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2011 Phys. Scr. 83 065008

Abstract
Based on the mechanism of vibrational resonance, we improve the weak low-frequency signal propagation in globally coupled bistable systems by time delay feedback. In the system chains, the weak low-frequency signal is added only to the first oscillator and the identical high-frequency signals are added to all of the oscillators. Both numerical and analytical results show that the response amplitude of the last oscillator to the low-frequency signal varies periodically with the delay parameter by two different periods, which equal the periods of the two exciting signals, respectively. In addition, the vibrational resonance can also be induced to improve signal propagation by adjusting the coupling strength. Comparing with the delay-free systems, with the cooperation of the high-frequency signal and time delay feedback, the weak low-frequency signal can be transmitted much more efficiently in the delayed systems.

Electromagnetic potentials without gauge transformations

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2011 Phys. Scr. 84 015009

Abstract
In this paper, we show that the use of the Helmholtz theorem enables the derivation of uniquely determined electromagnetic potentials without the necessity of using gauge transformation. We show that the electromagnetic field comprises two components, one of which is characterized by instantaneous action at a distance, whereas the other propagates in retarded form with the velocity of light. In our attempt to show the superiority of the new proposed method to the standard one, we argue that the action-at-a-distance components cannot be considered as a drawback of our method, because the recommended procedure for eliminating the action at a distance in the Coulomb gauge leads to theoretical subtleties that allow us to say that the needed gauge transformation is not guaranteed. One of the theoretical consequences of this new definition is that, in addition to the electric E and magnetic B fields, the electromagnetic potentials are real physical quantities. We show that this property of the electromagnetic potentials in quantum mechanics is also a property of the electromagnetic potentials in classical electrodynamics.

Coulomb screening of 2D massive Dirac fermions

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2011 Phys. Scr. 83 035002

Abstract
A model of 2D massive Dirac fermions, interacting with instantaneous 1/r Coulomb interaction, is presented in order to mimic the physics of gapped graphene. The static polarization function is calculated explicitly to analyze the screening effect at finite temperature and density. The results are compared with the massless case. We also show that various results in other works can be reproduced with our model in a straightforward and unified manner.

Amplification of weak signals via the non-adiabatic regime of stochastic resonance in a bistable dynamical system with time delay

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2011 Phys. Scr. 84 015003

Abstract
The non-adiabatic regime of stochastic resonance (SR) in a bistable system with time delay, an additive white noise and a periodic signal was investigated. The signal power amplification $\eta$ was employed to characterize the SR of the system. The simulation results indicate that (i) in the case of intermediate frequency $\Omega$ of the periodic signal, the typical behavior of SR is lowered monotonically by increasing the delay time $\tau$; in the case of large $\Omega$, $\tau$ weakens the SR behavior and then enhances it, with a non-monotonic behavior as a function of time delay; (ii) time delay induces SR when $A$ is above the threshold, whereas no such resonance exists in the absence of time delay; (iii) time delay induces a transition from bimodal to unimodal configuration of $\eta$; (iv) varying the particular form of time delay results in different phenomena.
Resolution of the Klein paradox

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2011 Phys. Scr. 83 025001

Abstract

We present a resolution of the Klein paradox within the framework of one-particle relativistic quantum mechanics. Not only reflection becomes total but the vacuum remains neutral as well. This is accomplished by replacing the physical pair production process with virtual negative energy ‘incidence’ within the barrier in a similar manner to what is done with virtual sources in optics and image charges in electrostatics.

On eigenvalue problems in quantum mechanics

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2011 Phys. Scr. 83 065003

Abstract

To solve quantum mechanical eigenvalue problems using the algorithmic methods recently derived by Nikiforov and Uvarov (1988 Special Functions of Mathematical Physics (Basel: Birkhäuser)) and Ciftci et al (2003 J. Phys. A: Math. Gen. 36 11807), one needs to first convert the associated wave equation into hypergeometric or closely related forms. We point out that once such forms are obtained, the eigenvalue problem can be satisfactorily solved by only imposing the condition that the regular infinite series solutions of the equations should become polynomials, and one need not take recourse to the use of the algorithmic methods. We first demonstrate the directness and simplicity of our approach by dealing with a few case studies and then present new results for the Woods–Saxon potential.

Accurate analytic approximation to the nonlinear pendulum problem

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2011 Phys. Scr. 84 015005

Abstract

This paper is concerned with the accurate analytic solution of the nonlinear pendulum differential equation. Instead of the traditional Taylor series or asymptotic methods, the homotopy analysis technique is used, which does not require a small perturbation parameter or a large asymptotic parameter. It is shown here that such a method is extremely powerful in gaining the pendulum solution in terms of purely trigonometric cosine functions. The obtained explicit analytical expressions for the frequency, period and displacement generate results that compare excellently with the numerically computed ones for moderate as well as sufficiently high values of the initial amplitudes. For larger initial amplitudes close to 180° Padé approximants of the found series solutions lead to fairly accurate results whose relative errors as compared with the exact values are less than 1%.
 Characteristics of multiplicity distribution of target fragments in forward and backward hemispheres in high-energy nucleus–nucleus interactions

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2011 Phys. Scr. 84 015201

Abstract

A detailed study on the mechanism of the evaporation of target fragments in the forward and backward hemispheres in 12C–AgBr interactions at 4.5A GeV, 28Si–AgBr interactions at 14.5A GeV, 16O–AgBr interactions at 60A GeV and 32S–AgBr interactions at 200A GeV is carried out in terms of the multiplicity distribution. The nature of the multiplicity distribution in the forward and backward hemispheres is found to be different across all the interactions. The asymmetry parameters and the forward–backward ratios were also calculated for the above-mentioned interactions. The asymmetry parameters and the forward–backward ratios from other nucleus–nucleus interaction data were compared with our results. The forward–backward ratios of target fragments are found to be nearly the same for all the nucleus–nucleus interactions. The forward–backward ratios of all the interactions are greater than 1, suggesting that the probability of emission of fragments in the forward hemisphere is higher than that in the backward direction. The multiplicity moment, entropy and reduced entropy, i.e. the ratio of entropy to average multiplicity of target fragments, are evaluated in both the forward and backward hemispheres for all the four above-mentioned interactions. The values of multiplicity moments are found to be energy independent up to 60A GeV energy in the backward hemisphere. The reduced entropy is also found to be almost energy independent to within experimental error in the backward hemisphere. No such observation can be made in the forward hemisphere. The total entropy of the target fragments is found to be higher in the forward hemisphere. A study of correlation in terms of the scaled variance was also carried out in both the hemispheres for all the nucleus–nucleus interactions. No systematic variation of correlation either with energy or with the size of the projectile nucleus has been noticed. The study yields quite interesting information on the mechanism of particle evaporation in the backward hemisphere.

The mechanical, electronic structure and thermodynamic properties of B2-based AgRE studied from first-principles

Xiaoma Tao1, Hongmei Chen1, Xingxiu Li1, Yifang Ouyang1,2 and Shuzhi Liao2

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2011 Phys. Scr. 83 045301

Abstract

The lattice constants, formation enthalpies, bulk modulus, elastic constants and electronic structures of B2-based AgRE (RE=Sc, Y and La–Lu) have been calculated by means of first-principles based on the density functional theory. The shear modulus, Young’s modulus and Poisson’s ratio have been estimated from the calculated elastic constants. The electronic structures were calculated to give insight into the bonding mechanism in AgRE compounds. In addition, the Debye temperature, heat capacity, thermal expansion and Grüneisen parameter of AgRE compounds were obtained by applying the Debye model. The calculated lattice constants, formation enthalpies and elastic constants are all in good agreement with the available experimental data and other theoretical results. The formation enthalpy of B2-AgRE varies linearly with the density of states at the Fermi level.
Optimization of the bubble radius in a moving single bubble sonoluminescence
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2011 Phys. Scr. 83 055403
Abstract
A complete study of the hydrodynamic force on a moving single bubble sonoluminescence in N-methylformamide is presented in this work. All forces exerted, trajectory, interior temperature and gas pressure are discussed. The maximum values of the calculated components of the hydrodynamic force for three different radii at the same driving pressure were compared, while the optimum bubble radius was determined. The maximum value of the buoyancy force appears at the start of bubble collapse, earlier than the other forces whose maximum values appear at the moment of bubble collapse. We verified that for radii larger than the optimum radius, the temperature peak value decreases.

Mixed convection boundary-layer flow about an isothermal solid sphere in a nanofluid
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2011 Phys. Scr. 84 025403
Abstract
The steady mixed convection boundary-layer flow of a nanofluid about a solid sphere with constant surface temperature has been studied for cases of both assisting and opposing flows. The resulting system of nonlinear partial differential equations is solved numerically using an implicit finite-difference scheme known as the Keller-box method. The solutions for the flow and heat-transfer characteristics are evaluated numerically for various values of the parameters, namely the nanoparticle volume fraction \( \phi \) and the mixed convection parameter \( \lambda \), at Prandtl numbers \( Pr = 0.7 \) and 6.2. The three different types of nanoparticles considered are \( \text{Al}_2\text{O}_3 \), \( \text{Cu} \) and \( \text{TiO}_2 \), using water-based fluid with \( Pr = 6.2 \). It is found that for each particular nanoparticle, as the nanoparticle volume fraction \( \phi \) increases, the skin friction coefficient and the heat-transfer rate at the surface also increase. This leads to an increase in the value of the mixed convection parameter \( \lambda \), which at first gives no separation.

U-shaped multi-band negative-index bulk metamaterials with low loss at visible frequencies
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2011 Phys. Scr. 84 035402
Abstract
We study bulk negative-index metamaterials made up of U-shaped cells at visible frequencies that can realize multi-band negative refractive index with very low loss based on high-order resonance. The mechanism of multi-band negative refractive index can be interpreted by analyzing the transmission modes, current distribution, effective LC circuit models and kinetic energy of electrons. In the low-frequency region, the multi-band resonances are mainly due to the cell itself; in the high-frequency region, they are mainly due to the interaction between adjacent cells. Compared with cut-wire pairs, U-shaped cells can realize resonances more easily at high frequencies and produce more negative-index transmission bands.

Propagation of shock waves in a viscous medium
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2011 Phys. Scr. 83 065402
Abstract
A theoretical model for entropy production in a viscous medium due to the propagation of shock waves has been developed. An exact general solution is achieved for plane, cylindrical and spherical symmetries of shock waves in viscous flow, which on numerical substitutions gives variations in the entropy production, temperature ratio and particle velocity in the shock transition region with the coefficient of viscosity, specific heat ratio, shock strength, initial density and initial pressure.

Optimization of the bubble radius in a moving single bubble sonoluminescence
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2011 Phys. Scr. 83 055403
Abstract
A complete study of the hydrodynamic force on a moving single bubble sonoluminescence in N-methylformamide is presented in this work. All forces exerted, trajectory, interior temperature and gas pressure are discussed. The maximum values of the calculated components of the hydrodynamic force for three different radii at the same driving pressure were compared, while the optimum bubble radius was determined. The maximum value of the buoyancy force appears at the start of bubble collapse, earlier than the other forces whose maximum values appear at the moment of bubble collapse. We verified that for radii larger than the optimum radius, the temperature peak value decreases.
Generation of continuous-variable entanglement in a three-level system coupled with a parametric oscillator

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2011 Phys. Scr. 83 025403

Abstract
We consider a nondegenerate three-level cascade laser driven by a classical field with a parametric oscillator. The dynamic evolution of the master equation is investigated and the steady-state entanglement between two modes is investigated. We show that introducing the parametric oscillator can enhance the entanglement between the two-mode cavity. In particular, with the help of the classical field, a high intensity of entangled light between the two modes can be achieved.

Power-flow formulation of a ray approach to the modelling of inhomogeneous waves

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2011 Phys. Scr. 84 025401

Abstract
In this paper, we elaborate on quite a simple analytical framework for the physically intelligible principle of a ray description of inhomogeneous wavefields on the basis of the generic properties of active and reactive wave power flows. While being very close to traditional geometric optics (GO) in the limit of lossless media, in substantially non-Hermitian systems this approach turns out to be a distinct method capable of keeping up ray trajectories in a real-valued domain. We also demonstrate that the ray method based on power-flow analysis is mostly free from the standard limitations of GO. In this regard, the proper use of the ray-tracing technique can be justified for modelling a wide range of non-regular wave phenomena if wave power transport is under consideration. The paraxial equations are shown to comply with the power-flow formulation, thus finding an extended range of applicability.

Nonplanar ion-acoustic solitary waves in electron–positron–ion plasmas with electrons following a $q$-nonextensive distribution

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2011 Phys. Scr. 83 065502

Abstract
Cylindrical and spherical Korteweg–de Vries equations were derived for ion-acoustic solitary waves in an unmagnetized three species plasma system comprised of cold ions, nonextensive electrons and thermal positrons by using standard reduction perturbation methods. The effects of nonplanar geometry and $q$-nonextensive electrons on the profiles of the amplitudes and widths of solitary structures were examined numerically.

The 3+1 dimensional Kadomtsev–Petviashvili Burgers’ equation in non-uniform dusty plasmas

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2011 Phys. Scr. 83 045501

Abstract
Using the perturbation method, the 3+1 dimensional modified variable coefficient Kadomtsev–Petviashvili (MKP) Burgers’ equation governing nonlinear dust acoustic shock waves is derived with the combined effects of non-adiabatic dust charge fluctuation, higher-order transverse perturbation and the non-thermally distributed ions in inhomogeneous dusty plasmas due to spatial gradients of dust charge and plasma densities for the first time. The MKP Burgers’ equation is reduced to the standard variable coefficient Kadomtsev–Petviashvili (KP) Burgers’ equation. A particular solution of this KP Burgers’ equation is also obtained. It is shown that the dust acoustic shock waves can exist in the KP Burgers’ equation.
Experimental and theoretical studies of the direct-current breakdown voltage in argon at micrometer separations

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2011 Phys. Scr. 83 045503

Abstract
In this paper, the dc breakdown in argon has been measured in the discharge system consisting of two parallel planar Cu electrodes at separations from 20 to 500 μm varying the pressure from 4.5 to 690 torr. The measured breakdown voltage curves were systematically analyzed and a corresponding scaling law was suggested. The estimation of the secondary emission coefficient γ as a function of the reduced electric field was based on experimental data and simple theoretical studies. Additionally, particle-in-cell/Monte Carlo collision simulations were performed to understand in more detail the processes involved in the dc discharge breakdown. Good agreement was found between experimental and simulation results.

Electron acoustic solitary waves with kappa-distributed electrons

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2011 Phys. Scr. 84 025507

Abstract
Electron acoustic solitary waves are studied in a three-component, unmagnetized plasma composed of hot electrons, fluid cold electrons and ions having finite temperatures. Hot electrons are assumed to have kappa distribution. The Sagdeev pseudo-potential technique is used to study the arbitrary amplitude electron-acoustic solitary waves. It is found that inclusion of cold electron temperature shrinks the existence regime of the solitons, and soliton electric field amplitude decreases with an increase in cold electron temperature. A decrease in spectral index, κ, i.e. an increase in the superthermal component of hot electrons, leads to a decrease in soliton electric field amplitude as well as the soliton velocity range. The soliton solutions do not exist beyond $T_c/T_h>0.13$ for $\kappa=3.0$ and Mach number $M=0.9$ for the dayside auroral region parameters.

Dust acoustic instability with Lorentzian kappa distribution

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2011 Phys. Scr. 84 035504

Abstract
The instability of dust acoustic waves (DAWs) driven by ions and electrons with different drift velocities in an unmagnetized, collisionless, isotropic dusty plasma was investigated based on kinetic theory. The electrons, ions and dust particles are all modeled by using the generalized Lorentzian kappa distributions. It is found that the instability growth rate depends not only on the mass, temperature, density ratios of the components and ion–electron drift velocity ratio, but also on the spectral index for each component. The effects of the indices on the instability growth rate of DAWs have been discussed in detail.

Instabilities in strongly coupled ultracold neutral plasmas

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2011 Phys. Scr. 83 015503

Abstract
In ultracold neutral plasmas the ions are strongly coupled in the liquid phase, while the electrons are weakly coupled. The effect of strong ion correlations on the dispersion relation of possible ion-beam plasma instabilities is considered.

Influence of gas pressure on the structure and dynamics of dust rotation in magnetized dusty plasmas

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2011 Phys. Scr. 83 025502

Abstract
The structure and dynamics of dust rotation under a magnetic field at different gas pressures in the sheath of a radio-frequency discharge are
investigated in this paper. The influence of gas pressure on the rotational properties of the dust particles located in different layers is studied in detail. Both rigid rotation (all the dust particles move with a constant angular velocity) and sheared rotation (the angular velocity of the dust particles has a radial distribution) of the dust particles induced by a magnetic field are observed. With increasing gas pressure, the angular velocity of the rotating dust particles in all layers decreases. Under specific experimental conditions, the angular velocity of the dust particles in the lower layer is lower than that of the dust particles in the upper layers. With increasing gas pressure, dust particles in the lower layer stop rotating earlier than those in the upper layers. At a critical (high) gas pressure, dust particles in the lower layers also reverse their rotation direction earlier than those in the upper layers. Within the same dust layer, particles located in the inner region stop rotating and reverse their rotation direction earlier than those in the outer region. At a sufficiently high angular velocity, a void (dust-free region) is formed in the dust cloud, leaving the dust particles rotating in a layer at the system edge. When the gas pressure becomes too high, the voids can be destroyed, and the dust particles are redistributed in the dust cloud. Finally, a 3D spindle-shaped configuration of the dust cloud in the plasma sheath destroyed, and the dust particles are redistributed in the dust cloud. Finally, a 3D spindle-shaped configuration of the dust cloud in the plasma sheath.

Condensed matter: structural, mechanical and thermal properties

Electrical properties of the double perovskite oxide Ho$_2$CuZrO$_6$

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2011 Phys. Scr. 84 015602

Abstract

The double perovskite oxide holmium copper zirconate, Ho$_2$CuZrO$_6$ (HCZ), was synthesized by a solid-state reaction technique. The crystal structure of HCZ shows a monoclinic phase. The dielectric relaxation of HCZ was investigated in the frequency range 44 Hz–1 MHz and in the temperature range 40–360 °C by using impedance spectroscopy. The complex impedance data were analysed by the Cole–Cole model. The ac conductivity follows the power law. The value of activation energy obtained from the temperature dependence of the dc conductivity plot indicates a hopping-type conduction mechanism. The scaling behaviour of the imaginary part of impedance indicates that relaxation in HCZ describes the similarity in frequency of charge boundaries. The dielectric loss tangent curves at room temperature exhibit dielectric relaxation peaks attributed to the similarity in frequency of charge hopping between the localized charge states and external fields. The relaxation peak shifts to higher frequencies for ferrites with nanosized grains.

Structural and dielectric properties of Cr-doped Ni–Zn nanoferrites

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2011 Phys. Scr. 83 025602

Abstract

Cr-doped Ni–Zn ferrite nanoparticles having the general formula Ni$_{1-x}$Zn$_x$Cr$_2$Fe$_{2-x}$O$_4$ ($x$=0.1, 0.3, 0.5) were prepared by the simplified sol–gel method. The structural and dielectric properties of the samples sintered at 750±5 °C were studied. X-ray diffraction (XRD) patterns confirm the single-phase spinel structure of the prepared samples. The crystallite size calculated from the most intense peak (3 1 1) using the Debye–Scherrer formula was 29–34 nm. Scanning electron microscope images showed that the particle size of the samples lies in the nanometer regime. The dielectric constant ($\varepsilon_r$), dielectric loss tangent (tan $\delta$) and ac electrical conductivity ($\sigma$) of nanocrystalline Cr–Ni–Zn ferrites were investigated as a function of frequency and Cr concentration. The dependence of $\varepsilon_r$, tan $\delta$ and $\sigma$ on the frequency of alternating applied electric field is in accordance with the Maxwell–Wagner model. The effect of Cr doping on the dielectric and electric properties was explained on the basis of cations distribution in the crystal structure.
Structural, electrical and magnetic studies of nickel–zinc nanoferrites prepared by simplified sol–gel and co-precipitation methods
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2011 Phys. Scr. 84 025603

Abstract
Ferrite nanoparticles, particularly nickel–zinc ferrite nanoparticles, are novel materials for high-frequency applications. Nanoparticles with a composition of Ni\textsubscript{0.5}Zn\textsubscript{0.5}Fe\textsubscript{2}O\textsubscript{4} were prepared by two different processes, namely the co-precipitation and simplified sol–gel methods. Powder x-ray diffraction (XRD) patterns confirmed the single-phase spinel structure for the as-prepared samples. Samples were sintered at 555 and 755 °C, after which the structural, electrical and magnetic properties were studied. The crystallite sizes, as determined from XRD data, increased with sintering temperature. The dc electrical resistivity measurements were performed as a function of temperature, with the two-probe method in the temperature range from room temperature to 450 °C. The activation energy and drift mobility were calculated from the temperature-dependent dc electrical resistivity measurements. The dielectric constant and dielectric loss tangent for all the samples were determined as a function of frequency, and the frequency range used was from 20 Hz to 3 MHz at room temperature. The samples prepared using the simplified sol–gel method have lower dielectric constant values compared to those of the samples prepared using the co-precipitation method, and those prepared by the former method are more suitable for high-frequency applications. For the magnetic properties, a vibrating sample magnetometer was used. Saturation magnetization and coercivity increased with an increase in sintering temperature.

Pseudopotential calculation of the bulk modulus and phonon dispersion of the bcc and hcp structures of titanium
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2011 Phys. Scr. 83 065603

Abstract
The structural stability of Ti in the hexagonal-closed-packed and body-centered cubic structures was studied by means of the full potential linearized augmented plane wave method. The effect of pressure on the bulk modulus of the crystal structures was investigated. In this study, the plane wave ultrasoft pseudopotential method was used to calculate the elastic constants, bulk modulus and phonon frequency of Ti. Phonon calculations were performed by employing the density functional perturbation theory in real space, using the calculated lattice dynamical force constants. All calculations were based on the density functional theory with the generalized gradient approximation and local density approximation, which well describe the properties of the above-mentioned metal.

Negative differential conductivity in bilayer graphene controlled by an external voltage and in the presence of a magnetic field
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2011 Phys. Scr. 83 015603

Abstract
The current–voltage characteristic of graphene bilayers was obtained in the case of strong electric and magnetic fields. Regions of negative differential conductivity were obtained as a function of frequency, and the frequency range used was from 20 Hz to 3 MHz at room temperature. The samples prepared using the simplified sol–gel method have lower dielectric constant values compared to those of the samples prepared using the co-precipitation method, and those prepared by the former method are more suitable for high-frequency applications. For the magnetic properties, a vibrating sample magnetometer was used. Saturation magnetization and coercivity increased with an increase in sintering temperature.

Effect of substrate temperature in the synthesis of BN nanostructures
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2011 Phys. Scr. 83 065601

Abstract
Boron nitride (BN) nanostructures were grown on molybdenum discs at different substrate temperatures using the short-pulse laser plasma deposition technique. Large numbers of randomly oriented nanorods of fiber-like structures were obtained. The variation in the length and diameter of the nanorods as a function of the substrate temperature was systematically studied. The surface morphologies of the samples were studied using scanning electron microscopy. Energy dispersive x-ray spectroscopy confirmed that both the elements boron and nitrogen are dominant in the nanorod structures. The x-ray diffraction (XRD) technique was used to analyse BN phases. The XRD peak that appeared at 26° showed the presence of hexagonal BN phase, whereas the peak at 44° was related to cubic BN content in the samples. Raman spectroscopic analysis showed vibrational modes of sp\textsuperscript{2} and sp\textsuperscript{3}-type bonding in the sample. The Raman spectra agreed well with XRD results.
The fabrication, characterization and electrochemical corrosion behavior of Zn-TiO$_2$ composite coatings

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2011 Phys. Scr. 84 035601

Abstract

Metal-nanoparticle composite coatings improve the hardness, wear resistance and corrosion resistance properties of metal coatings. In this work, TiO$_2$ nanoparticles were chosen as second-phase particles to generate anticorrosive Zn composite coatings. The TiO$_2$ nanoparticles were dispersed in a Zn plating solution to co-deposit them with Zn. The Zn-TiO$_2$ composite coatings were then characterized by scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDS) and x-ray diffraction methods. The presence of TiO$_2$ particles in the composite was confirmed by SEM images and EDS spectra. The Zn-TiO$_2$ composite coatings incorporated with different amounts of TiO$_2$ particles were tested for corrosion performance by polarization and electrochemical impedance spectroscopy, and the dissolution behavior of the coatings that had been immersed in corrosive media for a long time was studied. Improved corrosion resistance properties of the Zn-TiO$_2$ composite coatings were confirmed by polarization studies, fitted Nyquist plots, an increase in phase angle and a shift in the $R_\text{ct}$ characteristic peak of the Bode plot.

Physical and chemical properties of a Ga-doped ZnO crystal

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2011 Phys. Scr. 83 065604

Abstract

First-principles calculations based on density functional theory and strengthened by Hartree–Fock computations have been performed to study a Ga-doped wurtzite-type ZnO crystal. The large 108-atom supercell used throughout this work allows one to model a single point defect within the periodic supercell model. Thus, the Ga impurity produced purely local effects on the properties of the material. The electronic band structure was obtained for both pure and impurity-doped materials. The occurrence of free electrons in the conduction band was observed after the incorporation of Ga, implying the Ga dopant’s contribution to n-type electrical conductivity in the ZnO crystal, in agreement with known experimental data. An analysis of the charges on atoms and obtained atomic displacements in the region surrounding the defect showed that there is some alteration in the chemical bonding because of the presence of Ga atoms. In particular, the ionic bonding is strengthened in the defect’s neighbourhood.

The structural, elastic and vibrational properties of the DyX (X=P, As) compounds

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2011 Phys. Scr. 83 035601

Abstract

A detailed theoretical study of the structural, elastic and vibrational properties of DyX (X=P, As) compounds is presented in this paper by performing $ab$ $initio$ calculations based on density functional theory using the VASP code. For describing the interaction between electrons and ions, the projector-augmented wave method is used. The generalized-gradient approximation is chosen for the exchange-correlation functional. The calculated structural parameters, such as the lattice constant, bulk modulus and second-order elastic constants, are presented. The high-pressure phase of both compounds is investigated and the phase transition pressure from NaCl (B1) to high-pressure phase (B2) is determined. To gain further information, we have calculated the Zener anisotropy factor ($A$), Poisson’s ratio ($\nu$), Young’s modulus ($E$), shear modulus ($C$), elastic wave velocities, Debye temperature, phonon frequencies and one-phonon density of states for the B1 structure of these compounds. The temperature-dependent variations of some thermodynamic properties such as entropy, heat capacity, internal energy and free energy are also predicted for the same compounds in the B1 phase.

A carbon nanotube-based pressure sensor

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2011 Phys. Scr. 83 065703

Abstract

In this study, a carbon nanotube (CNT)-based Al/CNT/Al pressure sensor was designed, fabricated and investigated. The sensor was fabricated by depositing CNTs on an adhesive elastic polymer tape and placing this in an elastic casing. The diameter of multiwalled nanotubes varied between 10 and 30 nm. The nominal thickness of the CNT layers in the sensors was 10–30 nm. The resistance of the sensors decreased 3–4 times as the pressure was increased up to 17 kN m$^{-2}$. The resistance–pressure relationships were simulated.
Specific heat and magnetization studies of RMnO$_3$ (R=Sm, Eu, Gd, Tb and Dy) multiferroics

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2011 Phys. Scr. 83 045701

Abstract

A series of multiferroic materials with the compositional formula RMnO$_3$ (where R=Sm, Eu, Gd, Tb and Dy) were prepared by the well-known citrate gel technique. After characterizing the samples structurally, a systematic investigation of specific heat and magnetization studies were performed over the temperature range 4–300 K with different magnetic fields. Based on these studies, it was found that all the samples exhibit a transition in the temperature region 39–54 K and the transition is attributed to ordering of Mn$^{3+}$ ions (T$_N^{3+}$). Further, the samples GdMnO$_3$, TbMnO$_3$ and DyMnO$_3$ were found to exhibit another transition (T$_M$) in the temperature range 20–29 K. Finally, another transition was exhibited by all the samples and it is attributed to the antiferromagnetic (AF) ordering of rare-earth ion moments (T$_{AF}$). The entropy at the AF transition T$_{AF}$ was computed. Finally, using the specific heat data, the Debye temperature values were also calculated.

First-principles study of structural, elastic, electronic, lattice dynamic and optical properties of XN (X=Ga, Al and B) compounds under pressure

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2011 Phys. Scr. 83 065702

Abstract

We have applied the pseudo-potential plane wave method to study the structural, elastic, electronic, lattice dynamic and optical properties of GaN and AlN in the wurtzite lattice and BN with zinc-blende structure. We have found that all elastic constants depend strongly on hydrostatic pressure, except for C$_{44}$ in wurtzite AlN and GaN that shows a weaker dependence. AlN and GaN present a direct band gap $\Gamma$–$\Gamma$, whereas BN has an indirect band gap $\Gamma$–X. The indirect $\Gamma$–K band gap in AlN occurs at about 35 GPa. The top of the valence bands reflects the p electronic character for all structures. There is a gap between optical and acoustic modes only for wurtzite phases AlN and GaN. All peaks in the imaginary part of the dielectric function for the wurtzite lattice GaN and AlN move towards lower energies, while those in the zinc-blende BN structure shift towards higher energies with increasing pressure. The decrease of the static dielectric constant and static refractive index in zinc-blende BN is weaker and it can be explained by its higher elastic constants.

The photoluminescence and magnetism of nitrogen-implanted ZnO

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Abstract

Single crystal ZnO was implanted using nitrogen ions with an energy of 60 keV. The microstructure, photoluminescence (PL) and magnetism were studied in detail. Except for nitrogen, no other impurity can be detected by x-ray photoelectron spectra measurements. The room temperature PL of pure ZnO consists of a weak ultraviolet (UV) emission band and a strong green emission band. The PL and electrical conductivity can be suppressed by nitrogen implantation or by annealing in air. However, the two emission bands of pure ZnO can be enhanced intensively by Ar$^+$ etching. The PL is related to the structure defects. Moreover, the intensity of UV luminescence is likely correlated to the electrical conductivity. Ferromagnetism cannot be obtained in the nitrogen-implanted sample from 77 to 300 K. The absence of ferromagnetism in nitrogen-implanted ZnO may be because there is no strong interaction between N 2p and O 2p electrons as nitrogen is a deep acceptor in ZnO.

Electric field effects on the intersubband optical absorptions and refractive index in double-electron quantum dots

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Abstract

The linear and nonlinear optical properties such as optical absorption and refractive index change associated with intersubband transitions in a two-electron quantum dot (QD) in the presence of an external electric field have been investigated theoretically by using the perturbation method. The exchange force, which is a strictly quantum mechanical phenomenon, has also been considered. Numerical results on typical GaAs/AlGaAs materials show that an increase of the electric field decreases the oscillator strengths, the peak positions of absorption coefficients as well as the refractive index changes. Additionally, an increase of the confinement frequency (dot size) increases (decreases) the absorption coefficients but does not significantly affect the refractive index changes. It is also observed that the intensity of the illumination and the relaxation time have drastic effects on nonlinear optical properties. Finally, we note that the optical absorption coefficients and refractive index changes of two electrons are about five times higher than that of a one-electron QD.
Nonlinear transport through ultra-narrow zigzag graphene nanoribbons: non-equilibrium charge and bond currents

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Abstract
The electronic nonlinear transport through ultra-narrow graphene nanoribbons (sub-10 nm) was studied. A stable region of negative differential resistance (NDR) appears in the $I–V$ characteristic curve of odd zigzag graphene nanoribbons (ZGNRs) at both positive and negative polarity. This NDR originates from a transport gap induced by a selection rule that blocks the electron transition between disconnected energy bands of ZGNR. Based on this transition rule, the on/off ratio of the current increases exponentially with ribbon length up to $10^5$. In addition, charging effects and the spatial distribution of bond currents were studied by using the non-equilibrium Green's function formalism in the presence of electron–electron interaction at a mean-field level. We also performed an ab initio density functional theory calculation of the transmission through a passivated graphene nanoribbon to demonstrate the robustness of the transport gap against hydrogen termination of the zigzag edges.

Improvement in the luminous efficiency of MEH-PPV based light emitting diodes using zinc oxide nanorods grown by the electrochemical deposition technique on ITO substrates

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Abstract
Zinc oxide (ZnO) nanorods grown by the electrochemical technique have been used to enhance the luminance of poly[2-methoxy-5-(2'-ethylhexoxy)-1,4-phenylenevinylene] (MEH-PPV)-based polymer light-emitting diodes. The luminance of the device with ZnO nanorods is found to increase by more than two times as compared with the device without ZnO nanorods. The diameter of the nanorods used in device fabrication was ~145 nm. The size of the nanorods was estimated from field emission scanning electron microscope images. Optical and structural characterizations of the nanorods were also performed by using absorption, photoluminescence and x-ray diffraction, confirming the formation of ZnO nanorods.

Magnetic and transport properties of chemical solution deposited (100)-textured La$_{0.7}$Sr$_{0.3}$MnO$_3$ and La$_{0.7}$Ca$_{0.3}$MnO$_3$ nanocrystalline thin films

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Abstract
A study of the magnetic and electrical properties of (100)-oriented La$_{0.7}$(Sr,Ca)$_{0.3}$MnO$_3$ thin films prepared by an optimized chemical solution deposition process on a (100) SrTiO$_3$ single-crystal substrate is reported in this paper. The films were studied by high-resolution scanning electron microscopy, x-ray diffraction, vibrating sample magnetometer, ferromagnetic resonance and four-point-probe electrical measurements. A characteristic nanocrystalline texture with ~15 nm crystallites is observed in both films. Remarkably, the resistivities of these films are three orders of magnitude smaller compared with unoptimized films grown even on the same substrate. The magnetotransport properties were determined as a function of temperature and applied field magnitude, and compared with bulk crystals and vacuum-deposited single crystalline (epitaxial) thin films as well as manganite nanostructures reported in the literature. Both films display large values of colossal magnetoresistance at around room temperature. Significantly, the magnetoresistance in (100) La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin film is observed to be highly linear even at low fields near the metal–insulator transition temperature. However, the dependence of these promising properties on the nanocrystal size remains to be explored.
Effect of pressure on the global and local properties of cubic perovskite crystals

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Abstract

The influence of pressure on the structural, elastic, thermal and bonding properties of four perovskite-type oxides AMO₃ is studied from the point of view of the quantum theory of atoms in molecules. Ab initio investigations are performed by means of the full-potential linear augmented plane-wave method as implemented in the wien2k code. The integrated basin charges resulting from the topological analysis of electronic density provide a partition of the bulk modulus and compressibility into atomic contributions. Special attention is paid to the nonlinear behaviour of the local bonding properties.

Synthesis and characterization of Cu doped cobalt oxide nanocrystals as methane gas sensors

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Abstract

This work is devoted to identifying the degradation mechanism in various structures of a poly(3-hexylthiophene) (P3HT):6,6-phenyl C₆₁-butyric acid methyl ester (PCBM)-based solar cell. We have tried to identify the dominant initial degradation mechanism on the basis of experimental studies carried out on different structures of an organic solar cell. It is known that many of these problems can be solved by means of the following: using proper electrodes and a suitable annealing temperature and duration, improving the morphology of the active film and maintaining a donor–acceptor phase-segregated ordered network as far as possible. The present studies have been carried out both in the dark and under illumination, and it is suggested that initial degradation plays a key role in device performance. The dominant degradation mechanism is the growth of the donor–acceptor complex with time, which not only reduces the effective surface area but also hampers the charge separation. The little change in Vₜₚ and the significant change in Jₛₛₚ suggest that once the LiF/Al electrode is improved, one must modify the structure either by introducing a thin layer of high-molecular-weight P3HT between PEDOT-PSS (poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate)) and photoactive P3HT:PCBM layers or by introducing an optimized content of P3HT nanofibrils/nanoparticles into the P3HT:PCBM blend. The best structure was found to be ITO/PEDOT-PSS/P3HT:PCBM/LiF/Al and it can be improved by the above two methods.

Interdisciplinary physics and related areas of science and technology

Role of donor–acceptor domain formation and interface states in initial degradation of P3HT:PCBM-based solar cells

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2011 Phys. Scr. 84 055702

Abstract

In this paper, nanoparticles of copper–cobalt compound oxide have been prepared by the sol–gel technique with different mole ratios of Cu/Co (ranging from 0.05 to 0.15) for the detection of methane gas, which is chemically a very stable hydrocarbon. The structural properties and morphology of the powders were studied by x-ray diffraction (XRD), Fourier transform infrared spectroscopy and transmission electron microscopy (TEM). By XRD analysis, we confirm that Co₃O₄ and (CuO₆CoO₆) CO₃O₄ phases are formed and mean grain size is decreased with increasing Cu doping (from 28 to 24 nm). On the basis of TEM images, it is found that these particles possess a cubic structure with nearly uniform distribution. Also, gas-sensing measurements reveal that the optimal operating temperature is 300 °C, that the use of Cu as a dopant improved the sensing properties of cobalt oxide and that the sensitivity increased considerably with Cu concentration. The best sensitivity properties of nanosensors have been found at the mole ratios of Cu/Co of 0.125 and 0.15.
Lorentz-covariant quantum transport and the origin of dark energy
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Abstract
A possible explanation for the enigma of dark energy, responsible for about 76% of the mass–energy of the universe, is obtained by requiring only that the rigorous continuity equation (the Boltzmann transport equation) for quanta propagating through space should have the form of a Lorentz-covariant and dispersion-free wave equation. This requirement implies (i) properties of space–time that an observer would describe as uniform expansion in agreement with Hubble’s law and (ii) that the quantum transport behaves like in a multiplicative medium with multiplication factor $\nu = 2$. This inherent, essentially explosive multiplicity of vacuum, caused by the requirement of Lorentz covariance, is suggested as a potential origin of dark energy. In addition, it is shown (iii) that this requirement of Lorentz-covariant quantum transport leads to an apparent accelerated expansion of the universe.

Cosmic microwave background radiation in an inhomogeneous spherical space
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2011 Phys. Scr. 84 055901

Abstract
We analyse the cosmic microwave background (CMB) radiation in spherical three-spaces with nontrivial topology. The focus is on an inhomogeneous space which possesses observer-dependent CMB properties. The suppression of the CMB anisotropies on large angular scales is analysed with respect to the position of the CMB observer. The equivalence of a lens space to a Platonic cubic space is shown and used for the harmonic analysis. We give the transformation of the CMB multipole radiation amplitude as a function of the position of the observer. General sum rules are obtained in terms of the squares of the expansion coefficients for invariant polynomials on the three-sphere.

Dimensions, nodes and phases in quantum numbers
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2011 Phys. Scr. 83 018101

Abstract
Students of quantum mechanics encounter discrete quantum numbers in a somewhat incoherent and bewildering number of ways. For each physical system studied, quantum numbers seem to be introduced in their own specific way, some enumerating from 1 and others from 0, without a common uniting thread. This essay presents a point of view that builds on dimensions, boundary conditions and various inputs that, while known, are often not brought together to present a simple, consistent picture. At the same time, some surprisingly sophisticated connections are also made.

Testing Lorentz symmetry with atoms and light
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Abstract
This article reports on the Fifth Meeting on CPT and Lorentz Symmetry, CPT ’10, held at the end of June 2010 in Bloomington, Indiana, USA. The focus is on recent tests of Lorentz symmetry using atomic and optical physics.
Optical tomography of Fock state superpositions

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Abstract

We consider optical tomography of photon Fock state superpositions (FSS) in connection with recent experimental achievements. The emphasis is put on the fact that it suffices to represent the measured tomogram as a main result of the experiment. We suggest a test for checking the correctness of experimental data. Explicit expressions for optical tomograms of FSS are given in terms of Hermite polynomials. Particular cases of vacuum and low-photon-number state superposition are considered and the influence of thermal noise on state purity is studied.

On multiple adsorptions of hydrogen atoms on graphene

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Abstract

First-principles calculations using the Vienna Ab Initio Simulation Package (VASP) have been performed in order to scrutinize the hydrogen–graphene interaction. Emphasis has been placed on how surface relaxation and the prior chemisorption of one, two and three hydrogen atoms on graphene affect the adsorption properties of an encroaching gas phase hydrogen atom. Chemisorption at the para site was found to be barrierless, while it has been shown that a stable ortho adsorbate can form directly from the gas phase. Adsorption of the third and fourth H atoms was found in all cases to have a significant barrier. The resultant minimum energy structures show a reasonable agreement with scanning tunneling microscopy images obtained by Homekær et al (2007 Chem. Phys. Lett. 446 237).

The pairing mechanism of high-temperature superconductivity: experimental constraints

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Abstract

Developing a theory of high-temperature superconductivity in copper oxides is one of the outstanding problems in physics. It is a challenge that has defeated theoretical physicists for more than 20 years. Attempts to understand this problem are hindered by the subtle interplay among a few mechanisms and the presence of several nearly degenerate and competing phases in these systems. Here, we present some crucial experiments that place essential constraints on the pairing mechanism of high-temperature superconductivity. The observed unconventional oxygen-isotope effects in cuprates have clearly shown strong electron–phonon interactions and the existence of polaron and/or bipolaron pairs. Angle-resolved photoemission and tunneling spectra have provided direct evidence for strong coupling to multiple-phonon modes. In contrast, these spectra do not show strong coupling features expected for magnetic resonance modes. Angle-resolved photoemission spectra and the oxygen-isotope effect on the antiferromagnetic exchange energy J in undoped parent compounds consistently show that the polaron binding energy is about 2 eV, which is over one order of magnitude larger than J ≈ 0.14 eV. The normal-state spin-susceptibility data of hole-doped cuprates indicate that intersite bipolarons are the dominant charge carriers in the underdoped region, while the component of Fermi-liquid-like polarons is dominant in the overdoped region. All the experiments for testing the gap or order-parameter symmetry consistently demonstrate that the intrinsic gap (pairing) symmetry for the Fermi-liquid-like component is anisotropic s-wave and the order-parameter symmetry of the Bose–Einstein condensation of bipolarons is d-wave.

Comments section (CCMP)

High-temperature superconductivity: the explanation

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Abstract

Soon after the discovery of the first high-temperature superconductor by Georg Bednorz and Alex Müller in 1986, the late Sir Nevill Mott in answering his own question “Is there an explanation?” (1987 Nature 327 185) expressed the view that the Bose–Einstein condensation (BEC) of small bipolarons, predicted by us in 1981, could be the one. Several authors then contemplated BEC of real-space tightly bound pairs, but with a purely electronic mechanism of pairing rather than with an electron–phonon interaction (EPI). However, a number of other researchers criticized the bipolaron (or any real-space pairing) scenario as incompatible with some angle-resolved photoemission spectra, with experimentally determined effective masses of carriers and unconventional symmetry of the superconducting order parameter in cuprates. Since then, the controversial issue of whether EPI is crucial for high-temperature superconductivity or is weak and inessential has been one of the most challenging problems of contemporary condensed matter physics. Here I outline some developments in the bipolaron theory suggesting that the true origin of high-temperature superconductivity is in a proper combination of strong electron–electron correlations with a significant finite-range (Fröhlich) EPI, and that the theory is fully compatible with key experiments.
Comments section (CFRP)

Foundations of quantum mechanics?
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2011 Phys. Scr. 84 018501

Abstract
Does quantum mechanics have unsolved foundational problems? Is there a dividing line between the quantum and classical descriptions of the world? In this paper, I give an elementary introduction to the mathematical aspects of quantum and classical models which have prompted such questions.

Topical issue (T143)

Entanglement dynamics of a bipartite system in squeezed vacuum reservoirs
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2011 Phys. Scr. T143 014006

Abstract
Entanglement plays a crucial role in quantum information protocols; thus the dynamical behavior of entangled states is of great importance. In this paper, we suggest a useful scheme that permits a direct measure of entanglement in a two-qubit cavity system. It is realized through cavity-QED technology utilizing atoms as flying qubits. To quantify entanglement we use the concurrence. We derive the conditions that ensure that the state remains entangled in spite of the interaction with the reservoir. The phenomenon of entanglement sudden death in a bipartite system subjected to a squeezed vacuum reservoir is examined. We show that the sudden death time of the entangled states depends on the initial preparation of the entangled state and the parameters of the squeezed vacuum reservoir.

Entanglement dynamics of two independent cavity-embedded quantum dots
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2011 Phys. Scr. T143 014004

Abstract
We investigate the dynamical behavior of entanglement in a system made of two solid-state emitters, as two quantum dots, embedded in two separated microcavities. In these solid-state systems, in addition to the coupling with the cavity mode, the emitter is coupled to a continuum of leaky modes providing additional losses and is also subjected to a phonon-induced pure dephasing mechanism. We model this physical configuration as a multipartite system composed of two independent parts each containing a qubit embedded in a single-mode cavity, exposed to cavity losses, spontaneous emission and pure dephasing. We study the time evolution of entanglement of this multipartite open system, finally applying this theoretical framework to the case of currently available solid-state quantum dots in microcavities.

A smooth, holographically generated ring trap for the investigation of superfluidity in ultracold atoms
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2011 Phys. Scr. T143 014008

Abstract
We discuss the suitability of holographically generated optical potentials for the investigation of superfluidity in ultracold atoms. By using a spatial light modulator and a feedback enabled algorithm, we generate a smooth ring with variable bright regions that can be dynamically rotated to stir ultracold atoms and induce superflow. We also comment on its future integration into a cold atom experiment.
At the borderline between atomic and nuclear physics: two-body $\beta$-decay of highly charged ions

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Abstract

In this paper, we discuss the radioactive decay of highly charged ions. There are several motivations for performing this kind of research. One of them is that stellar nucleosynthesis proceeds at high temperatures and therefore the involved atoms are highly ionized. Highly charged ions also offer the possibility of addressing the decay of well-defined quantum-mechanical systems such as, for example, one-electron ions, where all the interactions with other electrons are excluded. These studies can be performed solely at ion storage rings or ion traps, where the high atomic charge states can be preserved for extended periods of time. Although we have focused on experiments conducted at the storage ring ESR of GSI, we have tried to describe the general requirements for such experiments.

Configuration and calibration of a flat field grating spectrometer in the wavelength range 7–60 Å with a Manson ultrasoft x-ray source

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2011 Phys. Scr. T144 014064

Abstract

An ultrasoft x-ray and extreme ultraviolet spectrometer built and calibrated in the wavelength range of 7–60 Å is reported here. Details of the alignment of this flat field spectrometer with both a laser and a telescope are presented. The light path function rather than a standard calibration function, i.e. a polynomial function, is introduced as the fit function, which gives good agreement with the spectrometer design values and makes the calibration more reliable when extended to the region outside the points used for calibration, compared with a standard calibration function. The calibration results of a Manson ultrasoft x-ray source (model 2) with source targets of Cu, Fe and Ti are presented with all the peaks marked.
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