introduction

Exact solutions to the Schrödinger equation (SE) for anharmonic potentials have been a subject of great interest for the last few decades [1–4] in their field theory applications in the fields of plasma [5, 6], quantum field theory [7], quantum and statistical physics [8, 9] and structural phase transitions [10–12]. In spite of theoretical insights of the phenomena of strong resonant fields, in general, it is required to incorporate higher order anharmonicities in model potentials. The solutions to the SE for a double anharmonic potential may be applied in their spirit [13–15] where one can solve exactly a problem of an inhomogeneous physical or circular wave guide with refractive index profile described by a sextic type potential. In addition, it also applicable to problems of the intermediate physics [16]. Several efforts had been made so far to find stationary state solutions to the SE for various harmonic and anharmonic potentials [17–20] via different techniques. Most of such studies, however, are restricted to one and three dimensional systems only.

Chau and Mishra [21] obtained the analytical solutions to the SE for the Coulomb plus linear harmonic (CPH) potential within the framework of the Kato-Balkin perturbation theory for the linear operators. Kumar and Chaud [22] also computed the eigenvalue spectra for the CPH potential using the power series technique and further used to find the mass spectra of mesons. Soni et al. [23] obtained the mass spectra and decay properties of heavy quarkonia using the Cornell potential model. They also calculated the dipionon, diphoton and dipion-decay of these systems. Using two-term relativistic quark models, the linear potential model, and the screened potential model, Cheng et al. [24] calculated the mass spectra of charmonium. Very recently, Kumar et al. [25] studied the mass spectra of some heavy and light mesons with the generalized Cornell and zero anharmonic potential.



Self-compression of elliptical g -Gaussian laser pulse in plasmas with axial density ramp

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Abstract. Theoretical investigation on self-compression of a laser pulse with a Gaussian spatial envelope profile propagating through underdense plasmas with axial density ramp has been presented. Particularly the dynamics of pulse width, beam width and axial phase of the laser pulse have been investigated in detail. Effect of the ellipticity of the cross-section of the laser pulse also has been investigated using numerical theory based on Lagrangian-coordinate settings part of differential equations (PDE) governing the evolution of the pulse envelope has been reduced to a set of coupled ordinary differential equations for the pulse width and beam width of the laser pulse. The evolution equation for the axial phase of the laser beam has been obtained by the Fourier transform of the parabolic structure of the laser pulse from Cartesian space to k - A space. The differential equations so obtained have been solved numerically to investigate the effect of laser-plasma parameters on the propagation dynamics of the laser pulse.

Introduction

The dream of manipulating light is as old as human civilization. Ancient people used lenses made up of glass or stone

light to focus pieces of paper. However, with the advent of laser [1] in 1960, the twentieth century witnessed a dramatic shift in our perception and understanding of light. The extraordinary properties of femtosecond, high-power and noncollimatedity of laser light have aroused the history of light-matter interaction.

When laser beam is focused into dielectric medium and afterwards reflect that is considered only “copy” that are of “conventional” nature, but more common to challenge and innovative progression is come. With this high-resolution as a breakthrough, the laser has proceed to becoming “best of a breed”. The laser has become ubiquitous in the global, every field of modern life (science and technology [2–6]), but the more applications are in physics and are waiting for their turn.

Self-compression of propagating the maximum of light with matter have been reported by the incident of shaped pulse interaction (IP) technique [7–10] in which a laser pulse is stretched, amplified and recompressed. The amplification method allows to generate very short laser pulses with peak powers up to petawatt range. Many applications of ultrashort pulse laser make use of the very high power that such pulse inevitably provide. Although the average power from the laser may be quite moderate and the total energy within a pulse may also be small, the extremely short duration of such pulse guarantees that the total interaction energy is large. In a typical system the length of the laser pulse is 100000 times longer than the pulse duration, and in the focal point is about 100000 times the average power. For example, a 100 femtosecond pulse with a carrier frequency of 1000 THz contains one enough energy to heat a drop of water to a temperature of a degree Celsius within a peak power of 10 megawatts.

When focused on a very spot, such high-power, ultrashort, ultraviolet, making ultrashort pulses a tool for

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Mass spectra and thermodynamic properties of some heavy and light mesons

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Abstract. An energy eigenvalue equation for a static, anharmonic interaction potential is derived by solving the Schrödinger equation analytically within the framework of the Nikiforov-Uvarov (NU) method. The resultant expressions are then used to calculate the mass spectra of some heavy and light mesons, $(c\bar{c}, \bar{c}c, b\bar{c}, \bar{c}b, \bar{c}d, d\bar{c}, \bar{c}s, \bar{s}c)$ and the results are found to be in good agreement with the other theoretical and experimental studies. The energy eigenvalue expressions is further used to compute some important thermodynamic quantities like partition function, specific heat capacity, free energy, internal energy, entropy and magnetization.

Keywords: Schrödinger equation, static potential, Nikiforov-Uvarov method, mesons, mass spectra, thermodynamic properties

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1. Introduction

Exact expressions of eigenfunctions and eigenvalues, if derived as solutions to the Schrödinger equation (SE) for a physical system, are of prime importance. These expressions provide a window to look into the underlying dynamics of a system. Also, with the help of bound state energy eigenvalues, one can obtain the partition function which can further be utilized to calculate other thermodynamic properties, such as specific heat capacity, free energy, mean energy, entropy, etc. In reality, however there are only a few potentials for which the radial SE can be solved exactly [1]. Numerical and analytical methods are then complementary to find exact or approximate solutions to the SE with/without the centrifugal term, $l(l+1)/r^2$, in the potential $V(r)$ for a particle. In the case of a quarkonium system, one can reproduce with a reasonable accuracy, the experimentally observed mass spectra within the state of the non-relativistic quantum mechanics with an ansatz for interaction potential. To this effect, many studies were carried out earlier and a brief overview of such studies is given here.

Inyang et al. [2] obtained the mass spectra of heavy mesons using a class of Yukawa potential by employing the series expansion method. Here potential was modifi-

ed to temperature-dependent by replacing the screening parameter with Debye mass. Baidyan et al. [3] obtained the masses, magnetic moments and charge decay widths of baryons with two heavy quarks involving non-relativistic quark model. Within the framework of the Cornell potential, Gupta and Mishra [4] numerically solved the non-relativistic SE and calculated the mass spectra of mesons. By using the perturbation method, Mousavi et al. [5] studied mass spectra and other properties of light and heavy mesons by considering a new potential, a combination of Cornell, Gaussian and linearly square interaction terms. Kumar and Chand [6–8] determined the mass spectra of heavy mesons and energy spectra of quarkonia ions by solving the N -dimensional radial SE using power series and the asymptotic iteration methods within the framework of Coulomb plus harmonic interaction potential.

Rani et al. [9] obtained the mass spectra of heavy and light mesons by considering a general interaction potential (generalized Cornell potential) by solving the non-relativistic SE via the asymptotic iteration method in three dimensions. Study et al. [10] investigated the mass spectra and thermodynamic properties of various baryons using extended Cornell potential by solving the N -dimensional radial SE using Nikiforov-Uvarov (NU)

On the solutions and applications of the generalised Cornell potential

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ABSTRACT

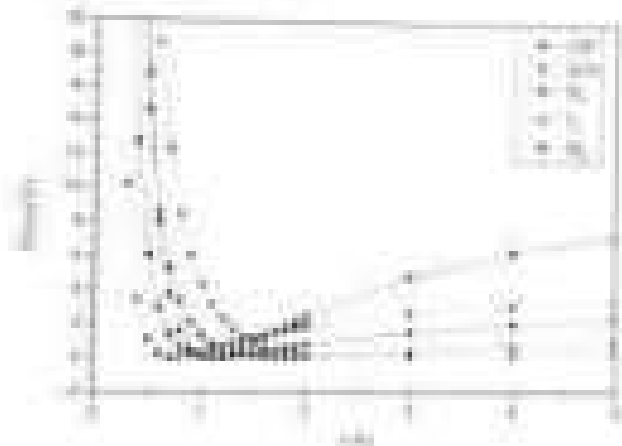
This work presents the solutions to the non-relativistic Schrödinger equation for the generalised Cornell potential using the Nikiforov-Uvarov functional analysis method and the General Algebraic Computational Scheme approaches and exact solutions are obtained for ground state eigenvalues spectra of some physical observables are also obtained from the generalised virial theorem, while the framework of the analysis and the constants associated generally, but restricted to the generalised potential, involve exponential spectra of diatomic molecules via the form $V(r) = A + B/r + C \exp(-\alpha r)$ and the exact spectra of H and H^+ molecules are determined respectively. We also compute the expectation values of position operator and its square, inverse average, and radius of gyration for the above diatomic molecules by employing the Hellmann-Feynman theorem. A clear agreement is obtained between the present results and previously published works.

ARTICLE HISTORY

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Schrödinger equation
generalised potential
exact solutions
diatomic molecules
virial theorem



1. Introduction

Since its inception in the last quarter of twentieth century, over the years, the quantum mechanics has progressed a lot. It studies upon almost every faculty of human knowledge and provides plausible explanation of diverse phenomena of nature. It basically involves three basic equations, the Schrödinger equation (SE), the Klein-Gordon (KG) equation and the Dirac equation. The solutions to the wave equations SE are very useful in explaining the thermodynamic properties of various systems [1], assignment of masses [2,3], optical and

rigidity properties of quantum dots [4,5], average spectra of diatomic molecules [6,7], quantum information entropy [8], etc.

In case of the diatomic molecules, the potential would generally include some important parameters like the dissociation energy (DE), equilibrium bond length (e), screening parameter α and inter-atomic separation (r). In past, many authors have investigated analytical and numerical solutions to the SE by using different potentials within the framework of a variety of methods like the Nikiforov-Uvarov (NU) method [9–11], asymptotic



Effect of Porosity on Hydromagnetic Boundary Layer Flow with Forced Convective Heat Transfer

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A numerical investigation has been carried out to study on the effect of porosity with forced convective flow through an steady hydromagnetic (MHD) flow the non-Newtonian magnetic nanofluid over a rotating disk. The governing nonlinear coupled partial differential equations together with the boundary conditions are first discretized into a nonlinear system by using differential equations along boundary transformations. Further, the numerical solutions are obtained using the general finite difference method and presented for the velocity, temperature and skin friction profiles through graphs. For a wide range of porosity, magnetic nanofluid having Prandtl numbers ranging from (1.1 to 10.0) are taken and consideration which included wall-normal water-based magnetic nanofluid having $\eta = 0.01$. Also, the flow profiles are from the disk surface, skin friction and thickness of the boundary layer are discussed. From the results, it is noted that the rise in the porosity of Darcy-Forchheimer the flow velocity is augmented as well as in axial direction. Further, there is an improvement in the heat transfer rate towards the outer environment with the increase in the Prandtl number.

Keywords: Magnetic field, Magnetic Nanofluid, Porosity, Prandtl number, Rotating Disk

1 Introduction

Magnetic nanofluids are colloidal liquids of nanoscale ferromagnetic particles suspended in a carrier fluid. A surfactant coating is required to avoid the clumping and to enhance its life. Because of its responsive behaviour over the magnetic field, the researchers and engineers vigorously attracted for investigation on them considering the wide range of industrial applications since last few decades (Shi et al., Sharma et al., Philip). The main aim of the spherical shaped particles enhances the heat dissipation due to increased surface area of the boundary layer. The phenomena of friction variation, heat/cooling, pressure drop, minimization of drag force, energy mass transport etc. in nano-suspension flow become more popular among numerous researchers.

In recent decades, the rotating disk flow has become a topic of interest among several researchers due to the commonly used circular shaped devices in mechanical engineering such as crystal growth

process, gas turbine systems, thermal power plants, high speed rotating machinery, etc. The thermal effect on the viscosity over a flat surface has been investigated by Vyasathi et al.¹ for flow and thermal behavior. Das et al.² published the work on the time-dependent convective flow for an oscillating porous plate taking into account of thermal radiation. Ram et al.³ investigated the convective heat transport phenomena of unsteady boundary layer flow of hydrocarbon-based nanosuspensions. For understanding the radiation impacts on the magnetic nanofluid flow, a range of Prandtl number $10 < Pr < 175$ is taken by Ram et al.⁴ Chaudhary⁵ applied Perturbation technique to investigate the unsteady flow of CNT-water nanofluid over a stretching plane with slip conditions. Also, many researchers⁶⁻¹¹ got published the results on the rotating disk problems for various nanofluid flow. Recently, Sharma et al.¹² discussed the Coriolis effect and viscous dissipation with forced convective heat transfer on steady flow of magnetic fluid considering the geometry of a rotating porous disk. Also, the impact of variable viscosity and

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Self-focusing of laser-driven ion acoustic waves in plasma with axial density ramp

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Abstract In the present work, dynamics of the laser-driven ion-acoustic waves (IAWs) in plasmas with axial density ramp has been investigated theoretically. The effect of propagation characteristics of the laser beam on self-focusing of IAW has been investigated in detail. During its propagation through the plasma, the laser beam excites an IAW at frequency ω_p , where the optical susceptibility of plasma and gets non-linearly coupled to the laser beam. First analytical solution of the coupled nonlinear wave equations for the pump wave and IAW have been obtained under WKB approximation technique using variational theory. It has been observed that propagation of the IAW is significantly affected by the self-focusing effect of laser beam.

Keywords α -plasma · Filamentary wave · Relativistic plasma · Self-focusing · Ion-acoustic wave · Chirping wave

Introduction

The fundamental necessity of our economic strategy is lighting our homes, giving our food and power our computers. There is no end to world's energy appetite. The need of energy is so great and growing so rapidly around the world

that alternate sources of energy to supply humanity's ever increasing demand of energy without doing any harm to global climate are required. In this regard, the quest to tap the energy of nuclear fusion (1) by employing neutral beam beams to create an ultra-hot plasma and generate electric power has been in progress since past few decades. The future power plants will be fueled by a beam of heavy hydrogen-based molecules—no water and will produce no harmful greenhouse—no dirty pollutants, no nuclear waste and no greenhouse gases. In laser-driven fusion, the goal is to deposit laser energy in a particular density to the plasma in order to create the compression and subsequent heating of the fuel pellet. If the pellet is compressed sufficiently, it may undergo fusion, leading to the release of a large amount of energy. It is so if there is a tiny fraction of the sun in Earth.

Both the vision and the challenges of fusion have been the focus of the laser physics world. Fusion fuel is abundant and cheap. The major advantages are: (1) The abundance of fuel—the most easily exploitable fuels are deuterium and tritium. Deuterium occurs naturally in all sources of water especially sea water. Tritium however, is normally available naturally, it can easily be manufactured inside the fusion reactor by the bombardment of lithium with neutrons, which also abundant in nature. (2) Cleanest source of energy—fusion does not produce nuclear waste directly. Although neutron is highly radioactive and requires activation of the reactor chamber to store which activated materials are now useful to industries waste disposal of neutrons demands its containment in the entire reactor assembly at the end of its life.

However, fusion only happens at the extremely high temperatures that are typical characteristics of stars, whereas fusion only happens at normal temperatures. The fuel with the lowest binding energy is a mixture of deuterium and tritium that ignites at temperatures around 50 keV (i.e., 50

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STIMULATED BRILLOUIN SCATTERING OF ELLIPTICAL μ -GAUSSIAN LASER BEAMS IN PLASMAS WITH AXIAL DENSITY RAMP: EFFECT OF SELF-FOCUSING

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Theoretical investigation on stimulated Brillouin scattering of incoming Gaussian laser beams interacting with axially non-uniform plasmas has been presented. A non-uniform density profile has modeled the axial inhomogeneity of the plasma and the optical nonlinearity of the plasma has been considered to be very strong owing to the dependence of the refractive index of the plasma plasma on laser intensity. An analytic study has been made through an propagating through plasma gets coupled with a propagating electromagnetic wave (HE) at frequency ω_1 and produces a back-scattered wave at frequency $\omega_2 = \omega_1 - \omega_B$. Using variational theory semi-analytical solution of the set of coupled wave equations for the pump at HE and a scattered wave have been obtained under R.F.E. approximation. It has been noted that the growth of the scattered wave is significantly affected by the self-focusing effect of the pump beam.

Keywords: plasma density ramp, refractive plasma self-focusing, stimulated Brillouin scattering

МОДЕЛЬ КАНАЛОВЫХ ВОЛН В НЕОДНОРОДНОЙ ПЛОСКОЙ ПЛАЗМЕ С РАДИКАЛЬНО НЕЛИНЕЙНОСТЬЮ И НЕОДНОРОДНОСТЬЮ ПЛОТНОСТИ ПО ОСИ

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Теоретическое исследование распространения падающей Gaussian-волны лазерного излучения взаимодействующей с осевыми неоднородными плазмой. Предположено, что неоднородность плотности плазмы моделируется осевой неоднородностью показателя преломления. Сильная зависимость показателя преломления плазмы от интенсивности падающей волны рассмотрена в рамках вариационной теории. Получены полуквантовые решения системы связанных волновых уравнений для накачки в канальной волне и рассеянной электромагнитной волне (HE) с частотой ω_1 и обратнорассеянной волне с частотой $\omega_2 = \omega_1 - \omega_B$. По вариационной теории получены аналитические решения для накачки в канальной волне и рассеянной волне в приближении Р.Ф.Е. Показано, что рост рассеянной волны существенно зависит от эффекта самосжатия накачки.

Ключевые слова: каналная волна, радиально нелинейная плазма, неоднородность плотности, лазерное излучение, взаимодействие волн

Introduction: Powering the world without burning the global climate is a recurring concern. That is the goal for decades, developed countries have added enormous amounts of solar, geothermal, wind and biomass power to discharge electrical power production. But these forms of renewable energy cannot match humanity's insatiable thirst for energy. At the moment, the prospect of utilizing nuclear fusion by its

RESEARCH ARTICLE

Generation of superthermal electrons by self-focused Cosh Gaussian laser beams in inertial confinement fusion plasma

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Abstract. Theoretical study on the generation of superthermal electrons by intense laser beams in hot dense plasma during inertial confinement fusion has been presented. In order to obtain uniform heating of the fuel pellet the irradiation over the target cross section has been modified by Cosh Gaussian profile. The effect of self-focusing of the laser beam on energy gained by the electrons has been investigated in detail. Following ionization theory and hydrodynamic fluid model of plasma coupled differential equations governing the evolution of beam width of the laser beam and energy of the superthermal electrons have been obtained. It has been observed that the uniformity of the irradiation over the target cross section enhances the energy of superthermal electrons considerably.

Keywords: Self-focusing; Superthermal electrons; Plasma; Chirp-pulse; Cosh-Gaussian

Introduction

The fundamental property of our universe is energy. It lights up the matter, gives our food and provides our computers. There is no end to world's energy appetite. The need of energy is so great and growing so rapidly around the world that alternate sources of energy to provide humanity's energy needs of energy without doing any harm to global climate are required. In this regard the quest to tap the energy of nuclear fusion (1, 2) by employing intense laser beams as

source of ultra hot plasma and generate fusion power has been in progress since past few decades. The fusion power plants will be fueled by a form of heavy hydrogen found in ordinary sea water and will produce no harmful environmental by-products, no nuclear waste and no greenhouse gases.

The basic idea of laser fusion is to split an intense laser beam into several smaller beams of equal intensity (3). The split beams are directed in energy and subsequently brought back together by a system of mirrors and lenses, the beams are thereby focused on a small region from different directions. A cylinder of deuterium and tritium fuel is enclosed in a spherical shell a few millimeters in diameter, made of plastic, glass or some other material, and the resulting fuel pellet is placed at the intersection of the beams, the pellet is then uniformly irradiated.

The laser beam almost uniformly heats the centre of the spherical part of the pellet, but the material in the spherical cap at the outer surface is exposed to a greater total laser energy. Incident energy is consequently absorbed in a denser layer of plasma that surrounds the deuterium-tritium fuel. The heated layer of plasma expands and ablates (4) at various velocities over time from the rest of the pellet, the velocity of the ablated plasma is typically 1000 kilometers per second. An equal and opposite force maintains the material inside the ablation layer intact, in accordance with Newton's third law, as if it was a rocket propelled by the plasma escaping all around it. In effect the system is a laser-powered spherical rocket whose payload is the rapidly contracting fuel pellet. The energy efficiency of the rocket engine is, however, less than 10 percent because the electron velocity (at the ablated material) is much higher than the velocity velocity (the imploding pellet). The necessary implosion time is sufficient to compress the remaining shell to a density of several hundred kilograms per second in a radius of a

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RESEARCH ARTICLE

Excitation of ion acoustic waves by self-focused q-Gaussian laser beam in plasma with axial density ramp

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Abstract Dynamics of the laser-driven ion acoustic waves (IAW) in plasmas with axial density ramp has been investigated theoretically. The effect of self-focusing of the laser beam on the power of laser excited IAW has been incorporated. During its propagation through the plasma, the laser beam excites an IAW at frequency ω , that due to the optical nonlinearity of plasma gets continuously coupled to the laser beam. Using variational theory, analytical/numerical solutions of the coupled nonlinear wave equations for the pump wave and IAW have been obtained under WKB approximation technique. It has been observed that power of the IAW is significantly affected by the self-focusing effect of pump beam.

Keywords q-Gaussian · Density ramp · Retarded plasma · Self-focusing · Ion acoustic waves

Introduction

Plasma is a collection of positively and negatively charged particles moving about so irregularly that they do not readily combine. Plasmas are everywhere in the universe [1]. They form the intensely hot gas under high pressure in the sun and the stars, as well as the ionized gas in interstellar space and in the ionosphere envelope surrounding the earth. Plasmas also exist close to hand. They are

present in the form of burning fuel and in gas-discharge devices such as neon signs. Plasma exhibits such an enormous variety of physical effects that physicists have studied their properties for about 200 years. This research on plasmas, particularly on gas discharges, led to the discovery of the electron and to the elucidation of atomic structure [2].

The unique interest in plasmas reflects two principal motives. The first one is technological. An understanding of plasma behavior is critical to the controlled release of electromagnetic energy [3–11]. An attempt is reported in a short-note shows the need of neutron sources based on laser ion. Another technical goal is the design of magnetron-driven plasmas [7], in which electron power is generated by jet of gas plasma traversing magnetic fields. The second broad motive for the study of plasmas is the importance of plasma phenomena, in space and in astrophysics. When a plasma is subjected to electromagnetic fields, the motion of the particles is no longer completely random. The resonant consequences of this imposed order is that a plasma can support certain kinds of waves that are related to electromagnetic waves but that have unique and various properties. These waves include high-frequency electron plasma waves [8, 9] (EPWs) and low frequency ion-sound ion acoustic waves [10, 11] (IAWs).

IAW can be excited in plasmas due to characteristic properties of anisotropy and collision between. Plasma is a state of matter that contains enough heat for ions, but their interactions. The negatively charged electrons are not attracted by positively charged nuclei, but they are not bound together. This gives a plasma some unusual properties unlike most kind of ordinary matter—solids, liquids and gases—the free floating electrons and ions of a plasma are strongly affected by electric and magnetic fields. Plasma is a whole is quasiparticle, but it

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Optical guiding of q-Gaussian laser beams in radial density plasma channel created by two prepulses: ignitor and heater

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Abstract Self-action effects such as focusing and self phase modulation of q-Gaussian laser beam in plasma channel created by ignitor laser (prepulse) have been investigated theoretically. The ignitor laser creates radial expansion of q . The laser beam from the plasma channel and propagation in parabolic channel and also through the channel like by defining the channel like expansion. The third laser (Gaussian beam) is guided in the plasma channel under the combined effects of density nonlinearity of the parabolic channel and refractive index nonlinearity of the plasma channel. Formulation is based on studying the numerical solution of stationary Schrödinger wave equation (SWE) by the field of focused laser beam with the help of vector theory approach. Physical analysis is done on dynamical variations of the spot size of the laser beam and longitudinal phase shift of the guided beam with distance of propagation.

Keywords Self-Focusing · Self-Trapping · Phase Modulation · Focused Laser Beam · Propagating Wave

Introduction

Over the past few decades [1] are characterized by the use of the most successful treatments of 19th century science. What was made available in 19th, were simply called a solution or search of a problem. Today, many have returned

first place in almost every aspect of life, including such as biology like (DNA) proteins, super matter (dark matter) in physics and technology. With the advent of optical pulse amplification (OPA) technique [2] the use of low density has provided a gain that is less technology leading to a breakthrough in the field of light-wave interaction. This advancement in laser technology has given birth to an entirely new field of science known as laser-plasma interaction. An application of multiple laser beams (i.e., picosecond, nanosecond, [3, 4] laser systems, petawatt, [5, 6] kilojoules, [7] ultrashort wavelength [8], [9, 10] ultraviolet or more than photo ionization.

A major impetus toward the investigation on laser-plasma interaction was provided by the proposal of converting fusion reactions [11, 12] to viable energy production by using intense laser beams. Fusion is considered to be the ultimate source of energy as there will be no emission of radioactive and produce and green house gases. Thus, it opens the promise to search humanity's solution that is energy without making any harm to global climate. Along the way the field of laser-plasma interaction has branched into a number of practical applications: the laser-driven accelerators [13, 12] X-ray lasers [14, 15] higher harmonic generation [5, 6], etc. The ultimate benefit of most of these applications depends on stable guiding of intense laser beams over large distances, without significant energy loss. However, due to light natural wave property of diffraction, a light beam focusing on vacuum or in a medium always focuses in the absence of an optical guiding mechanism. Diffraction broadening of the laser beam is due to the modulation phenomenon that impairs the stability of electron acceleration by reducing the efficiency of laser-plasma coupling. Hence, there is urgent need to explore the methods that may act to increase the

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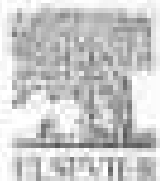
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Advancements in net-zero pertinency of lignocellulosic biomass for climate neutral energy production

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ABSTRACT

The lignocellulosic biomass is one of the most abundantly available natural resources for green energy production. The heterogeneous organic and inorganic composite structure of lignocellulosic biomass comprises numerous carbohydrates, proteins and lipids. The cellulose, hemicellulose, lignin, and other organic components with varied groups, chemical, and physical compositions are found in the biomass as preferred by organisms. This review article describes the use of lignocellulosic biomass in sustainable source of energy in solid, liquid and gas and its industrial uses in diverse energy industries. The effects of various acid physical, chemical, and biological treatments on biomass are discussed with their effect on biomass during conversion of energy sources. Further, the production of liquid energy generated in solid, liquid and gas are described in comparison to conventional solid fuels to assess a sustainable transformation towards their conversion from coal. This review article's objective is centered in the light of our progress concerning current utility of lignocellulosic biomass.

1. Introduction

The progress of the global economy, production, and production over the last decades has been significantly enhanced as the consumption of the primary limited fossil fuels for green generation [1,2]. It is estimated that conventional CO₂ emissions are one of the primary causes of climate change. It helps in the rising the industrial revolution, making the developed countries such as the United States, which were an early transition to a fossil fuel-based economic system, also an early gas is contributing to these advances, as illustrated in Fig. 1 [3]. However, low and non-renewable resources have reduced about industrial activities and/or economic activities. In order to reduce energy resources are used in conventional form across the countries this year has, as shown in Fig. 1, alternative and sustainable (RES) sources have energy sector is around 14%, agricultural, forests and land use activities (24%), health and recreation (covering roughly 3.2%) and industrial uses (roughly 14%) [4]. It is clear from the statistics that a range of sectors which accounts 60–70% emissions, that of which energy and agriculture were essential

in a large amount. To deal with this, primary energy needs can be substituted with utilizing alternative and renewable energy fuels, resulting in the green energy crisis alleviation.

The numerous renewable energy sources, including wind, solar, and hydroelectric energy are on the rise in most of the energy demands [5]. The benefits of these energy resources include reduced greenhouse gas emissions, improved return on foreign funds, and creating economic growth through manufacturing and installation jobs. Despite the fact that these technologies are sophisticated enough to meet current energy demands, they do have their limitations. The primary disadvantage of these technologies is their geographical location, as solar, wind, and wave energy are irregular in nature, covering millions of square meters land utilizing these renewable energy sources. Considering the geographically remote locations for renewable technologies, the additional aspects such as natural fires, water preservation, etc. might hamper implementation of renewable energy technology of optimal location.

Electricity increasingly replaced coal-fired, gas, and solid fuels that are derived primarily from renewable sources. Germany, a country of high

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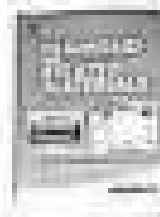
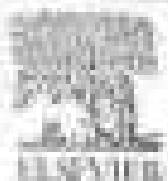
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Effect of chirality and defects on tensile behavior of carbon nanotubes and graphene: Insights from molecular dynamics

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ABSTRACT

Carbon nanotubes (CNTs) and graphene have attracted significant attention due to their unique mechanical properties. In this study, the mechanical properties of pristine as well as defected CNTs and graphene are investigated using molecular dynamics (MD) simulation. The effect of various defects such as Stone-Weissert (SW) and Stone-Wales (SW5) defects on the mechanical properties and ultimate strength have been explored under uniaxial tension. The simulation revealed that the ultimate strength of graphene sheets and CNTs with the strength and failure strain were found to decrease with an increase in the number of defects. The results strongly suggest that the failure of loading the graphene in the uniaxial direction is dependent on loading in the other direction due to the existence of the interconnection bond in the structure loading direction. The fracture strength of the pristine zigzag graphene sheet is higher than for the pristine armchair graphene sheet in case of uniaxial tensile loading. The failure mode of the zigzag graphene sheet is higher than the pristine graphene sheet. This has a great impact on the simulation of strength of composites from the SW defects. The higher the number of defects, the lower is the strength of the nanotubes.

1. Introduction

In designing, modeling, manufacturing, and processing, nanotechnology has been primarily dominated by advances in materials and device levels. This sector is a broad discipline encompassing various fields, science and engineering. To enhance the quality of life in the world, nanotechnology is currently leading the advanced and innovative materials [1–3]. Nanotechnology is found to be one of the most progressive fields, particularly in terms of manufacturing [4,5]. Also, nanotechnology is considered for usage in nanotechnology devices of various sizes, the advances of nanotechnology system including, their application in the nanotechnology research because of their extraordinary mechanical, thermal, and chemical properties [6]. Nanotechnology has also been widely used as a platform for improving mechanical properties of composite systems continuously increasing their weight due to their high strength, stiffness, and mechanical quality.

Over the past few years, nanotechnology advances have emerged that stress to explore various phenomena. Many of these phenomena are now being described using research and practical tests, with many others being predicted due to technological limitations of the lack of experimental equipment. That is why advanced nanotechnology, such as fabrication

and modeling methods, are being established. Based on this concept, modern modeling techniques have been found useful as a connection between nanoscale molecular understanding and macroscopic mechanical engineering. Nano-mechanics perform an essential role in the growth and evolution of molecular engineering. The disparity between atomic and macroscopic mechanics and materials with the emerging device in nanotechnology has reduced due to the availability of new methods and techniques. These technologies have also enabled scientists to observe the movement of atoms in such a manner that laboratory experiments cannot show [7].

Nanotechnology that are used primarily to improve the properties of nanocomposites are graphene [8–10], and carbon nanotubes (CNTs) [11–13]. Due to their outstanding mechanical properties, CNTs and graphene have become some of the most viable reinforcements in composite nanocomposites. From various observations, it has been revealed that the modulus and strength of CNTs are either equal or greater than the best graphite fibers [14]. Few weight percentage of CNTs and graphene in other materials are thought to be beneficial because the great properties of polymer-based composites, in expanding the mechanical properties of CNTs and graphene because nanotubes [15]. Graphene and CNTs unique structure and various

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Effect of defects and boundary conditions on the vibrational behavior of carbon nanotube and graphene: A molecular dynamics perspective

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ABSTRACT

The presence of defects like a equiflute defect on the longitudinal and circumferential properties of carbon nanotubes (CNTs) and graphene. The vibrational properties of single layered graphene sheet (SLGS) and single wall carbon nanotube (SWCNT) have been investigated in this research. Molecular dynamics simulations have been carried out to explore the vibrational modes and acoustic phonons of CNTs with consideration of (i) boundary conditions of both fixed or periodic and (ii) defects (equiflute) on the CNTs with different boundary conditions to investigate the effect of the defect concentration such as chirality, defect type, boundary conditions, and type and number of defects on the longitudinal and circumferential modes of CNTs and graphene sheets. It was observed that for the different boundary conditions, dispersion curves for the vibrational frequency as compared to the large size of the system (number of the unit). The results are not a consistent effect on the natural frequency of CNTs. Regarding graphene sheet, it was observed that increasing the size of the graphene sheet decreased the fundamental natural frequency of SLGS. As compared to fixed/clamped defects, the missing defects were found to have more impact on the dispersion of the natural frequency of CNTs and GNS.

1. Introduction

Advanced and versatile have opened the horizon of the materials world's recent years that include potential for significant improvements in mechanical and physical properties when compared to conventional natural materials. However, nanotechnology is a major scientific field that allows a new range of properties throughout the world [1]. The development of various devices and devices with size of less than a μm , typically between 1 nm to 100 nm (e.g., in terms of nanotechnology) in the presence of emerging particles in an infinite pattern and creating various materials with various qualities. Carbon based nanomaterials including high strength and multifunctional composite materials have been produced by a set combination of the nanoscale world over the last decade [2,3]. Carbon nanotubes (CNTs) and graphene, especially, have gained growing in interest development [4,5]. CNTs and graphene are the members of nanotechnology structures that have long been explored in depth from various perspectives owing to their exceptional features when compared to other materials [6]. Their nanostructures have various applications because of their size and mechanical characteristics (see Fig. 1).

Single-walled carbon nanotubes (SWCNTs) have various features

like (i) 1D, which is comparable to diamond [7], SWCNTs are also the most lighter and stronger than steel. However, nanotubes have a tensile strength of up to 100 GPa, which is almost 10 times that of the steel with the highest ultimate strength [8]. Several technical and medical devices in nano-scale-mechanical systems (MEMS), which include catheters, stents, and various devices. We are knowledge of nanomaterials relative behavior [9,10]. Additionally, vibrations are very likely for nanoscale systems for the subsequent production of carbon based nanomaterials, such as CNTs and graphene [11]. As a result, studying a precise model of carbon-based nanomaterials to observe the natural frequency and mode shapes are a critical issue.

Chen et al. [12] provided a complete study of the vibrational behavior of CNTs and their composites using different methodologies to identify the behavior of CNTs and graphene. Three types of approaches were used: (i) dynamic methods such as molecular dynamics (MD) and finite element method; (ii) continuum methods, and (iii) acoustic resonance methods (e.g., finite element method (FEM)). Acoustic resonance is particularly a 3D analysis, interacting with one another via a family of potential fields. The differential equations of partial vibrations are converted to the natural. As a result, this method takes a long time and requires a lot of processing. Acoustic mode fields are represented

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Confluence of Existential Concerns and the Concepts of Shrimad Bhagwadgita in the Western literature

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Abstract: *The present research paper is an extensive of confluence of the existential concerns and the concepts of Shrimad Bhagwadgita in the Western literature, carried out on the Bhagwad Gita. The main purpose of this article is to explore philosophical insights embedded in this historical scripture and help the readers to gain its greater understanding and insights from the of view of existential concerns. It also searches metaphysical principles contained in the Bhagwad Gita and provides answer of the existential questions: what metaphysical principles can be seen in the Bhagwad Gita? How can it be interpreted? How the metaphysical principles of the Bhagwad Gita connect/interrelates with existential theory? Considering the questions, the Bhagwad Gita provides theory of creation, cycle of creation and destruction (birth and death cycle). It also includes theory of being (existence). Since these explain, as it exemplifies in the Bhagwad Gita, the form of existentialism, i.e., making human beings confront human reality, awakened up in his present, existence precedes essence. It means that man first of all exists, constructs himself, surges up in the world—and defines himself afterwards. The Shrimad Bhagwadgita is one of the most widely respected Hindu scriptures in existence and has been a source of inspiration for many people. However, there are many other influences that the Gita has on many aspects of different cultures. The Gita affected many influential American and European in the past centuries. The notion of the Gita, Arjuna's dispute, and final realization of Truth touch on many different aspects of Hindu belief but central is the concept of dharma and an ordered universe where each person has a responsibility to do what they have been placed on earth to do and which no one else can accomplish. In the end, all are a part of the cosmos of the Universe and can only begin to work toward this realization by first recognizing it as the truth among Hindu texts, the Gita is the fullest expression of this concept of the human toward self-realization and liberation which free the soul from the illusion, which cause suffering and reward*

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**Exploring Intermolecular Interactions in some halogen substituted benzyl
Cyanurins and their DFT studies**

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ABSTRACT
The present study reports on the synthesis of benzyl cyanurins through the
reaction of benzyl cyanide with cyanuric acid in the presence of sodium
hydroxide. The structure of the synthesized benzyl cyanurins was confirmed
by IR, ¹H NMR and mass spectroscopy. The structure of the synthesized
benzyl cyanurins was confirmed by IR, ¹H NMR and mass spectroscopy.
The structure of the synthesized benzyl cyanurins was confirmed by IR,
¹H NMR and mass spectroscopy.

KEYWORDS
Benzyl cyanurins, intermolecular interactions, DFT studies, cyanuric acid, benzyl cyanide, sodium hydroxide, IR, ¹H NMR, mass spectroscopy.

1. Introduction

Exploring intermolecular interactions among the synthesized benzyl cyanurins is a topic of interest for chemists, as it provides insight into the field of molecular chemistry. The study of intermolecular interactions in complex systems is crucial for understanding the structure and properties of materials. Intermolecular interactions, such as hydrogen bonding, van der Waals forces, and dipole-dipole interactions, play a significant role in determining the physical and chemical properties of molecules. The study of these interactions is essential for understanding the behavior of complex systems, such as polymers, biological molecules, and materials. The study of intermolecular interactions is also important for understanding the properties of complex systems, such as polymers, biological molecules, and materials. The study of these interactions is essential for understanding the behavior of complex systems, such as polymers, biological molecules, and materials.

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Exploring Intermolecular Interactions in Some 3-Halo-7-oxabicyclo [3.1.0]hexane and their Derivatives Functional Groups Studies

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ABSTRACT The present manuscript is based on the determination of various interactions in the crystal structure of 3-Halo-7-oxabicyclo [3.1.0]hexane. The different crystallographic parameters were assessed to quantify structural changes through intermolecular interactions. The crystal structure and intermolecular nature is made of both the intermolecular C-H...O and C-H...N interactions. Various intermolecular parameters such as range of bond length, contact distance and angle and bond lengths description have been explained through hydrogen bond network. The hydrogen bond network that has been proposed is as follows: O1-H2...O1 and O1-H2...N1. The presence of charge transfer between donor (ammonia) and acceptor (nitro) groups, was also explained by electron density based charge transfer (σ-donation, charge transfer and π). The molecular cell structure of different compounds have been investigated by X-ray technique in their reduced form. Powdering, which is the analysis included the presence of strong hydrogen-bonding interactions. Moreover, it is observed that $C(2)-H(2) \cdots O(1)$ which is found to be 2 times than that of crystallographic hydrogen bonds which is 40×10^{-3} a.u.

KEYWORDS Hydrogen bonding network, Hydrogen bond, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding, Hydrogen bonding.

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INTRODUCTION

The study of intermolecular interactions is an ongoing task in crystal chemistry. Intermolecular interactions of molecules depends to a great extent on the presence of non-covalent interactions such as aromatic stacking, allylic and aromatic hydrogen bonds. Functional groups such as carbonyl, amino and nitrile etc. are important for intermolecular interaction through hydrogen bonding. The interactions participating in intermolecular interactions depend upon nature of complementary sites in terms of strong and aromatic hydrogen bond. There are a number of examples of hydrogen bonding in crystalline structure. It explains the crystallographic

hydrogen bonding. Appropriate preparation of complementary hydrogen bonding species resulted into multiple hydrogen bonds which can be explained in the formation of base as well as one-hydrogen-bonded intermolecular interactions. Multiple intermolecular interactions can be possible in crystalline which are right intermolecular angle and both interacting groups together. Intermolecular interactions through hydrogen bonding network is one of important aspects of molecular structure and formation of crystal and the crystal packing patterns. With the advancement, the field in the synthesis of intermolecular interactions and their structures is an ongoing work. Various intermolecular interactions often coexist together such as σ-donation or different intermolecular.

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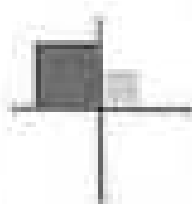
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EXPLORING INTERMOLECULAR INTERACTIONS IN SOME 4-METHYL COUMARINS DERIVATIVES AND THEIR DFT STUDIES

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Gulab Singh

Volume 10 of 100 The Journal of Oriental Research Madras

Transformation in Real Life through Raju: A Critical Study of R.K. Narayan's *The Guide*

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Published on 28 May 2022, Corresponding Author: Naveen Kumar

Abstract

It is an established fact that tradition of literature depicts life on pages and oscillates it in real life. It expresses true picture of life in different hues and colours in relation to the outer and inner world. Oral and written traditions of life and literature must be in practice. Reality and imagination both creates true picture of life through ideas, emotions and actions of man. Man bothers about life but life does not wait, as life is an amalgamation of our ideas and actions. Sometimes, either the circumstances favour us or we create circumstances favourable to us. Between this what is hidden is not understandable. There is a course of life that takes us backward or forward or vice-versa. Our ideas and actions play an indispensable role in our life and help us in our transformation.

Either man is picture of life or life creates a picture to give him a proper shape. It means that life is ready to give him a finer and finer shape. The life is a shadow that moves and mixes with us to give us a mature work. In the *Guide*, R.K. Narayan, through Raju's character, gives us such ideas of the transformation of life. Now, we can affirm that the life is good shaper for man and woman both.

Keywords: Fiction, Foundation, Idea, Action, Reality, Tradition, Cause, Transformation, Shape.

Introduction:

My endeavour, here, is to present a life of ideas and actions in totality, the manifold and shape of a good life. On number of occasions, we the human beings don't take a good chance to others that they may understand us or not. Life and society do take their course respectively. Society, more or less, overcomes life or life overcomes society. We know that



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Multicomponent synthesis, *in vitro* cytotoxic evaluation and molecular modeling studies of polyfunctionalized pyrazolo(3,4-*b*)pyridine derivatives against three human cancer cell lines

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ABSTRACT

A series of diversely polyfunctionalized pyrazolo(3,4-*b*)pyridines were synthesized by the multicomponent reaction of phenylacetamidocetyl hydrazide and 1-oxo-2-hydroxyacetamide with 1,3-dicarbonyl under solvent-free and solvent-catalyzed conditions; various pyrazolo(3,4-*b*)pyridine derivatives were screened for their anticancer activity against three human cancer cell lines namely HCT116, SK-N-SI, and MCF-7. Nonfluorinated 1-(2-oxo-2-phenylacetamidoethyl)-2-oxoacetamide (1) displayed better cytotoxicity results compared to other tested derivatives. The compound 1-(2-oxo-2-phenylacetamidoethyl)-2-oxoacetamide(1) (Compound 14) was identified as the most active derivative with 50% cell growth inhibition nearly equal to the standard drug doxorubicin (50%) in case of HCT116, SK-N-SI, and MCF-7 cell lines. Among the fluorinated derivatives, compound 1-(2-oxo-2-(2-fluoroethyl)acetamidoethyl)-2-oxoacetamide(1) (Compound 24) was identified as the compound with 50% cell growth inhibition against all the tested cell lines. Compound 14 was found to display subtle binding interaction mode for active site of HCT116 cancer enzyme.

ARTICLE HISTORY

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KEYWORDS

Cytotoxicity; *in vitro* studies; multicomponent synthesis; pyrazolo(3,4-*b*)pyridines; structure

GRAPHICAL ABSTRACT



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Agarwal

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Molecular iodine mediated transition-metal-free oxidative dehydrogenation of 4,7-dihydropyrazolo[3,4-b]pyridines

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ABSTRACT

A transition-metal-free iodine-I₂/CO₂ catalyzed efficient oxidation of 4,7-dihydropyrazolo[3,4-b]pyridines has been developed for the practical synthesis of corresponding pyrazolo[3,4-b]pyridines. The method is suitable for synthesis of various substituted pyrazolo[3,4-b]pyridines as it is free from tedious purification steps and gives pure products in high yields. Molecular iodine (I₂) being inexpensive, environmentally benign, and easy-to-handle reagent, was used to carry out the dehydrogenation under mild reaction conditions.

ARTICLE HISTORY

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KEYWORDS

iodine; pyrazolo[3,4-b]pyridine; oxidative dehydrogenation; transition-metal-free; environmentally benign; reaction rate; low pressure

GRAPHICAL ABSTRACT



Metal free
Simple efficient procedure
Green strategy

Introduction

Pyrazolo[3,4-b]pyridine, an important fused 6-membered ring, is associated with several biological and medicinal properties.¹ Therefore, this nucleus has been extensively investigated from its synthetic and medicinal viewpoints.^{2–7} There are several marketed drugs possessing pyrazolo[3,4-b]pyridine as core scaffold, to name a few, the antiplatelet drug cangrelor (1), Sildenafil (2) (glycogen synthase kinase-3 (GSK-3) inhibitor), and EL-1864 (3) (Figure 1).⁸

Dehydrogenation of 4,7-dihydropyrazolo[3,4-b]pyridine nucleus can lead to their aromatic counterparts pyrazolo[3,4-b]pyridines.^{9–11} A large number of oxidizing agents like molecular oxygen-N-hydroxyphthalimide (NHPI) and Cu(OAc)₂,¹² PCC in acetic acid¹³, lead tetraacetate¹⁴, 30% H₂O₂ and 10 mol% AlCl₃/Et₂O¹⁵, *m*-chloroperoxybenzoic acid in-CPBA/tetrahydrogaphthalimidine (TH) chloride [HCTPPC]¹⁶,

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Boundary layer flow with forced convective heat transfer and viscous dissipation past a porous rotating disk

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ABSTRACT

The steady-state flow and convective heat transfer over a porous rotating disk with viscous dissipation has been investigated. The similarity of the boundary layering under the action of the rotation or suction of the fluid at the disk surface is used to reduce the governing equations to a set of ordinary differential equations. Further, the similarity solution is obtained and the corresponding system of ordinary differential equations. Further, the similarity solution is obtained in terms of similarity variables. The velocity profiles are shown for various values of the suction parameter and the effect of the porous medium is also shown. The effect of the porous medium is also shown for various values of the suction parameter. The effect of the porous medium is also shown for various values of the suction parameter.

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1. Introduction

The rotating disk surface boundary layer flow is one of the most interesting problems for research in fluid mechanics with the field from the viewpoint of its important applications, both theoretically and practically for rotating disk systems, where a fluid rotates, porous media may be subjected by various forms instead of water flows. This flow is defined as an apparent definition of rotating objects when they are seen from a particular reference frame.

Heat transfer problems in the presence of porous media has become steadily important in engineering applications. Various fields such as heat exchangers in cooling systems, electronic devices having cooling parts, heat processing, swimming, etc. (Suman and Bhadwaj, 2011) has given the need impetus to the work on convective heat transfer fluids to transfer the heat of high viscosity. The applications of these fluids include the heat fluids, porous media and saturated flow (Suman et al., 2011) and Suman et al. (2011) give the details for various effects due to convection is revealed for their numerous applications in various fields of in-

terests. Recently, Suman et al. (2011) reported flow through porous media.

The governing study due to the rotating disk flow of convective porous fluid flow was given by Suman et al. (2011). They studied the porous medium in rotating the rotating disk surface differential equations and coupled system of ordinary differential equations. Suman, Bhadwaj, Suman, et al. (2011) and S. Mahapatra et al. (2011) studied flow through porous media over a rotating disk with convective heat transfer. They studied the results on convective heat transfer for the porous media.

S. Mahapatra et al. (2011) studied the effect of porous medium in engineering for porous gas turbine cooling (2011) and rotating disk flow (2011). Suman and Bhadwaj (2011) studied the heat transfer and porous medium effect on rotating disk flow over a porous medium surface. The influence of porous medium on convective heat transfer in porous media over a rotating surface has been studied by Suman et al. (2011). Suman et al. (2011) discussed the effect of porous medium and porous medium on convective heat transfer over a rotating disk over a porous medium. Suman et al. (2011) studied the heat transfer flow of an incompressible rotating fluid over a rotating disk by using various porous media. Mahapatra et al. (2011) presented a study on porous medium in a porous medium which is probably adequate for most of the porous media. By taking various convective effect and heat transfer through

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RELATIVISTIC EFFECTS ON STIMULATED BRILLOUIN SCATTERING OF SELF-FOCUSED q -GAUSSIAN LASER BEAMS IN PLASMAS WITH AXIAL DENSITY RAMP

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Abstract

We investigate the phenomenon of stimulated Brillouin scattering (SBS) of q -Gaussian laser beam relativistically interacting with inhomogeneous plasma. When an intense laser beam with frequency ω propagates through plasma, due to electron-ion two-stream instability of plasma electron, it gets coupled to a counter-propagating acoustic wave (AW) at frequency ω_p . The nonlinear interaction of pump beam with the AW produces a back-scattered wave at frequency $\omega - \omega_p$. In view of the relativistic effects on electron-ion two-stream instability of the relativistic electron-ion system for the time-varying plasma, the relativistic effects under the Wentzel-Kramers-Brillouin (WKBJ) approximation, describe that the relativistic effects are significantly affected by the self-focusing effect of the pump beam.

Keywords: q -Gaussian beam, density jump, relativistic plasma, stimulated Brillouin scattering, self-focusing

1. Introduction

Ever since the proposal of relaxing nuclear fusion via intense laser beams (IT) for viable energy production [1] without producing any harm to global climate, there was considerable interest in the nonlinear interaction of intense laser beams with plasma. In laser-driven fusion, the goal is to deposit the laser energy at a particular density in the plasma in order to create the compression and subsequent heating of the hot spot. If the pellet is sufficiently compressed, it can undergo fusion, with the release of a large amount of energy. However, the laser may interact with the plasma at a density referred to as the critical density leading to several undesirable effects [2–4] and preventing the effective ignition of the target.

Due to their remarkable properties of transparency and collective behavior, plasmas possess a number of natural modes of oscillations [5–8]. Thus include high-frequency electron plasma waves (EPWs) and low-frequency ion-acoustic waves (IAWs), the latter ones correspond to resonant phenomena, as do the

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Scattering of Laser Light in Dielectrics and Plasmas: A Review

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A review on some nonlinear phenomena associated with light-matter interactions has been presented. Emphasis is put on explaining the basic physics of the phenomena while minimizing the mathematics. Particularly the phenomena of Rayleigh scattering, stimulated Raman and Brillouin scattering have been discussed in detail. As a special case scattering of intense laser beams with finite size of matter (i.e. plasma) also has been discussed.

Keywords: Scattering of light, nonresonance, stimulated scattering, Brillouin scattering.

1 INTRODUCTION

Laser[1] is one of the most successful pieces of apparatus gifted by 20th century science. When laser made its debut in 1960 people considered it to be solution which is searching for its problem. Since its invention the impact of laser on our lives has changed with time and still is changing. Now laser is ubiquitous in every aspect of life: from super market barcode scanners, security checkpoints, CD writers to high end applications like medical diagnosis and surgery[2][3], optical confinement fusion[4][5]. The extent of diversity in the applications of laser can be estimated from

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Potential Well Dynamics of Self Focusing of Quadruple Gaussian Laser Beams in Thermal Quantum Plasma

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This paper presents theoretical study on self-action effects of intense laser beams interacting with laser plasma. Potentially the physics associated with the nonlinear defraction of the laser beam has been investigated in detail. In order to see the effect of anisotropy of the distribution over the laser phase front on its propagation character, since the radiation profile of the beam has been modeled by multiple Gaussian (G) profile. Following Variational theory approach, the nonlinear partial differential equation (PDE) for the laser envelope has been reduced to a set of coupled ordinary differential equations, by the evolution of laser width and axial phase. The equations so obtained have been solved numerically to observe the effect of laser as well as medium parameters on the propagation characteristics of the laser beam.

1. INTRODUCTION

The quest to realize nuclear fusion by employing intense laser beams [1–3] for quench and fast start of nuclear fire, without harnessing the global climate is at the vanguard of research since past few years. This will be similar to

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Dynamical invariants for time-dependent real and complex Hamiltonian systems

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ABSTRACT

The Schrödinger and Heisenberg (SH) approach is revisited in real space to solve dynamical invariants for one- and two-dimensional time-dependent Hamiltonian systems. The latter, deriving the SH-conditions in all complex phase space-dimensionalities $(n = 1, 2, 3, \dots)$ and considering real and complex physical systems, the obtained quantum invariant consists a function $\mathcal{I}(t)$ exhibiting particularity of time flow (not under differential equation). We further capture this approach into extended complex phase space defined by $(q = (x, y, z), p = (p_x, p_y, p_z))$ to construct a quantum invariant for a time-dependent system. The derived invariants show its applicability into real and complex systems of arbitrary time-dependent Hamiltonian systems.

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1. INTRODUCTION

The concept of dynamical invariants is an important branch of nonlinear dynamics. Their discovery is a major research tool and revealed considerable insight on the development of efficient methods to solve complex problems and their physical interpretation and utility to understand the underlying dynamics of a physical system.^{1–5} Invariant plays a vital role in the study of the motion of fluids, such as their vorticity, vorticity and time-dependent, plasma physics, impulsive, quantum system, and quantum state.^{6–10} The particle production in cosmological models,^{11–13} can be explained by knowing invariants of the underlying system, however, also help to find solutions of nonlinear differential equations by reducing them to quadratures. Classical dynamical invariants also proved useful in some special cases of systems, time-dependent (TD) systems.^{14–16} These invariants also provide a new technique to analyze of solutions to differential equations (not of them),^{17–19} and also derivation of invariant invariants of various time-dependent (TD) systems.^{20–22} The higher order invariants,^{23–25} offer the optimal character of physical systems, particularly in studying of dynamics. Complex invariants,^{26–28} had also been discussed in the past, in the context of understanding various motion and quantizing CP-converting two-flavor neutrino system, were presented in the particle physics, etc. The applications of invariants in a variety of fields, dynamics theory which is a continuous to find the invariant that are generally non-integrable, structure in an asymptotic sense.^{29–31} To this effect several methods have been developed in the literature for the construction of invariants with varying degree of utility.

An important method discussed conserved quantities (explicitly) TD dynamical systems. The latter shows relationship properties of a physical system to its corresponding conserved quantities. The simplicity of such invariants are arbitrary, all physics are independent (invariantly) under time evolution with energy conservation in the corresponding conserved quantity and its constant with respect to change in position, as the case regarding conserved quantity. These invariants also of them, which are also conserved in their domains are desirable aim. To show this, we have used to integrate the equations of motion. As our work is play in the context of specific invariants properties of real systems. The latter approach,^{32–34} is based on the introduction of Noether's theorem, and used in the

ORIGINAL RESEARCH ARTICLE

A theoretical study of (9, 0) Singlewalled Carbon Nanotubes using quantum mechanical techniques

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ABSTRACT

First-principles calculations studies using the density functional theory have been performed on (9, 0) Singlewalled Carbon Nanotube (SWCNT) to investigate its structural, optical and thermodynamic properties using CASTEP (Cambridge Sequential Total Energy Package) and DFTB (Density Functional based Tight Binding) module of the Material Studio Software version 7.0. Various functionalities and sub-functionalities available in the CASTEP Module using Pulay Density Mixing technique of accuracy and various algorithms and scanning schemes available in the DFTB module using exact algorithms have been tried out to study on the electronic structure. The analytically derived values of the band gap observed were compared with the experimentally determined value reported in the literature. By comparison, combination of Newton stopping scheme and parallel diagonalizer produced best results in DFTB module while in the CASTEP module, GGA (General Gradient approximation) functionals with RPEE (Revised-pseudo-Block-Eigen) as Sub-Functional was found to be the most convenient. These optimized parameters were then used to determine various structural, optical and thermodynamic properties of (9, 0) Singlewalled Nanotube. (9, 0) Singlewalled Nanotube, which is extensively being used for sensing H₂, CH₄ & NO₂, has been picked up in particular as it is reported to exhibit a finite energy band gap in contrast to its expected metallic nature. The study is of utmost significance as it not only probes and validates the simulation route for predicting suitable properties of nanomaterials but also sheds light on the comparative efficacy of the different approximations and re-optimization quantum mechanical techniques used in simulation studies.

Keywords: Simulation, Density Functional Theory, Molecular Modeling, CASTEP, DFTB, SWCNT

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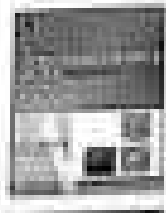
1. Introduction

Since the advent of Carbon Nanotubes by Iijima in 1991^[1] and subsequent synthesis of Singlewalled Carbon Nanotubes (SWCNTs) by Iijima^[1] & Terasma^[2]. Singlewalled Carbon nanotubes have gained immense attention because of their interesting electrical^[3], mechanical^[4-6] and optical properties^[7-9]. This multidimensional nanoscale one-dimensional roll of a single layer of graphite (graphene) has revealed highly promising applications in future molecular electronics^[10] over the last few decades. The remarkable electronic properties of these 1-D structures make them suitable for various applications in nanotechnology, optoelectronics, and other fields of materials science as chemical sensors^[11-13], actuators^[14], nano-biomaterials^[15-17], conductive heating filaments^[18,19], conductive transparent electrode^[20-22], conductive nanowires^[23], nano-SPiEs^[24-26], and display backlights, flat lamp and field emitters^[27,28] etc. This has involved interest in the experimentalists as well as theoreticians



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Effect of conjugation on the vibrational modes of a carbon nanotube dimer



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ABSTRACT

The Raman-scattered profiles using the density functional theory have been performed to investigate the effect of conjugation on vibrational modes across two CNTs of different diameters, are tied together to constitute an interconjugated dimer. Raman spectra of a (1, 0) CNT + a (50) CNT and a (1, 0) + (50) CNT dimer (comprising of parallel (1, 0) and (50) CNTs) tube to tube but not tube to tube were simulated. Various vibrational modes in different frequency regions have been simulated in detail. A red shift is observed around the G bands owing to the coupling and occurrence of the acoustic phonons by conjugation of CNTs. In the 1600–1800 cm⁻¹ region (D bands), higher additional peaks can be seen owing to the coupled vibrations. If both parts of the dimer carry the G bands peaks of both the CNTs, a shoulder in the Raman spectra is observed. In the G band region of the dimer spectrum, a low-frequency component with Lorentzian shape and a weak high-frequency component with a low-intensity tail (G₁) band of low shape suggest acoustic nature of the interconjugated CNT dimer.

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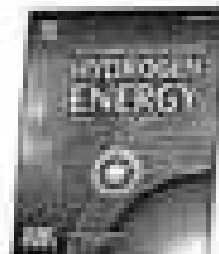
1. Introduction

The advancement of Raman spectroscopy as a characterizing tool for the carbon nano materials is indispensable. It provides useful information about significant properties of carbon nanotubes (CNTs) like chiral index (n, m) [1], diameter [1–3], strain analysis [3], purity index, doping levels [4], functionalization ratio [5] and the inter-tube [6,7] especially for studying the inter-tube vibrational modes of carbon nanotubes. Raman spectroscopy techniques serve as a well-tuned tool. Various techniques and techniques, various dimensions of structural properties, various electronic modes are experimental as well as theoretical aspects of vibrational analysis of CNTs have been well reported including Raman spectroscopy of a dimer to study the vibrational behavior of CNTs. Study of the inter-tube vibrational modes, phonons, and phonons is very useful for predicting or characterizing the optical and electronic properties. SWCNT (single-walled carbon nanotube) being the dimensional structure, the role of these inter-tube phonons were more efficient and occurrence of interaction between these vibrations greatly influenced their physical properties.

Spectroscopy studies themselves provide significant input as far as optimization of the design of nanotube vibrational spectroscopic CNT device design is concerned and offers a key to understand better explore their phonon modes (Phonon Index) [8–11].

Understanding the intriguing features of CNTs is conjugation with other nanomaterials makes their conjugated hybrid nanomaterials useful multidimensional structures having various potential applications like supercapacitors, lithium ion/battery electrodes, solar cells, sensors, photovoltaics, photocatalysis [12–15]. High dimensional pressure resistance, optical tunable devices, electromagnetic absorbers and highly efficient biosensors [12–14]. To utilize the potential characteristics of these one-dimensional developed through conjugation, are need to thoroughly study their molecular structure and that is where the vibrational spectroscopy methods come into the picture. As the vibration based applications of these 1-D tubes are based on their quantum regime, understanding of quantum coupling between electronic and phonon systems necessary for which Raman spectroscopy is the ultimate tool. A number of spectroscopic studies, experimental as well as theoretical, have already been reported in the literature that the effect of conjugation of CNT with metal or with another CNT with same or different chirality is still to be explored well. Conjugation of two free standing SWCNTs (not tight but by weak Vander Waal's interaction constitute a SWCNT dimer). In 2014, Saito et al. [16] the first free standing dimer of SWCNTs

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Effect of transition metal (Cu and Pt) doping/ co-doping on hydrogen gas sensing capability of graphene: A DFT study

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- Modified structure and chemical properties of dopant-free graphene
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ABSTRACT

Carbon nanomaterials are found to demonstrate good hydrogen gas sensing capability and transition metal (TM) modified derivatives are enhanced sensitivity. Studies have confirmed improvement in sensing performance of graphene when doped with Pt or Cu or Pt-Cu. However, effect of the doping of graphene with transition metals of comparable size as its hydrogen sensing properties has not yet been studied. In the present study, we investigated the sensitivity of pristine graphene, Pt doped graphene, Cu doped graphene and Pt-Cu co-doped graphene toward hydrogen molecule adsorption utilizing density functional theory (DFT) by ab initio method. The adsorption energies for the optimized graphene structures for hydrogen sensing in addition, the electronic properties for various charge transfer analysis, band gap and density of states have also been taken into consideration. The reactivity of graphene surface for hydrogen adsorption was found to be greatly enhanced with Pt-Cu co-doped graphene surface as demonstrated by the adsorption energies and electronic properties.

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Effect of the magnetic field on the energy spectra of a quantum dot system

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Abstract. Analytical solutions to the radial Schrödinger equation are obtained for a two-dimensional semiconductor quantum dot system under the influence of a parabolic confinement potential using the Taylor expansion method. The calculated results are compared with other theoretical results to check the efficacy of the present method. Effects of the Zeeman interaction, the parabolic potential energy and the magnetic field on the energy spectra of quantum dot systems are also highlighted.

Keywords: Eigenvalue spectra; Taylor expansion method; quantum dot

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1. Introduction

Over the last few decades, low-dimensional structures like quantum wells, quantum wires and quantum dots (QDs) have drawn a significant attention of researchers. Various properties of such structures can now be manipulated as per practical requirement by providing sophisticated experimental facilities. These systems are now rapidly gaining acceptance in design and fabrication for small and low-power-consuming electronic devices. After over the above mentioned nano-structures, a QD, also referred to as artificial atom, is that enough as its properties can be controlled by controlling its shape and size (1–4). A QD created by physical leads through tunnel junctions is normally called a single electron transistor, or Enomoto island, a two-dimensional electron gas and wire. A barrier through such an artificial atom or the suppression between its leads can be varied even by transporting a single electron (2, 5). Thus, an confinement of electrons in all the three spatial directions, the energy spectra of a QD become completely

quantized and exotic quantum experiments (7, 8) are facilitated (9, 10) opportunities to study correlated single particle and collective dynamics of such systems at the atomic scale.

Due to their remarkable structural and optical properties, QDs find widespread technological applications in optoelectronics (11). QDs are also suitable for light absorption and emission at well wavelengths, which make them interesting candidates to design LEDs, diode lasers and solar cells. These are widely used to increase focus for high speed data transfer, TV and computer displays, laser printing, eye viewing and Langmuir-Blodgett film thin to several nanometre thickness. In the realization of quantum computers, QDs are expected to be the main building blocks. QDs are also gaining popularity in research and applications in medicine. These are mainly used to study molecular processes, cancer tumor targeting, to the construction of cell labelling, diagnostics and cellular imaging at high resolution and to treat various cancer infections. These are also used to design memory chip, nanowire and photon sensors and catalyst to split hydrocarbons from carbon dioxide.

In 2001, a lot of research work has been carried out on two-dimensional semiconductor QD systems (12–16) which

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Classical invariants for non-Hermitian anharmonic potentials

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Abstract. Invariant theory for integrability of complex dynamical systems, as introduced by Liouville, is extended to non-Hermitian potentials, invariant or non-invariant. For this purpose, the corresponding Liouville's integrability condition for the class of the complex potential phase space systems, the integrability criteria are extended to deal with invariant and a stability criterion. An example of non-integrability of a two-degree-of-freedom system is given.

Key words. Classical mechanics; non-Hermitian potentials; complex dynamical systems; integrability; invariant; Liouville's integrability condition; complex phase space systems.

Mathematics subject classification. 34C30, 34E05, 37J30, 37J46, 70F05, 70F10, 70F20, 70F40, 70F45, 70F50, 70F55, 70F60, 70F65, 70F70, 70F75, 70F80, 70F85, 70F90, 70F95, 78A05, 78A10, 78A15, 78A20, 78A25, 78A30, 78A35, 78A40, 78A45, 78A50, 78A55, 78A60, 78A65, 78A70, 78A75, 78A80, 78A85, 78A90, 78A95, 79A05, 79A10, 79A15, 79A20, 79A25, 79A30, 79A35, 79A40, 79A45, 79A50, 79A55, 79A60, 79A65, 79A70, 79A75, 79A80, 79A85, 79A90, 79A95, 80A05, 80A10, 80A15, 80A20, 80A25, 80A30, 80A35, 80A40, 80A45, 80A50, 80A55, 80A60, 80A65, 80A70, 80A75, 80A80, 80A85, 80A90, 80A95, 81A05, 81A10, 81A15, 81A20, 81A25, 81A30, 81A35, 81A40, 81A45, 81A50, 81A55, 81A60, 81A65, 81A70, 81A75, 81A80, 81A85, 81A90, 81A95, 82A05, 82A10, 82A15, 82A20, 82A25, 82A30, 82A35, 82A40, 82A45, 82A50, 82A55, 82A60, 82A65, 82A70, 82A75, 82A80, 82A85, 82A90, 82A95, 83A05, 83A10, 83A15, 83A20, 83A25, 83A30, 83A35, 83A40, 83A45, 83A50, 83A55, 83A60, 83A65, 83A70, 83A75, 83A80, 83A85, 83A90, 83A95, 85A05, 85A10, 85A15, 85A20, 85A25, 85A30, 85A35, 85A40, 85A45, 85A50, 85A55, 85A60, 85A65, 85A70, 85A75, 85A80, 85A85, 85A90, 85A95, 86A05, 86A10, 86A15, 86A20, 86A25, 86A30, 86A35, 86A40, 86A45, 86A50, 86A55, 86A60, 86A65, 86A70, 86A75, 86A80, 86A85, 86A90, 86A95, 87A05, 87A10, 87A15, 87A20, 87A25, 87A30, 87A35, 87A40, 87A45, 87A50, 87A55, 87A60, 87A65, 87A70, 87A75, 87A80, 87A85, 87A90, 87A95, 88A05, 88A10, 88A15, 88A20, 88A25, 88A30, 88A35, 88A40, 88A45, 88A50, 88A55, 88A60, 88A65, 88A70, 88A75, 88A80, 88A85, 88A90, 88A95, 89A05, 89A10, 89A15, 89A20, 89A25, 89A30, 89A35, 89A40, 89A45, 89A50, 89A55, 89A60, 89A65, 89A70, 89A75, 89A80, 89A85, 89A90, 89A95, 90A05, 90A10, 90A15, 90A20, 90A25, 90A30, 90A35, 90A40, 90A45, 90A50, 90A55, 90A60, 90A65, 90A70, 90A75, 90A80, 90A85, 90A90, 90A95, 91A05, 91A10, 91A15, 91A20, 91A25, 91A30, 91A35, 91A40, 91A45, 91A50, 91A55, 91A60, 91A65, 91A70, 91A75, 91A80, 91A85, 91A90, 91A95, 92A05, 92A10, 92A15, 92A20, 92A25, 92A30, 92A35, 92A40, 92A45, 92A50, 92A55, 92A60, 92A65, 92A70, 92A75, 92A80, 92A85, 92A90, 92A95, 93A05, 93A10, 93A15, 93A20, 93A25, 93A30, 93A35, 93A40, 93A45, 93A50, 93A55, 93A60, 93A65, 93A70, 93A75, 93A80, 93A85, 93A90, 93A95, 94A05, 94A10, 94A15, 94A20, 94A25, 94A30, 94A35, 94A40, 94A45, 94A50, 94A55, 94A60, 94A65, 94A70, 94A75, 94A80, 94A85, 94A90, 94A95, 95A05, 95A10, 95A15, 95A20, 95A25, 95A30, 95A35, 95A40, 95A45, 95A50, 95A55, 95A60, 95A65, 95A70, 95A75, 95A80, 95A85, 95A90, 95A95, 96A05, 96A10, 96A15, 96A20, 96A25, 96A30, 96A35, 96A40, 96A45, 96A50, 96A55, 96A60, 96A65, 96A70, 96A75, 96A80, 96A85, 96A90, 96A95, 97A05, 97A10, 97A15, 97A20, 97A25, 97A30, 97A35, 97A40, 97A45, 97A50, 97A55, 97A60, 97A65, 97A70, 97A75, 97A80, 97A85, 97A90, 97A95, 98A05, 98A10, 98A15, 98A20, 98A25, 98A30, 98A35, 98A40, 98A45, 98A50, 98A55, 98A60, 98A65, 98A70, 98A75, 98A80, 98A85, 98A90, 98A95, 99A05, 99A10, 99A15, 99A20, 99A25, 99A30, 99A35, 99A40, 99A45, 99A50, 99A55, 99A60, 99A65, 99A70, 99A75, 99A80, 99A85, 99A90, 99A95.

Keywords. invariant theory; Liouville's integrability condition; complex dynamical systems; integrability; invariant; Liouville's integrability condition; complex phase space systems.

1. Introduction

In the last few decades, several efforts have been made to extend the idea of Liouville's integrability to the generalized class of dynamical systems [1–7]. The existence of invariant integrals helps in understanding and classifying the dynamical properties of a dynamical system. Such invariants can be constructed only for the systems that exhibit some of the dynamical features and hence their construction involves their use in identifying the class of dynamical systems for a certain type of potential energy involving a finite number.

The integrability of a real dynamical system can be studied on the basis of real time and real energy conservation. But both conservation are not invariant to the transition to complex systems [8–12]. The invariants obtained are expected to give an important insight into the field, such as checking the stability of the dynamical differential equation, to obtain the energy of a steady system, to distinguish a Hamiltonian system, and to check the accuracy of numerical solution [13–17]. These aspects are also useful in various fields, such as laser physics, plasma physics, astrophysics, nonlinear optics, hydrodynamics, and wave effects, and their uses, etc. [18].

Some physical properties of a dynamical system can be studied under the nature of real Hamiltonian systems, but there are some other aspects of dynamical systems that can be studied by complex dynamical systems. For example, phenomena like the optical states of a quantum resonator, standing or wave, dispersion, and resonance phenomena, the study of complex systems from the viewpoint of non-Hermitian systems, wave propagation, optical bistability, quantum biology, and the non-Hermitian resonant effect [19–21].

Approximation to a real dynamical system of complex Hamiltonian [22–25], a quantum dynamics in steady state systems in the field of optical resonators, and the study of quantum propagation, are further open and arise in both the classical and quantum dynamical fields.

There are several methods available in the literature to study the integrability of systems. It has been shown in [26] that the Liouville's integrability condition is not sufficient to study the integrability of a dynamical system.

1. In quantum mechanics, and also there is study on differential equations problems, the transformations $x \rightarrow y$, $t \rightarrow \tau$ and $\psi \rightarrow \phi$ that are applied to the wave function $\psi(x, t)$ and the Schrödinger equation $i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$, which are called unitary transformations for non-Hermitian systems are the first, because there are not required a unitary transformation transformations, as the system evolves in time, it has a complex energy. The later studies the unitary transformation for the construction of complex invariants that are the study of real dynamical systems, introduced by Manton [27], and the real number group associated to a Hamiltonian system by Margulies [28].
2. A generalized version of the Liouville's integrability condition, which is constant, can also be found that influences the possibility of non-Hermitian dynamical systems are shown as complex numbers. This is a complete result in [29] given by $\alpha, \beta, \gamma, \delta$, and ϵ given [30].
3. A complex invariant method can also be studied as an alternative to the Liouville's integrability condition [31]. A detailed study of the method is reported in [32] and [33]. The corresponding complex valued Hamiltonian H_c is defined from $H_c = H_c^* + i\Gamma$, where H_c^* is the complex conjugate of H_c and Γ is the real part of H_c .

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INVESTMENT BEHAVIOUR OF WOMEN INVESTORS IN THE COMPETITIVE MARKET: A FACTOR ANALYSIS APPROACH

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ABSTRACT

The present paper attempts to have a better understanding of the behaviour of women investors while making an investment decision. The main objective of the study was to investigate the main factors, which play an important role in the choice of investment of women investors. The major factors that influence the women investors will be helpful for the financial service provider. This study is based on the sample survey of 330 women investors in Haryana. Factor analysis has been used to analyse the data. The analysis revealed the six factors related to financial attitude and behaviour i.e. Perceived ROI, Rationality, Investment Consistency, Risk Aversion, Higher Risk Propensity and Conservation Investment. The result showed that most of the investors are worried about their financial affairs.

Keywords: women investors, Competitive Market, Investment Behaviour.

INTRODUCTION

Individuals invest their savings in different ways. The choice of investment is made by the family's net worth, family income, stage in life cycle, employment status of spouse, etc. (Kamdar, 2011). Investment is a wisdy function of our needs and goals. Every investor may have multiple numbers of investment objectives and requirements which they want to fulfill by their investment portfolio. Investors might be concerned with more than many measurable factors such as risk and return.

The general opinion is that women cannot bear more risk than men. But now the time has changed as women have great propensity to save and invest. Today, a great number of women are employed, having good career and are earning their livelihood. Now the women's attitude towards investment avenues has been changing. Behavioral finance also plays an important role in the investment decision of women investors. Hence, the woman's expectation and objective may be differs from person to person.

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AN ANALYSIS OF INVESTMENT PATTERN OF WOMEN INVESTORS IN HARYANA

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ABSTRACT

This paper examines the investment pattern of women investors regarding various investment options available in India. This study is based on the investment pattern of the respondents in the state Haryana only. The objective of this study was to determine the preference and objective behind the various investment tools. This study was conducted on the women investors across the government sector, private sector and house wives in the Haryana. The data was collected by distributing a self-administered questionnaire to 100 women respondents. The outcome of the study suggests that majority of the respondents preferred to invest their savings in traditional investment avenues such as bank deposit, insurance policies, post office schemes etc.

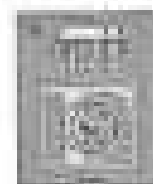
Keywords: Investment Pattern, women respondents, House Wives.

INTRODUCTION

Investment is the commitment of funds made in the expectation of some positive return on it. Every investor carefully plan, evaluate and allocate funds in various investment avenues which offer greater return with safety of principal amount. Hence, the investment decision making is one of the crucial challenges faced by the investors. Every investor differs from the other in many aspects due to various factors like demographic causes, socio-economic background, education level, marital status, age and gender. The investor should consider his financial goals, risk tolerance level and other constraints while designing the investment portfolio (Zabihalla, 2013). The present study is undertaken to estimate the attitude of women investors towards various investment avenues.

REVIEW OF LITERATURE

Pardey and Kishanvarayan (2013) in the study titled "Investor's Perceptions Towards Alternative and Preferences" aimed at to find out the investment preferences towards the various investment



Synthesis, characterization, *in vitro* DNA photocleavage and cytotoxicity studies of 4-arylamino-1-phenyl-3-(2-thienyl)-5-hydroxy-5-trifluoromethylpyrazolines and regioisomeric 4-arylamino-1-phenyl-5-(3-(2-thienyl)-3(5)-trifluoromethylpyrazoles



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ABSTRACT

1-(2-Thienyl)-3-(2-arylamino-4-(trifluoromethyl)-5-hydroxy-5H-pyrazol-5-yl)-2-phenyl-2H-pyrazole (1) and 1-(2-thienyl)-3-(2-arylamino-4-(trifluoromethyl)-5-hydroxy-5H-pyrazol-5-yl)-2-phenyl-2H-pyrazole (2) were used as starting materials to prepare the regiosomeric 4-arylamino-1-phenyl-3-(2-thienyl)-5-(3-(2-thienyl)-3(5)-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (3) and 4-arylamino-1-phenyl-5-(3-(2-thienyl)-3(5)-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (4) by heating with phosphorus pentoxide in sealed conditions. All the synthesized compounds 3, 4, 5, 6 and 7 were screened for their DNA photocleavage activity on plasmid pUC19. Compounds 3 and 4 showed 100% cleavage at 365 nm UV light without any additive. The results in terms of photocleavage activity (3) photolysis showed DNA level after the photocleavage 3-(5-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (3) and 4-arylamino-1-phenyl-5-(3-(2-thienyl)-3(5)-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (4) were similar to that of 3-(2-thienyl)-3(5)-trifluoromethylpyrazole (5). *In vitro* cytotoxicity studies of 3-(5-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (3) and 4-arylamino-1-phenyl-5-(3-(2-thienyl)-3(5)-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (4) were similar to that of 3-(2-thienyl)-3(5)-trifluoromethylpyrazole (5). The cytotoxicity against four tested cell lines using MTT assay, 3-(5-trifluoromethylpyrazol-5-yl)-2-phenyl-2H-pyrazole (3) was similar to the most potent compound with an IC₅₀ value of 0.4 ± 0.4 μM against MCF7 cell line.

1. Introduction

Pyrazole derivatives have increasingly attracted attention in the recent years due to their biological and chemotherapeutic importance as anticancerals [1,2], anti-infective [3–5], anti-inflammatories [6,7], anti-oxidant [8,9], anti-epileptic [10,11], anti-convulsant [12] and anti-arrhythmic [13,14] agents. Various reports show that pyrazole derivatives having appropriate groups at N1, C2, C4 and C5 can act as tyrosine and DNA photocleavage agents for anticancer cells. For example, pyrazole derivatives having one group at position-4, C4(OR), (5) (3 or 4) was identified as novel anti-proliferative agent having activity for cancer cells [15,16]. Derivatives containing one group have also been reported to possess cancer biological activities like anticancer [17] and anticancer properties [18]. The presence of electron withdrawing group can lead to cleavage of carbon nitrogen bond leading to the release of nitrogen and the

formation of aryl radicals which act as effective agents against DNA binding and photocleavage [19–21].

Moreover, 3-(2-thienyl)-2-phenyl-2H-pyrazole (2) was reported for its ability to inhibit cell migration and tumor lung cancer growth [22] (Fig. 1). The compounds containing thienopyrazole ring such as 4-(2-thienyl)-2-(2-thienyl)-2H-pyrazole and its derivatives are well known single target inhibitors and phototoxic agents [23–25].

Additionally, compounds containing thienopyrazole ring possess cancer cell-inhibitory effect at cellular level [26]. Incorporation of aryl/thienopyrazole group into the thienopyrazole leads to extension of properties of the compounds. A large number of fluorinated anti-proliferative agents are being used for the treatment of cancer [27]. 4-(2-thienyl)-2-(2-thienyl)-2H-pyrazole (2) (Fig. 1) has been used for the treatment of metastatic of human pancreatic cancer [28] (Fig. 1). Thus, in view of the

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Mass Spectra of Heavy and Light Mesons Using Asymptotic Iteration Method

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Abstract. The non-relativistic radial Schrödinger equation is consistently solved using asymptotic iteration method within the framework of a general two-body potential (like Cornell, Coulomb plus harmonic oscillator). The energy eigenvalues (masses) is derived in three-dimensional space, which is further used to calculate the mass spectra of ψ , χ , η , η' , χ and ψ mesons. The obtained results of the work are in good agreement with experimental and other theoretical results and well supported in comparison with other non-relativistic meson studies.

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Key words: Schrödinger equation, asymptotic iteration method, mass spectra, mesons.

1. Introduction

The quarkonium mass spectra can be addressed theoretically via two different approaches. The first one is a direct calculation using quantum chromodynamics (QCD) [1–5]. These calculations can be done with lattice QCD, but are complex and computationally very expensive. The other technique is the use of potential models to describe the bound states, which is simpler by the description of energy levels in quarkonium systems. The experimentally observed mass spectra of the quarkonium states can be reproduced with a certain potential model for the use of an interaction potential in non-relativistic quantum mechanics. As this approach, the potential $V(r)$ is taken as a function of the relative separation r between quark and an antiquark and the problem is then handled consistently by solving the two-body Schrödinger equation (SE) for $V(r)$. Many the heavy quark potential is represented by the Cornell potential $V(r) = -\frac{4}{3}\alpha_s + \sigma r$.

Bakker et al [6] obtained the mass spectra of ψ meson within the framework of non-relativistic approximation. Haja's using two types of interaction potentials i.e. QCD potential potential, power law potential, harmonic and Cornell potentials had also studied the exclusive decay of excited states of ψ meson. Hajar et al [7] calculated the mass spectra of mesons using Cornell potential by solving the non-relativistic SE consistently. Hammad et al [8] obtained the mass spectra of mesons by solving the Klein-Gordon equation with Cornell interaction between mesons [9] and also calculated [10] the masses and wave functions of heavy baryons by solving the radial SE using relativistic theory. Hammad et al [11] solved the radial SE using variational method and studied the properties of light and heavy mesons by considering Cornell interaction. Hajar et al [12] studied mass spectra and exclusive decay rates of charmonium, bottomonium and ψ mesons

using relativistic quark model based on quasipotential approach.

Wang [13] obtained the mass spectra of quarkonium by using temperature dependent Yukawa potential defined from lattice gauge calculations. Ma [14–17] analytically solved the Schrödinger radial SE using Nikitin-Dunne method and obtained the mass spectra of charmonium and bottomonium using Cornell and Cornell plus harmonic potentials. Hajar et al obtained the mass spectra of heavy mesons by considering Cornell plus harmonic (Cornell potential) interaction between quarks by solving Schrödinger radial SE using power law [18] and soft repulsive interaction potentials (SRIP) [19]. They also studied the SE using Nikitin-Dunne method and obtained energy spectra of a new charmonium state in a magnet field [20].

With a view to generate improved results for quarkonium states, in the present work, we consider a general interaction potential

$$V(r) = -\frac{4}{3}\alpha_s + \sigma r + \frac{A}{r} + \frac{B}{r^2}, \quad (1)$$

where α_s , σ , A and B are of the positive potential parameters, which will be fixed by considering experimental data later on. The additional term of $\frac{1}{r}$ in Cornell plus harmonic (CPH) potential represents the behaviour of potential at the origin $r = 0$ due to possible better confinement and leads to improved results as compared to CPH potential [21].

The other important interaction potentials like Cornell and Cornell plus harmonic potentials are special cases of potential (1). This potential has also been used to calculate the energy eigenvalues spectra of quarkonium states [22–26] and we also successfully applied the same potential to calculate bound energy states of a number of diatomic molecules [27]. Recently Hajar et al [28] study and discussed the mass spectra of mesons by solving the Schrödinger radial SE using most accurate method

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Bound state solutions to the Schrödinger equation for some diatomic molecules

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Abstract. The bound state solutions to the radial Schrödinger equation are obtained in three-dimensional space using the series expansion method within the framework of a potential well whose potential. The energy eigenvalues of the pseudo-harmonic and Kratzer potentials are given as special cases. The obtained analytical results are applied to several diatomic molecules, i.e., N_2 , CO , NO and CH . In order to check the accuracy of the present method, a comparison is made with some results obtained in the literature by using other techniques.

Keywords. Schrödinger equation; bound state; eigenvalues; pseudo-harmonic potential; Kratzer potential; series method.

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1. Introduction

In the realm of quantum physics and quantum chemistry, the most challenging task is to obtain exact analytic solutions to the radial Schrödinger equation (SE) with a given interaction potential [1–3]. The 1D case solutions to the SE, in particular, find special interest in chemical physics and molecular spectroscopy. To describe the spectra of diatomic molecules, anharmonic potentials, such as the Morse potential, are generally utilized. The harmonic oscillator potential can be used only for low-state calculations. The Kratzer and pseudo-harmonic potentials are regarded as intermediate ones between anharmonic and harmonic oscillator potentials. This is the reason of the anharmonic potentials in molecular physics, molecular spectroscopy, chemical physics and biology. The bound state (i.e., l -state) solutions to the relativistic and non-relativistic SE have been studied by several researchers in the past. A brief account of such studies is as follows:

Qiang *et al.* [4, 5] obtained the eigenvalues and eigenfunctions of the SE with the pseudo-harmonic potential in two-dimensional (2D) and then established the relation and annihilation operators directly from the regularization with the factorization method. Wang *et al.* [6] took with the factorization and eigenfunctions of the curved and the eigenvalues and eigenfunctions of the SE with the harmonic and pseudo-harmonic potentials in an arbitrary D -dimensional space. Qiang *et al.* [7]

presented the analytical solutions to the radial SE for the rotating Morse potential. The energy levels and state functions of all bound states were also obtained for the three diatomic molecules (NO , CO and LiH) and the molecules by the molecular potential were in good agreement with the results of other studies. Analytical expressions of eigenvalues and eigenfunctions were derived by Sun [8] and obtained the energy of the bound states of the diatomic molecules using the Morse potential, which is frequently used to calculate the vibrational energies of diatomic molecules.

Kaymak *et al.* [9] obtained the exact analytical solutions to the radial SE for the Kratzer potential for various values of α and β and calculated the bound state energy eigenvalues and corresponding eigenfunctions for CO , NO , O_2 and F_2 diatomic molecules. The exact solutions to the radial SE for the Morse and pseudo-harmonic potentials were obtained by Selim *et al.* [10, 11] for arbitrary values of λ . The calculated eigenfunctions were expressed in terms of Jacobi polynomials and the energy bound states were applied to several diatomic molecules such as N_2 , CO , NO and CH . Özveren *et al.* [12] presented the exact analytical solutions to the SE in N -dimensional space for the pseudo-harmonic oscillator potential. The bound state energy eigenvalues, normalized wave functions, and expectation values for r^{-1} , r^2 , T , V , H and p^2 were also obtained. From these values, they found that the results obtained in each



Integrability of a Time-Dependent Coupled Harmonic Oscillator in Higher Dimensions

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Abstract

Within the framework of extended complex plane space characterized by $z = x + iy$, $\bar{z} = x - iy$, $\bar{\bar{z}} = z$, we investigate the exact 4d real-time integral for coupled harmonic system in time dimension. For this purpose, Lie-algebraic method is employed and the results obtained in this work may play an important role in studying the exact of differential equations solutions of Coupled system and to check the consistency of a numerical algorithm.

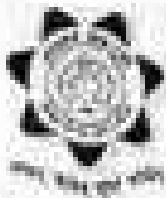
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1. Introduction

Various physical properties of a dynamical system can be explained by the real Hamiltonian systems [1,2] but there are some other aspects of a dynamical system which can not be explained in this way. It is the complex Hamiltonian which explain such aspects of a system successfully [3-4]. The complex Hamiltonian helps to understand the several phenomena in the area of physical systems [5,6] like phenomena pertaining to resonance scattering in atomic, molecular and nuclear physics, population growth in biology [7] and study of delocalization transition for the understanding of various of type-II superconductors [8] and to some chemical reactions also. In addition to this complex Hamiltonian has been used to study some other theoretical concepts i.e. complex eigenvalues with regard to the calculation of a semiclassical coherent state propagator in the path integral method have attracted a particular interest in laser physics [9].

There are various ways of constructing a given Hamiltonian, but here we use the scheme given by Karim and de Azavedo [9], used to develop an algorithm for the computation of semiclassical coherent state propagator to irregular potentials in extended complex plane space approach (ECPSA). The real and imaginary parts of i

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Performance Evaluation of MSME Before and After Enactment of MSME Act 2006

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Abstract

The micro, small and medium enterprises is an important segment of Indian economy. It is playing an important role to growing the Indian economy. Although big industries that not come under the MSME sector are playing important role in the Indian economy but we cannot ignore the role of MSME sector in Indian economy. By taking this point in mind we have greater need to understand the status of MSME sector in Indian economy with the point of working enterprises, employment, export and the total investment under the MSME sector. With the help of this paper we will understand the concept of MSME and to find out the impact of MSME act 2006 on this sector by comparing the performance of MSME sector before and after the enactment of MSME act 2006.

Key-Words : Small Scale Industry, SMEs,

Introduction

The small scale industry is an important segment of Indian economy. It has been accepted as the engine of economic growth due to their contribution in the country's industrial production, employment, growth rate and export. The micro, small and medium enterprises are also referred to as small and medium enterprise (SMEs) and small and medium sized business (SMBs) in some countries. The abbreviation SME occurs commonly in the European unions and in international organization, such as the World Bank, the united unions and the world trade organization. The term small and medium sized business (SMB) is predominately used in the united state of America. In the European unions and USA, SMBs are companies whose fixed

Cost or turnover falls below certain limits. The business is classified as per the number of employee employed in the business. In South Africa the term SMME is used for small, medium and micro enterprises. In Africa they use MSME for micro small and medium enterprises. In Indian economy this sector is generally known as the micro small and medium enterprises (MSME). Thus the MSME sector includes the three type of industry namely micro, small and medium enterprises. These industries can be different from each other on the basis of total investment in plant & machinery or investment in equipment in each industry. These industries are the basis foundation of Indian industrial sector. These industries provide the opportunities of doing business in India to different type of entrepreneur.



CORPORATE SOCIAL RESPONSIBILITY: AN INITIATIVE OF SOCIAL DEVELOPMENT

Pardeep Kumar

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ABSTRACT

When we talk about the responsibility of a business organization towards the society in the context of legal, social, geographical, environmental and economically then it is known as corporate social responsibility (CSR). Without the existence of society the business organization can't survive because the society provides the framework to operate business organization. The CSR is an initiative of corporate sector towards the society. With the help of the CSR any business organization can perform their responsibility towards the society. Now the CSR has become an important part of business strategy. The motive of this paper is to understand the concept of CSR, responsibilities of business organization to society, impact of CSR on rural development and evaluation of CSR in the context of different parties of the society. To gather the information about the above objectives the secondary data used because paper is conceptual in nature.

KEYWORDS: corporate social responsibility, social development, corporate sector.

INTRODUCTION

Every business organization survive in the society and use the many resources whether human or non human for achieving their goal. These resources are the components of the society. If a business achieves their goal with the help of society then some responsibility of business organization creates towards the society. In other words we can say that a business organization responsible towards the society by legally, socially, geographically and environmentally. When we talk about the responsibility of a business organization towards the society in the context of legal, social, geographical, environmental and economically then it is known as corporate social responsibility (CSR). Without the existence of society the business organization can't survive because the society provides the framework to operate business organization. The CSR is an initiative of corporate sector towards the society. With the help of the CSR any business organization can perform their responsibility towards the society. If a company has started such type of business that creates the pollution problems by their operation then it becomes the organizations responsibility to provide the preventive measures to society. The society also keeps the expectations about these measures. If a company does this very well then we will say that the company performing their responsibility. Now the requirement of these responsibilities has increased because the business organization has become customer oriented instead of sale oriented. If business organization perform their CSR functions towards the society with effective manner then their importance among the society definitely increase. In few years ago the society was not aware about their rights but now the every part of society aware about their rights. So there is more need to implement CSR in effective and better way.

REVIEW OF LITERATURE:



ITMR: An Experiment to ACO based Multipath Routing

Shashi Agarwal, Pardeep Kumar, Shashita Upadhyay

Abstract—As the volume of big data and cloud computing are growing day-by-day, the need of multipath routing is also getting more and more look into. Without using multipath routing the handling of big data is almost impossible. This paper is an attempt in the direction of finding and calculating multiple paths in a network. This paper compares the similarities and differences between the ACO based approaches to routing i.e. ITMR, AntNet and ABC algorithm. The ITMR has been performed for a network and the results are found as per expectation i.e. the algorithm is able to find the multiple paths for data transmission depending upon the conditions.

Index Terms—ITMR, AntNet, AntNet, ABC

I. INTRODUCTION

Multipath routing is a technique by which multiple paths may be used in parallel to transmit the data via a network. A previous number of benefits viz., more bandwidth, load balance, better security, etc. There are three main components needed for the implementation of multipath routing viz., Multipath Calculation Algorithm, Multipath Forwarding, and Multipath Link-Link protocol.

This paper considers the first component of the multipath routing implementation i.e. A multipath algorithm, which explores multiple paths between source and destination nodes depending on previous metrics. Metrics can be throughput, delay, reliability, bandwidth, distance, security, cost etc.

II. MULTIPATH CALCULATION ALGORITHM

A multipath calculation algorithm has number of characteristics. The major two characteristics are quality and quantity of paths.

The quality of a path does not always mean the best path, rather it depends on path specification. A path which fulfills the requirements of the flow specification will be termed as a better quality path. For example, if the flow specification is either low-cost or higher bandwidth or higher throughput, then the multipath algorithm should be able to find multiple paths with low cost or available higher bandwidth or higher throughput, whichever is desirable. Multiple paths which are identified should have other attributes such as path quality and path independence.

Path quantity means how many paths are generated by a multipath calculation algorithm. Although more paths means more overhead, yet the number of paths found by the

algorithm should be considerable as one can not want excessive routes for selecting a limited number of paths depending upon the requirements. However, main focus of the algorithm should be on computing quality paths.

III. ACO-BASED ROUTING

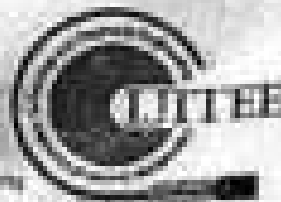
Traditional approaches to multipath routing yields good results, but in some cases it may be improved to find and consider all possible paths for traffic transportation due to large overhead, and therefore, only a limited number of good paths need to be considered. In such cases, some inspired computational intelligence techniques provide optimum solutions to the problem of finding and utilizing the multipath way towards NP-hard.

Ant Colony Optimization (ACO) is a very natural approach to determine the routes in the distribution as the ants are also doing the same thing to get the requirements of network routing. Therefore in this paper ACO [1] has been contemplated as one of the basis for identifying the routes from a source to a destination.

A multipath routing strategy with adaptation of ACO approach has been formalized in [2]. Modification aspects of both ABC[3] and AntNet[4] variations of ACO [5] have been evident in the strategy of the strategy. Table 1 addresses various features present in ACO based routing and their implementation strategy in ABC and AntNet. The third column derives the formulation of the ITMR algorithm [7] indicating a comparison as well as similarity with ABC and AntNet.

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INDIVIDUAL'S PREFERENCE FOR INVESTMENT - A REVIEW OF LITERATURE

RUSMAN DEVI

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ABSTRACT

In this modern time, the money plays an important role in everybody's life. Every individual need first start-up consumption for the benefits of future requirements. Saving of people is required in various aspects for fulfilling future needs. Investment is the commitment of funds which have been saved from current consumption with the hope that some benefits will be occurred in the future. Thus it is a reward for waiting for money. Saving of the individual are invested in assets depending on their risk and return demands, safety money, liquidity, the available avenue for investment, various financial institutions, etc.

For the achievement of above goals appropriate decisions have to be taken through this study, an attempt has been made to see the preference of investors towards various investment avenues. This paper is based on the research work done on the said subject. For the purpose of study the research papers were selected from various national and international journals & conference proceedings.

Keywords: Investment avenues, Risk and return.

INTRODUCTION

Investment is the purchase of financial assets or other form of value with expectation of desirable future returns. The most crucial problem faced by the investors is perhaps in the area of taking investment decisions. Every investor differs from the investors in all aspect due to various like demographic factors, socio-economic background, marital status, educational qualification, age, gender, etc. The other problem in investment is the lack of awareness about various investment alternatives. In India many investment avenues are available in which some are highly risky or some are marketable and liquid. The investor has to choose particular avenue depending upon his specific need, risk preference and return expected (Kothari 2014). We categorize the investment avenues according to their risk level in many parts such as:



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paper helps to understand the various investment needs such as future needs, good returns, tax benefits and risk factor. Finally, the study concludes that there is significant difference

A STUDY OF DIFFERENT INVESTMENT NEEDS OF WOMEN INVESTORS IN BARTANAL CONTEXT

Sanjay Singh

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 Kurukshetra University, Kurukshetra

ABSTRACT

Individual behavior is goal oriented and without needs there are no goals. Every individual invest their money to improve their monetary wealth for present and future both. Investment decisions are influenced by the investment objectives or expectation perceived by the investor. Investor increases their wealth effectively by protecting it from stock, inflation and other factors. The present research work is an attempt to explore the differences in importance of the investment needs between single and married women investors and also various level of education. The research

KEYWORDS: Investment, Income, Future Needs, Tax benefits

INTRODUCTION

The income that a person earns may be used for purchasing goods and services that he currently requires or it may be saved for the goods and services that he may require in the future. In other words, income can be spent for current consumption or saved for the future consumption. In this nature investment plays an important role. All investments are made by the expectation of some future benefits or the overall success.

This study deals with the investment needs of women investors in Haryana context to find the better investment context. A) for all the category to

developing, the thinking of the people is also changing rapidly. Some decade back, the first place of women is considered at home. But now the time has changed and even the position of women is rising. Women are working equally to men in every field. Now, many women want to invest but lacking in a best investment strategies.

LITERATURE REVIEW

Warner and Charles (2010) in the study titled "Factors Influencing Indian Individual Investors' Behaviour: Survey Evidence" finds that the psychological issues such as conservatism and under-confidence are playing a significant role in determining the individual investors' behaviour.

Singh and Bhat (2012) made an

attempt to study the investor's perception towards investment objectives with regard to Internet Stock Trading in India. This study suggested that perceived risk coverage is the most important factors towards investment objectives.

Emmons and Hwang (2010) in his article "Life Insurance & Working Women: A Critical Study of Factors Affecting The Purchase Decision" proves that the decision to purchase an insurance policy is mainly affected by the advice of husband and even women blindly follow advice of their family without searching any other information regarding investment or the policies. Their main objective of purchasing policy is to save income tax.



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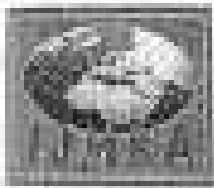
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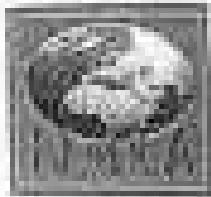
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Exploring *Embedded* Narratives in Muriel Spark's *The Finishing School*

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INTRODUCTION

Exploring *Embedded* Narratives in Muriel Spark's
The Finishing School

"What is the story? How does it develop?
 Historical events – they have to develop. How ...?"
 "No idea, Rowland, I can't foresee the future,
 All I know is the story will happen."
 – *The Finishing School*, 11

The novel as a form became the centre of critical analysis with the beginning of modernist movements and in the postmodern era this critical study with the form of novel led to several radical changes. Muriel Spark from the beginning of her novel writing career explored new narrative strategies. She is an increasingly celebrated novelist whom each novel is a literary event. Spark underlines the existential problems in God-created world without any orthodox perspective and rejects the traditional style of narrative. Spark's experiments with the form and technique of the novel provide wider perspective to understand the postmodern concerns.

Genette's work has "its focus, not the tale itself, as he speaks, but how it is told" (Story 227). He approached the theory of narratology in different ways in *Narrative Discourse: An Essay in Method* (1972). The term *embedded* narrative is used by Genette in *Narrative Discourse* and it denotes the short narratives inserted by the main plot. Generally it is told by other narrators from other narrative perspectives. This is a rather common technique that adds diversity to the narrative act as well as increases the complexity of the narrative. The aim of the present paper is to explore the *embedded* narratives in Muriel Spark's *The Finishing School*.

The Finishing School is Spark's last novel and it was published in 2004. It gives the impression of being mildly experimental, even when it deals with events such as publishing and selling the rights with which the author is profoundly familiar. *The Finishing School* is about relationship between a teacher and student. It narrates how a young student student Chris is writing a novel and how he provides his teacher Rowland for writing a novel. Theoretically this novel appears only what was already created. It doesn't present the novel conflicts like her previous novels, so the readers are not able to believe in Spark's detachment towards her characters.

The Finishing School is written in three layered complicated structure and inter-text layer presents *embedded* narrative. According to Genette's narrative typology, the level of this novel's narrative structure can be divided in four parts and these four parts is discussed in three categories. The following table is showing the same division:

S. No.	Object	Levels	Narrative Content
1	Frame Story	Extradiegetic	Introductory Narrative
2	Event Story	Intradiegetic	Story about a school and two aspiring Writers
3	Embedded Level Story	Homodiegetic	Rowland and Chris Writing their Novels
4	Embedded Narration	Metadiegetic	<ul style="list-style-type: none"> ➤ Chris' Home-made Novel: <i>The Filled Jarley?</i> ➤ Rowland's novel <i>The School Observed</i>

Metafictional Study of Muriel Spark's *Loitering with Intent*

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ABSTRACT

Muriel Spark's *Loitering with Intent* projects metafiction as its key feature with regard to its complex narrative structure and it has several instances of fiction-within-fiction and interrupts the reader's expectations of a genre by violating the generic boundaries. The present paper tries to uncover the self-reflective and self-conscious personality of Spark as a writer which she tries to portray through metafiction. It also explains her art of narrative and creation of fiction. Along with it, the paper also reflects its impact on her future novels which she wrote after *Loitering with Intent*.

Key Words: Metafiction, Narratology, Narratives, Narration, Novel, Muriel Spark, Fiction, Postmodern

INTRODUCTION

"When people say that nothing happens in their lives I believe them. But you must understand that everything happens to an artist: there is always rehearsal, nothing is lost and nothing never exists."
-*Loitering with Intent*

"Metafiction" is a semiological literary device and genre of fiction, which means fiction about fiction or fiction within fiction. It has become a powerful tool in late modern and postmodern fiction but it is rooted in former authors and works. An history of metafiction moment is seen in Homer's *Odyssey*, Chaucer's *The Canterbury Tales* (1400), Laurence Sterne's *The Life and Opinions of Tristram Shandy* (1759) etc., but it is highly practiced by the fiction writers in the 21st century and Muriel Spark is also one of those selected authors who used this complicated layered metafictional technique to form a fiction-within-fiction. Muriel Spark's *Loitering with Intent* projects metafiction as its key feature with regard to its complex narrative structure and it has several instances of fiction-within-fiction and interrupts the reader's expectations of a genre by violating the generic boundaries. The present paper tries to uncover the self-reflective and self-conscious personality of Spark as a writer which she tries to portray through metafiction. It also explains her art of narrative and creation of fiction. Along with it, the paper also reflects its impact on her future novels which she wrote after *Loitering with Intent* (1981).

Since Muriel Spark (July 1, 1918 – April 13, 2006) occupies an important place among the post-war British novelists. In 1981, Spark was nominated for the second time in her career, for Booker McConnell Prize for *Loitering with Intent*. Though the title was the prize but her novel received enough critical attention. This novel is one of Muriel Spark's most accomplished books or novels. Since its publication, *Loitering with Intent* has been explored from various aspects. However, not many critics have in-depth studies on its metafictional features. A few critics, like Doyak, Page, Winkler, narrate that the novel is a metafiction, but they only draw a general conclusion without providing sufficient arguments in a comprehensive and convincing way. Indeed, *Loitering with Intent* is a typical metafiction and distinguishes itself from others by its extremely wide range of metafictional characteristics. In terms of its structure, the novel has the complicated "fiction within fiction". As to its content, it not only foregrounds the artificiality of the novel itself but also has literary-structure as its fictional object.

Loitering with Intent is unique for its multi-layered structure. At first sight, it seems to be a simple autobiography-in-novel. However, careful reading can reveal its complex structure as fiction-within-fiction, or meta-fictionary. Though genre not "In metafictional novels, diverse literary devices range from ironic within stories and self-conscious worlds or mutually contradictory situations" (Wright, 88).

Multi-component reaction to access a library of polyfunctionally substituted 4,7-dihydropyrazolo[3,4-b]pyridines

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ABSTRACT

A practical approach to polyfunctionally substituted 4,7-dihydropyrazolo[3,4-b]pyridine derivatives from heteroaryl hydrazones, 2-aryl-2-isocyanoacetates and aldehydes have been described in this report. The present catalyst-free protocol involves the multicomponent of heteroaryl aldehyde and isocyanoacetate, which undergoes in situ Michael addition to afford ring compounds in moderate to good yields. All the steps were conducted consecutively to render the procedure as practical and straightforward as possible. The sequential synthetic protocol requirement takes less than one hour and shows broad substrate scope.

GRAPHICAL ABSTRACT



- ✓ Short time
- ✓ Short reaction time
- ✓ Simple efficient practical experimental procedure
- ✓ Good multi-component strategy

KEYWORDS

Hydrazine, 4,7-dihydropyrazolo[3,4-b]pyridine

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Introduction

Heterocyclics are ubiquitous scaffolds in pharmaceuticals, natural products, and biologically active compounds. Pyrazolo[3,4-b]pyridine system, in particular, constitutes a privileged substructure and has gained special attention of the researchers in the last few decades. These compounds have been reported to exhibit antineoplastic,^{1,2} anti-inflammatory,^{3,4} A1 adenosine receptor inhibitor,⁵ anticancer,^{6,7} glycogen synthase

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Good

RESEARCH ARTICLE

Electron plasma wave excitation by self-focused cosh gaussian laser beams in axially inhomogeneous plasma: effect of density ramp

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Abstract Excitation of the laser driven electron plasma wave (EPW) in plasma with axial density ramp has been investigated theoretically. The effect of self focusing of the laser beam on the growth of laser excited EPW has been investigated during its propagation through the plasma. The laser beam excites an EPW at frequency ω_p that due to the optical bistability of plasma gets nonlinearly coupled to the laser beam due to the postnonlinear bistability of electron electrons. Using variational theory and analytical solution of the coupled nonlinear wave equations for the pump wave and EPW have been obtained under WKB approximation technique. It has been observed that growth of the EPW is significantly affected by the self focusing effect of pump beam.

Keywords Self focusing; Electron plasma wave; Postnonlinear; Resonance; Gain; Chirp ramp

Introduction

Inhomogeneity or coupling of linear laser beams with plasma set at the verge of instability when gain loss balance due to its important in many practical applications such as laser fusion [1–11], plasma wake field acceleration [12–15], free laser [16–18], relativistic generation [19], etc. The ultimate extent of these applications depends on the efficiency of laser plasma coupling, which is further decided by many

different nonlinear processes [9–11]. These processes range from collisional absorption to excitation of trapped laser driven resonances [12–15]. These nonlinearities can be further extended to the resonant coupling of the incident laser beam with two daughter waves. In the context of current context both these daughter waves can be electron plasma waves, or acoustic waves along with a scattered electromagnetic wave.

EPWs can be viewed as plasma surface laser mode; all properties of gain instability and collisional behavior. Plasma is a state of matter that consists enough free the atoms lose their individuality. The negatively charged electrons are still attracted by positively charged nuclei, but they are not bound together. This gives a plasma some overall properties unlike most kind of ordinary matter where, liquid and gases do free floating electrons and ions of a plasma are strongly affected by magnetic and magnetic fields. Plasma is a where is quasi neutral, but as the electrons and positively charged ions are separated, a distribution in various regions of air separates and not present charges along the by plane of a charged parallel plate capacitor. Both an excess charge, fluxes of charges results in an electric field forming from positive to negative regions. The electric field pulls the electrons and ions towards each other with equal force. Due to their large mass ions get lagged and this is mean as ions and the electrons move towards the ions. As the electrons move towards the ions, they steadily gain velocity and momentum. It is a paradoxical moving towards an mean position from an extreme position. Due to this gain in momentum the electrons maintain their opposite low potential resulting in reversing the direction of electric field. Now the reversed electric field opposes the electron motion like them down and turning them back again. The process repeats itself establishing an electron oscillation. In the presence of thermal velocity these electron oscillations tend to a longitudinal collective compression and rarefaction regions of electrons

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EXCITATION OF ELECTRON PLASMA WAVE BY SELF FOCUSED COHERENT GAUSSIAN LASER BEAMS IN COLLISIONLESS PLASMAS: EFFECT OF DENSITY RAMP

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Excitation of the laser driven electron plasma waves (EPWs) in plasmas with axial density ramp has been investigated theoretically. The effect of self-focusing of the laser beam on the growth of laser excited EPW has been incorporated. During its propagation through the plasma, the laser beam excites an EPW of frequency ω_p that due to the spectral nonlinearity of plasma gets nonlinearly coupled to the laser beam. Using variational theory some analytical solutions of the coupled nonlinear wave equations for the pump wave and EPW have been obtained under R.F.E. approximation technique. It has been observed that growth of the EPW is significantly affected by the self-focusing effect of pump beam.

Keywords: self-focusing, electron plasma waves, nonlinearities, parametric decay

ВЛИЯНИЕ РАМКИ ПЛОТНОСТИ НА ВОЗБУЖДЕНИЕ ЭЛЕКТРОННОЙ ПЛАЗМЕННОЙ ВОЛНЫ КОГЕРЕНТНЫМИ ЛАЗЕРНЫМИ ПУЧКАМИ В КОЛЛИЗИОННОЙ ПЛАЗМЕ

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Исследовано возбуждение электронно-плазменных волн когерентными лазерными пучками (ЭПВ) в плазме с осевой рамкой плотности. Эффект самосфокусировки лазерного пучка на рост возбужденной ЭПВ учтен. В процессе распространения в плазме лазерный пучок возбуждает ЭПВ с частотой ω_p , которая из-за спектральной нелинейности плазмы нелинейно взаимодействует с лазерным пучком. Используя вариационную теорию, получены аналитические решения связанных нелинейных уравнений для волны накачки и ЭПВ в приближении Р.Ф.Е. Наблюдено, что рост ЭПВ существенно зависит от эффекта самосфокусировки лазерного пучка.

Ключевые слова: самосфокусировка, электронно-плазменные волны, нелинейности, параметрическое распад

Introduction. Investigations on coupling of intense laser beams with plasmas is at the vanguard of research since past few decades due to its importance in many potential applications including laser fusion [1-11], plasma wake field accelerators [12, 13], X-ray lasers [14, 15], terahertz generation [16] etc. The ultimate limits of these applications depend on the efficiency of laser-plasma coupling, which is further decided by

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RESEARCH ARTICLE

Self-focusing, self-trapping and self-phase modulation of elliptical q -Gaussian laser beams in collisionless plasma

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Abstract Theoretical investigations on optical self-action effects of intense q -Gaussian laser beams interaction with collisionless plasma has been investigated in detail. Emphasis is put on investigating the dynamics of beam width and axial phase of the laser beam. Effect of the elongation of the cross-section of the laser beam also has been incorporated using variational theory based on Lagrangian formulation, nonlinear partial differential equation (PDE) governing the evolution of beam amplitude has been reduced to a set of coupled ordinary differential equations for the beam width of the laser beam along the transverse direction. The evolution equation for the axial phase of the laser beam has been derived by the Fourier transform of the amplitude structure of the laser beam from coordinate space to (k_x, k_y) space. The differential equations so obtained have been solved numerically to estimate the effect of laser pulse parameters on the propagation dynamics of the laser beam.

Introduction

Since [1] is the one of the most important scientific revolution of the twentieth century. When laser made its debut, it was referred to be relative to study of a problem. Today laser has become ubiquitous or ubiquitous technology, from CD players to sophisticated chemical systems. Higher and applications of lasers are also shown. This includes medical

diagnosis and treatment [2], optical fiber [3], particle acceleration [4], disassembly of explosives [5], etc. The diversity in the applications of lasers can be felt from the fact that currently this technology is being used for heating as well as for ultra-cold cooling. The laser systems can produce extremely low state of matter [6] (ultra-cold as well as extremely cold state of matter [7]) (Bose-Einstein Condensate). The output of laser is varying too changed over time, and is self-changing. Already lasers have provided the perfect solution to an impressive variety of real-world situations, and it is expected that biotechnology will have an amazing quality of life and will contribute greatly to the world economy.

In case of its applications, the laser intensity is the key parameter that decides their ultimate result. Currently, due to the light's inherent wave property to diffract, the laser power has gotten too wasteful at the corner of low performance. Ideally, it was believed that diffraction of the laser beam cannot be avoided during its propagation neither through vacuum nor through material media. However, in 1968 Chu et al. [8] showed that in media whose index of refraction depends on the intensity of light, the spreading of an optical beam is possible and be observed. Hence, the expansion of optical beam due to diffraction is in fact counterable and controllable.

Self-focusing and self-trapping are two examples of nonlinear optical effects which may arise from any of many physical mechanisms. Self-focusing describes the formation of a light-induced channel in an inhomogeneous medium which confines the optical beam. This channel occurs in a few self-trapping occurs when self-focusing substantially exactly counteracts beam spreading due to diffraction. When this happens, the cross-section of the light-induced channel remains substantially constant with propagation distance over the distance of the self-trapping.

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Optical properties and effect of magnetic field on energy spectra of a GaAs spherical quantum dot

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Abstract In the present work, optical absorption coefficient and refractive index changes of a GaAs spherical quantum dot are investigated within the framework of the Fröhlich dielectric theory. In this effect, analytical expressions for energy eigen values and corresponding eigen functions are obtained by solving the radial Schrödinger equation by utilizing the potential of Yukawa–Hulthén method. Thereafter, using the density matrix formalism, expressions for linear and third-order nonlinear absorption coefficients along with refractive index changes are computed and plotted. Effect of the radius of quantum dot, the potential height and the incident light intensity on these quantities are further investigated and found to good agreement with literature results. The effect of external magnetic field on the energy spectra of the quantum dot is also presented.

1 Introduction

The study of low-dimensional structures have attracted considerable attention in the past few decades, in order to their potential applications in different fields. Among the low-dimensional systems, the quantum dot (QD) is particularly being extensively being studied in the past [1–6]. A QD is regarded as a system zero-dimensional (0D) structure, because electron confined itself in quantum confinement of carriers which further defines formation of discrete energy levels. With great technological advancement in the field of semiconductor processing, it is now possible to fabricate high-potential (H) junctions (QDs) of different shapes such as cylindrical [7, 8], spherical [9–16], ellipsoidal [11, 12], disc-shaped [13, 14], cubic [15], ellipsoid [16], hemispherical [17], etc. Such quantum confinement structures can be used for various applications in physics, chemistry and biology.

To explore the wide-ranging and consequently wide range of technological applications of QDs, various potential results have been used in the past, particularly, the Coulomb diamond pattern [18, 19], Mollow lines pattern [20], Mollow lines pattern [21], strongly quantum Hall-dotted potential [22], Rydberg pattern [23], Mollow-Yukawa potential [24], generalized Fermi integral [25], Fermi potential [26], parabolic-like potential [27], generalized Fermi potential [28], inverted quantum Yukawa–Hulthén potential [29], strongly quantum Hall-dotted Fermi potential [30] to name a few. In the literature, various potential of QDs. Most of the potential results indicate that, in comparison to the bulk materials, the quantum confinement effects in low-dimensional semiconductor systems greatly improve the nonlinear optical effect.

Effect of various parameters like temperature, magnetic and laser field, spin-orbit coupling, impurity charge, dot radius and refractive index of QDs have previously been studied by many researchers [27–30], along with the linear optical properties of QDs, their nonlinear properties have widely been studied. It is well known that nonlinear optical effects, such as the absorption coefficient (AC) and the refractive index changes (RIC), are conventionally be used to characterize many nonlinear potential applications [31]. Therefore, the study of the nonlinear optical properties of QDs continues to be a challenging task in materials.

A theoretical description of linear optical absorption and nonlinear absorption is based on solving the corresponding Schrödinger equation (SE) for a specific geometry and composition of QDs. Keeping in view the importance of optical and electronic properties of QDs, the basic purpose of the current research work is to theoretically investigate the changes in susceptibility (χ_1 and χ_3) in Yukawa–Hulthén (YH) within the framework of Coulomb plus Yukawa potential (CPY) potential. To the best of our knowledge, the linear and nonlinear optical properties of a spherical QDs using the CPY potential [32–34] has not been reported so far.

The present work is organized as, in Sect. 2, we have solved the SE with the CPY potential in 3D to discuss the energy eigenvalues and eigen functions. Analysis is expressed by the linear and nonlinear optical (AC and RIC) along with the effect of

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RESEARCH ARTICLE

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Ro-vibrational energy spectra and thermal properties of some diatomic molecules

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ABSTRACT

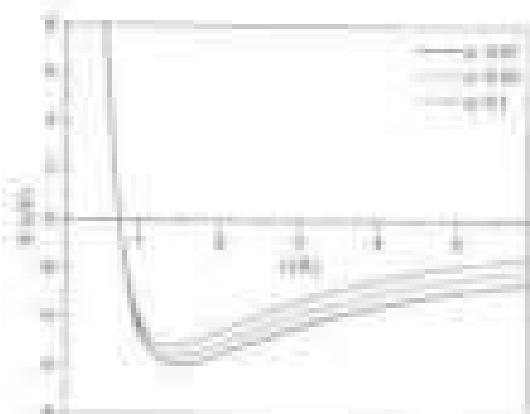
The present work deals with the solution to the radial Schrödinger equation for harmonic plus anharmonic Morse potential (HMP) within the framework of the Hellmann-Heisenberg functional approach method. The Langer-Witch approximation is used to handle the anharmonic energy levels of the HMP. Following the trial wavefunction and semi-empirical potential, the energy spectra of selected diatomic molecules, i.e. (LiH, NaCl), $^{23}\text{Na}^{35}\text{Cl}$ and $^{39}\text{K}^{87}\text{Rb}$ are computed. Further, the equations for dependence of various parameters, including energy of position $\langle r^{-1} \rangle$, square of inverse of position $\langle r^{-2} \rangle$, electric energy $\langle T \rangle$ and the square of momentum $\langle p^2 \rangle$ are obtained involving the Hellmann-Heisenberg theorem. Results of this study are compared with other earlier published studies. The analytical expressions for partition function and other thermodynamic properties of the diatomic molecules are determined.

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1. Introduction

Over the decades, the approaches to exact solution to the Schrödinger equation (SE) for various scattering potentials attracted the attention of researchers due to their vital practical and theoretical implications. In reality, not all physical potentials but a few can yield exact solutions to the SE. Numerous attempts have been made in the past to determine exact or approximate bound state solutions to the SE using various potential models. The spectroscopic properties of diatomic molecules can be better understood using

potential models. Experimentally observed energy spectra of diatomic molecules can be interpreted successfully by fitting a suitable scattering potential model. In general, a diatomic interaction potential can be defined in order of dissociation energy (D_0), equilibrium bond length (r_0), interatomic separation (r_1) and scattering parameter (α). The next logical step is to find the solutions to the non-relativistic SE with an energy potential by using an appropriate method out of available ones. In the past, numerous techniques were used to solve the SE with various potential models, including

STIMULATED RAMAN SCATTERING OF COSH-GAUSSIAN LASER BEAMS IN PLASMA WITH AXIAL DENSITY RAMP: EFFECT OF SELF-FOCUSING

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Abstract

We present analytical study of stimulated Raman scattering (SRS) of cosh-Gaussian (CG) laser beams interacting with axially nonuniform plasma. The axial intensity profile of the plasma is controlled by a conical density profile and the radial nonuniformity of the plasma is controlled by the rise in the quadrupole laser field on the plasma surface. As cosh laser beam with frequency ω_0 propagates through plasma jet coupled with a propagating electron plasma wave (EPW) with frequency ω_1 and produces a backscattered wave at frequency $\omega_2 = \omega_0 - \omega_1$. Using the nonlinear theory, we obtain a semi-analytical solution of the set of coupled wave equations for the pump beam, EPW, and scattered wave under the WKB approximation. We show that the SRS efficiency of plasma is significantly affected by self-focusing of the laser beam.

Keywords: self-focusing, stimulated Raman scattering, cosh-Gaussian beam, quadrupole laser beam

1. Introduction

Investigation on coupling of laser laser beam with plasma laser beam at the temporal of century is for the past few decades due to their application in many potential applications including laser fusion [1–4], plasma wakefield acceleration [5, 6], Free laser [6, 7]. The generation [8, 9]. The ultimate benefit of these applications depends on the efficiency of laser-plasma coupling, which is governed by many different nonlinear processes [9–11]. These processes range from collisional absorption to excitation of several laser-driven instabilities [12–15]. These instabilities can be represented as resonant coupling of the incident laser beam with two daughter waves. In the absence of an external magnetic field, these daughter waves can be either ion plasma wave (IPL) or acoustic wave, as well as scattered electromagnetic wave. In addition to the above-mentioned instabilities, there is one more possibility when the amplitude of the laser over the propagation of the laser beam produces directly excitation of plasma wave, as this leads to self-focusing or filamentation of the laser beam.

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Effect of Self Focusing on Stimulated Raman Scattering of Elliptical q -Gaussian Laser Beam in Underdense Plasma with Axial Density Ramp

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Stimulated Raman scattering (SRS) of elliptical q -Gaussian laser beam interacting with axially inhomogeneous plasma has been investigated theoretically. An intense laser beam with frequency ω_0 propagating through plasma gets coupled with a pre-existing electron plasma wave (EPW) at frequency ω_{pe} . Due to ponderomotive condensation on plasma electrons excited by the laser beam, the nonlinear interaction of pump beam with EPW produces a back-scattered wave at frequency $\omega_s = \omega_0 - \omega_{pe}$. Using variational theory with analytical solutions of the coupled nonlinear wave equations for the three waves (pump, EPW and scattered) have been obtained under WKB approximation technique. It has been observed that self focusing of the laser beam significantly affects the power of back scattered wave.

1. INTRODUCTION

Laser [1] is one of the most successful pieces of apparatus gifted by 20th century science. When laser made its debut in 1960 people considered it to be solution which is searching for its problem. Since its invention the impact of laser on our lives has changed with time and still is changing. Now laser is ubiquitous in every aspect of life: from super market barcode scanners, security checkpoints, CD writers to high end applications like medical diagnosis

Mass Spectra of Charmonium and Bottomonium Using the Coulomb Perturbed Potential

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Introduction

In heavy quarkonium, the properties of heavy and light quarks are of great interest. With the help of a hybrid-type equation (HE) we can predict various properties of quarks by the semi-relativistic potential models using different methodologies. It is generally believed that the quarkonia, which are composed of bound states of a quark and an antiquark are essentially non-relativistic. Therefore, in order to calculate various properties of quarks, a potential model based approach has been more successful [1]. Also a theoretical study should be able to predict various different properties in addition to mass spectra. To do so, we can use the Coulomb perturbed potential (CPP) [2] to predict the mass spectrum of various quarkonia. There are only a few available experimental and theoretical studies. Here, the semi-relativistic potential used is

$$V(r) = \alpha^2 + \beta r - \frac{\gamma}{r} \quad (1)$$

where α , β and γ are constant potential parameters and will be fixed later on.

Formalism

In the present work, the Nikiforov-Fuchs-Sokoloff method (NFS) method [3] is used to calculate the energy eigenvalues and corresponding eigenfunctions for CPP. The Schrödinger equation is written as [4]

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equation of radial HE for CPP is written as

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E - \alpha^2 - \beta r - \frac{\gamma}{r} - \frac{\hbar^2 \kappa^2}{2\mu r^2} \right] R(r) = 0 \quad (2)$$

where, $\kappa = (E_0 + E - 2\mu^2)$. By using the Greene-Mitchell approximation scheme and the NFS methodology [3], the final energy eigenvalue equation is given as

$$E = -\frac{\beta^2 \hbar^2}{2\mu} \left[\frac{2\mu + \alpha^2 + \beta + \gamma}{2\mu + \alpha} \right]^2 + \frac{\beta^2 \gamma \hbar^2}{2\mu} \quad (3)$$

where

$$\alpha = \frac{2\mu\beta}{\beta^2 + \kappa^2} + \frac{\beta\gamma}{\beta\kappa^2} \quad (4)$$

$$\beta = \frac{2\mu\gamma}{\beta^2 + \kappa^2} - \frac{2\beta\gamma}{\beta\kappa^2} - \frac{\beta\gamma}{\beta\kappa^2} + (E_0 + E - 2\mu^2) \quad (5)$$

and

$$\kappa = \frac{1}{2} \left[\beta \sqrt{4\mu + 4\beta\gamma + \beta^2} + \beta\gamma \right] \quad (6)$$

and the corresponding radial function is given as

$$R(r) = N \left(\frac{r}{\beta} \right)^{\alpha_1 - 1} \left(1 - \frac{r}{\beta} \right)^{\alpha_2 - 1} e^{-\frac{r}{\beta}} \mathcal{P}_n^{\alpha_1, \alpha_2} \left(\frac{r}{\beta} \right) \quad (7)$$

where N is normalization constant and $\mathcal{P}_n^{\alpha_1, \alpha_2} \left(\frac{r}{\beta} \right) = 1$ is hypergeometric function. Here, the parameters α_1 , α_2 and β are defined as

$$\begin{aligned} \alpha_1 &= \left(4 + \mu + \sqrt{\mu} \right) \\ \alpha_2 &= \left(4 + \mu - \sqrt{\mu} \right) \\ \beta &= 4 + 2\mu \\ \beta &= \beta_1 - \beta_2 + \beta_3 \end{aligned} \quad (8)$$

Spectrum Analysis of Mesons using Nikiforov-Uvarov Functional Analysis Method

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Keywords: Schrödinger Equation, CPP Potential, NUFA Method, Mesons, Mass Spectra

Abstract. The analytical expressions for the energy eigenvalues and eigenfunctions are computed for Coulomb perturbed potential by solving the Schrödinger equation within the framework of the Nikiforov-Uvarov functional analysis method and applying the Lippman-Schwinger approximation. Using the energy eigenvalues expression, we have determined the mass spectra of π and ρ mesons. The results of present study are in good agreement with experimental, theoretical and other relevant works available in the literature.

Introduction

As we know that most of the quantum mechanical systems can be studied by determining the bound state solutions to Schrödinger equation (SE) within a suitable potential model. Thereby, within the framework of an appropriate potential model and a proper mathematical approach, one can understand the behavior of quantum mechanical systems. Such theoretical models also help us to investigate the complicated systems, the mass spectra and radiative transitions width of various mesons. In non-relativistic quantum mechanics, experimentally observed vital physical properties can be reproduced with a suitable interaction potential model which, at present, is a function of relative separation between quark and antiquark pairs. In literature, there exist several important models related to computation of mass spectra of mesons; a brief of them is as follows:

Jiang et. al. [1] studied a temperature dependent Yukawa potential by replacing the screening parameter with the Debye mass and obtained mass spectra of heavy mesons by solving the SE with series expansion method. Mostani et. al. [2] solved the SE with the Cornell potential and calculated the mass spectra of some mesons. Using power series and asymptotic iteration method, Bannock et. al. [3, 4] calculated the mass spectra of charmonium and bottomonium by solving the 3-dimensional SE. By considering a generalized interaction potential, Raha et. al. [5] solved the SE via asymptotic iteration method and calculated the mass spectra of some heavy and light mesons. Some other important studies related to mass spectra of mesons are available in refs. [6-9].

So, to obtain better results for meson systems, here, we use the Coulomb perturbed potential (CPP) as an interaction potential i.e.

$$V(r) = -\frac{\alpha}{r} + br - \frac{c}{r^2} \quad (1)$$

where α , b and c are potential parameters and should be chosen appropriately such that the obtained results be comparable with available experimental and other theoretical resources.

Travelling and Solitary Wave Solutions of (2+1)-Dimensional Nonlinear Evolution Equations by Using Khater Method



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Abstract The most of the physical systems are nonlinear by nature which can be represented by various nonlinear partial differential equations. Here, we present a simple technique say Khater method to find the Travelling and Solitary Wave solutions of (2+1)-dimensional nonlinear evolution equations. This method is a very powerful tool for obtaining the exact solutions of various nonlinear differential equations. In this study, modified Korteweg–de Vries–Zakharov–Kuznetsov (mKdV–ZK) equation is taken as an example of nonlinear evolution equation which is used in astrophysics to study various space phenomena, dynamics of plasma etc.

Keywords mKdV–ZK equation · Khater method · Travelling wave solutions · Solitary wave solutions

1 Introduction

The concept of solitary wave was introduced by Zabusky and Kruskal in 1965 in their well known experiment on KdV equation. It gain interest of researchers working in areas of nonlinear dynamics. Various phenomena such as prolongation structures, space curves, gauge equivalence, Lie-algebraic properties, singularity structures are related to the concept of solitons and can be described by different nonlinear evolution equations/NLEEs [1–3]. The investigation of travelling and solitary wave solutions of these equations is a major component of the

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