Part A

Decoherence and quantum computers

Spin effects in electronic transport through quantum dots

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Electronic transport through quantum dots coupled to ferromagnetic leads will be discussed in detail with particular emphases on novel phenomena arising from the interplay of charge and spin degrees of freedom. When coupling between the dot and leads is weak, one finds effects typical of Coulomb blockade phenomenon. Some new and interesting effects occur in both the cotunneling and sequential tunneling regimes. The most intriguing one seems to be the zero bias anomaly in differential conductance, which originates from the interplay of spin accumulation on the dot and single-barrier cotunneling processes. A different anomaly occurs in transport through a quantum dot in the strong coupling regime, where the Kondo correlations become relevant. It turns out, that ferromagnetism of the leads has a significant influence on the Kondo anomaly in transport properties. First of all, ferromagnetism of the electrodes gives rise to splitting of the Kondo peak in the density of states, and therefore leads to splitting and suppression of the Kondo anomaly in transport properties. The full Kondo effect can be restored by applying an external magnetic field that compensates the level splitting due to exchange field created by ferromagnetic electrodes. Electronic transport through quantum dots coupled to magnetic leads with noncollinear magnetizations will also be considered. Exchange coupling between the dot and ferromagnetic electrodes gives then rise to precession of the spin accumulated on the dot. The spin precession has a significant influence on transport characteristics of the system.

References:

[1] J. Martinek, Y. Utsumi, H. Imamura, J. Barnaś, S. Maekawa, J. Koenig, and G. Schoen, Phys. Rev. Lett. 91, 127203 (2003).

[2] J. Koenig, J. Martinek, J..Barnaś, G. Schoen, Lecture Notes in Physics 658, 145 (2005).

[3] I.Weymann, J..Barnaś, J. Koenig, J. Martinek, G. Schoen, Phys. Rev. B 2005.

[4] W. Rudziński, J. Barnaś, Świrkowicz, M. Wilczyński, Phys, Rev. B 71, 205307 (2005).

[5] R. Świrkowicz, M. Wilczyński, J. Barnaś, cond-mat/0501605.

Geometric Aspects of Quantum Mechanics and Quantum Entanglement

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It is shown that the standard non-relativistic Quantum Mechanics gives rise to elegant and rich geometrical structures. The space of quantum states is endowed with nontrivial Fubini-Study metric which is responsible for the "peculiarities" of the quantum world. We show that there is also intricate connection between geometry and quantum entanglement.

Possibility of reducing the number of experiments without significant loss of gained information

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The paper presents a new concept of so called second generation of the design of experiment (DOE) based on artificial intelligence methods. Specifically speaking, the concept applies so called smart experiments which utilize artificial neural networks. They are being developed in technical areas thanks to prof. Polanski's initiative.

One of the features of the smart experiment plan is the possibility of reducing the number of measurements required during the experiment without significant loss of information. This brings mostly economical advantages in practical applications.

Reducing pure dephasing of quantum bits by collective encoding in quantum dot arrays

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Discrete, atomic-like spectrum of confined carrier states in quantum dots (QDs) suggests that these systems should be suitable for quantum information processing (QIP). Indeed, QIP schemes based on charge states in QD systems [1, 3] have been proposed. The most natural choice is to encode qubit values as the presence or absence of a confined exciton and to use sub-picosecond optical pulses to coherently control the system. These theoretical proposals were recently supported by an experimental demonstration [3]. However, the QD implementation of QIP is affected by serious limitations resulting, on one side, from the finite lifetime of charge states used for information encoding. On the other side, optical experiments [4] have demonstrated that pure dephasing processes destroy the coherence of the system state to a large extent within a few picoseconds after creating the state. This has been attributed to the carrier-phonon interaction [5] and interpreted in terms of spontaneous relaxation of the lattice after the optically induced change of the confined charge distribution, accompanied by emission of phonon wave packets [6], which leaves a kind of *which way* trace in the crystal, distinguishing between the qubit states. This effect may be avoided to some extent by pulse shaping [7] but it is completely eliminated only in the limit of adiabatic control, which requires long operation times and leads to a tradeoff situation with the finite lifetime restriction [5]. As a result, maximum fidelity of a coherent quantum control operation on a given system is limited.

In this presentation we use a perturbative theory describing the open system evolution under arbitrary driving [5, 6, 10] to show that pure dephasing may be reduced by collective encoding of logical qubits in an array of QDs. The idea relies on the fact that this dephasing mechanism is of purely dynamical character and results exclusively from the nonadiabaticity of the driving [5]. Thus, for a given speed of rotation in the qubit space, only slow modes that cannot follow the evolution of the charge distribution are involved while faster modes follow adiabatically and reversibly. In this way, only a long wavelength part of all the coupled modes is relevant for the dynamics. Since the range of these slow modes is selected dynamically, independently of the system geometry, it may correspond (under suitable driving conditions) to wavelengths larger than the QD array. Certain states of the array (with the same total number of excitons) cannot be distinguished by long-wavelength modes and may therefore be used for noiseless encoding of logical qubit values. This scheme works

only for relatively slow evolution and the resulting fidelity gain is again restricted by finite lifetimes but, as we will show, experimentally measured exciton lifetimes allow one to reduce the overall error. Although the proposed collective encoding is similar to the earlier idea of implementing logical qubits robust against real transitions on QD arrays [1] (noiseless encoding, closely related to the effect of sub-radiance), our scheme does not assume that the individual dots in the register are identical, which is essential for its possible implementation in artificial semiconductor structures.

References

[1] Zanardi P and Rossi F 1998 *Phys. Rev. Lett.* **81** 4752

[2] Biolatti E, Iotti RC, Zanardi P and Rossi F 2000 *Phys. Rev. Lett.* **85** 5647

[3] Li X, Wu Y, Steel D, Gammon D, Stievater T, Katzer D, Park D, Piermarocchi C, and Sham L 2003 *Science* **301** 809

[4] Borri P, Langbein W, Schneider S, Woggon U, Sellin RL, Ouyang D and Bimberg D 2001 *Phys. Rev. Lett.* **87** 157401

[5] Vagov A, Axt VM and Kuhn T 2003 *Phys. Rev. B* **67** 115338

[6] Jacak L, Machnikowski P, Krasnyj J and Zoller P 2003 *Eur. Phys. J. D* **22** 319

[7] Axt VM, Machnikowski P and Kuhn T 2005 *Phys. Rev. B* **71** 155305, cond-mat/0408322

[8] Alicki R, Horodecki M, Horodecki P, Horodecki R, Jacak L and Machnikowski P 2004 *Phys. Rev. A* **70** 010501(R), quant-ph/0302058

[9] Grodecka A, Jacak L, Machnikowski P and Roszak K. Phonon impact on the coherent control of quantum states in semiconductor quantum dots. In Ling PA, editor, *Quantum Dots: Research Developments*. Nova Science, Hauppauge NY 2005, cond-mat/0404364

[10] Roszak K, Grodecka A, Machnikowski P and Kuhn T 2005 *Phys. Rev. B* **71**(19) 195333, cond-mat/0404647

Qubit systems and invariant theory

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The properties of multi-qubit states are intimately related to problems in classical invariant theory. A brief introduction to this will be given. Then, by way of illustration, a complete analysis will be given of the ring of invariants of a mixed two-qubit system. We show in particular that this ring is a Cohen-Macauley ring, despite some initial appearances to the contrary. In carrying out this analysis the Molien function and corresponding Hilbert series are derived using some quite general methods. The syzygies necessary to confirm the completeness of the set of invariants are also discussed.

Dynamical dephasing of optically controlled charge qubits in quantum dots

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Quantum dots (QDs) are promising candidates for implementing quantum information processing (QIP) schemes due to their atomic-like discrete spectra, controllable properties, feasibility of building arrays of many coupled QDs (providing for scalability) and availability of fast optical control methods. Indeed, proposals for QD-based quantum computing [1, 3] were recently followed by an experimental demonstration of a controlled-NOT gate [3]. On the other hand, the progress of coherent control over confined charge states in QDs encounters serious obstacles resulting from strong dephasing effects due to the dynamics of the surrounding crystal environment. In self-assembled dots, the dominating dephasing scenario is related to carrier-phonon interactions.

In this presentation we review our recent results on the dynamically induced pure dephasing of charge qubits in QDs due to lattice dynamics. We describe the physical mechanism of dephasing resulting form spontaneous formation of coherent phonon dressing around an exciton created by an ultrafast optical pulse ("acoustic polaron") [6], which leads to emission of phonon packets and leaves a *which way* trace in the crystal. Next, we introduce a method that allows one to perturbatively include phonon effects for arbitrary optically controlled dynamics (which is treated exactly) [5, 6]. Using this method, we show that the dephasing effect may be reduced by slowing down the system dynamics towards the adiabatic limit, to the degree allowed by the lifetime of the exciton state [5]. We show that the contrary requirements imposed by the dynamical dephasing (slow dynamics) and by the accumulation decoherence resulting from finite lifetime (short operation) leads to a trade-off situation and limits the possibility of reducing dephasing. An alternative method to partly avoid decoherence is to use shaped pulses. In particular, astonishingly large reduction of dephasing is obtained by driving the system with just a few (3-4) short pulses [7]. Finally, we show how phonon-induced pure dephasing explains the observed damping of pulse-area-dependent Rabi oscillations on a single QD [8]. Resonant character of interaction between phonons and oscillating charge distribution in the dot [9] leads to the unexpected prediction that the damping should decrease not only for short but also for long control pulses.

References

[1] Zanardi P and Rossi F 1998 *Phys. Rev. Lett.* **81** 4752

[2] Biolatti E, Iotti RC, Zanardi P, and Rossi F 2000 *Phys. Rev. Lett.* **85** 5647

[3] Li X, Wu Y, Steel D, Gammon D, Stievater T, Katzer D, Park D, Piermarocchi C, and Sham L 2003 *Science* **301** 809

[4] Jacak L, Machnikowski P, Krasnyj J, and Zoller P 2003 *Eur. Phys. J. D* **22** 319–331

[5] Alicki R, Horodecki M, Horodecki P, Horodecki R, Jacak L, and Machnikowski P 2004 *Phys. Rev. A* **70** 010501(R) quant-ph/0302058

[6] Grodecka A, Jacak L, Machnikowski P, and Roszak K. Phonon impact on the coherent control of quantum states in semiconductor quantum dots. In Ling PA, editor, *Quantum Dots: Research Developments*. Nova Science Hauppauge, NY 2005. cond-mat/0404364

[7] Axt VM, Machnikowski P, and Kuhn T 2005 *Phys. Rev. B* **71**(11) 155305 cond-mat/0408322

[8] Zrenner A, Beham E, Stufler S, Findeis F, Bichler M, and Abstreiter G 2002 *Nature* **418** 612

[9] Machnikowski P and Jacak L 2004 *Phys. Rev. B* **69** 193302 cond-mat/0305165

Quantum Monte Carlo simulations of interacting electrons

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Abstract not received.

Quantum Market Games: Implementing Tactics Via Measurement

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A major development in applying the quantum mechanical formalism on various fields has been made during the last few years. Quantum counterparts of game theory, economy, as well as diverse approaches to quantum information theory has been found and currently are being explored. Using connections between quantum game theory and quantum computations, an application of the universality of a measurement based computation in quantum market theory is presented.

"Which way" interpretation of the dephasing of charge qubits in quantum dots

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A property of quantum systems that distinguishes them from classical ones and provides the unusual power for quantum computing schemes is the ability of a quantum system to remain in a superposition of states. However, a fundamental difficulty in sustaining the phase coherence of such a quantum superposition is the interaction between the quantum system and the surrounding world. In the course of joint evolution of the system and its environment, this interaction establishes phase correlations between the former and a macroscopic number of degrees of freedom of the latter. Such correlations perturb and eventually erase internal phase information of the quantum system. This effect, known as *decoherence* or *dephasing*, not only seems to be one of the most fundamental aspects of the quantum theory [1] but also presents serious limitations to quantum computing schemes, where maintaining system coherence over many control operations is of primary importance [2]. Thus, not only quantitative estimates but also qualitative understanding of dephasing processes is of great interest.

In this presentation we study the dephasing of exciton states in quantum dots (QDs), which are the most obvious implementation of a charge qubit [3], from a more general point of view. We exploit the idea that dephasing of quantum superpositions is due to the trace that the system leaves in its environment (*which way* information) [1]. In QDs, the level of purity of a superposition state may be experimentally determined by measuring the amplitude of coherent dipole radiation emitted by a confined exciton [4]. The observed decrease of this amplitude has been accounted for by a theory [5] invoking interaction with acoustical phonons. On the other hand, the fast dynamics of optically driven confined carrier states is accompanied by spontaneous lattice relaxation and emission of phonon packets [6, 7] which correlate the charge state with remote parts of the crystal and may be identified as the physical carrier of *which way* information.

Here, we will use a quantitative measure for information on the system state broadcast into the environment in the course of the dephasing process [8, 9] to show that the degree of system coherence (expressed by the amplitude of coherent radiation) is related to the amount of information transfered to the environment by a *quantitative* relation. In this way, we prove a complementarity between the knowledge of the system state (which refers to the exciton as a particle-like, indivisible entity) and the degree of coherence retained by the system.

References

[1] Zurek WH 2003 *Rev. Mod. Phys.* **75**(3) 715–775

[2] DiVincenzo DP and Loss D 1998 *Superlattices and microstructures* **23**(3/4) 419

[3] Biolatti E, Iotti RC, Zanardi P, and Rossi F 2000 *Phys. Rev. Lett.* **85** 5647

[4] Borri P, Langbein W, Schneider S, Woggon U, Sellin RL, Ouyang D, and Bimberg D 2001 *Phys. Rev. Lett.* **87**(15) 157401–1–4

[5] Vagov A, Axt VM, and Kuhn T 2003 *Phys. Rev. B* **67** 115338

[6] Jacak L, Machnikowski P, Krasnyj J, and Zoller P 2003 *Eur. Phys. J. D* **22** 319–331

[7] Vagov A, Axt VM, and Kuhn T 2002 *Phys. Rev. B* **66** 165312

[8] Englert B-G 1996 *Phys. Rev. Lett.* **77**(11) 2154–2157

[9] Jaeger G, Shimony A, and Vaidman L 1995 *Phys. Rev. A* **51**(1) 54–67

Some applications of $\widehat{P}$-matrices in orbit spaces and invariant theory

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In many physical problems or applications one has to study functions that are invariant under the action of a symmetry group G and this is best done in the orbit space of G if one knows the equations and inequalities defining the orbit space and its strata. It is reviewed how the $\widehat{P}$-matrix is defined in terms of an integrity basis and how one determines the equations and inequalities defining the orbit space and its strata using the $\widehat{P}$-matrix. When there is at most one syzygy, a $\widehat{P}$-matrix may be determined using some general algebraic and differential conditions on its matrix elements. The $\widehat{P}$-matrix is also a useful tool of constructive invariant theory, in fact, when the integrity basis is only partially known, calculating the $\widehat{P}$-matrix elements, one is often able to determine the integrity basis completely.

Paths, Virasoro characters and fermionic expressions.

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Baxter's corner transfer matrix method enables the one-point functions of certain 2D statistical models to be expressed as generating functions of weighted paths. In the case of the Forrester-Baxter models, the generating functions are Virasoro characters associated with the conformal minimal models M(p,p'). By combinatorially manipulating the paths, we obtain a quasiparticle description of the ensemble of paths. This directly leads to fermionic expressions for the Virasoro characters.

Multiple CSLs for cubic lattices

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Ordinary Coincidence Site Lattices (CSLs) are defined as the intersection of a lattice Γ with a rotated copy $R\Gamma$ of itself. They are useful for classifying grain boundaries and have been studied extensively some decades ago. Recently the interests turned to so-called multiple CSLs, i.e. intersections of n rotated copies of a given lattice Γ, in particular in connection with lattice quantizers. In this talk we consider multiple CSLs for 3-dimensional cubic lattices, in particular we discuss the spectrum of coincidence indices and their multiplicity as well as the possible CSLs.

Part B

The role of combinatorics in classification of solution for exactly solvable models

The completeness of the set of Bethe-Hulthen solutions for the linear Heisenberg system

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In this work we formulate the standard form of the solutions of the Heisenberg chain with periodic boundary conditions and show that these solutions can be transformed into the well-known Bethe-Hulthén solutions.

The standard form is found by solving the secular problem, separated according to the irreducible representations of the translation group. The relevant parameters $exp(ik)$ of the Bethe-Hulthén solutions may be found from a set of linear equations with co-efficients derived from the standard solutions.

Feynman Graphs and related Hopf Algebras

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We consider two aspects of the product formula for formal power series applied to combinatorial field theories. Firstly, we remark that the case when the functions involved in the product formula have a constant term is of special interest as often these functions give rise to substitutional groups. The groups arising from the normal ordering problem of boson strings are naturally associated with explicit vector fields, or their conjugates, in the case when there is only one annihilation operator. We also consider one-parameter groups of operators when several annihilators are present. Secondly, we discuss the Feynman-type graph representation resulting from the product formula. We show that there is a correspondence between the packed integer matrices of the theory of noncommutative symmetric functions and these Feynman-type graphs.
We obtain new Hopf algebra structures over the space of matrix quasi-symmetric functions : a natural cocommutative Hopf algebra structure on the space of diagrams themselves which originates from the formal doubling of variables in the product formula and an infinitesimal Hopf structure.
The two coproducts are specialisations of a one-parameter deformation.

Stationary space-times and generators of algebraic curvature tensors

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Algebraic curvature tensors $\mathfrak{R}$ are covariant tensors of order 4 which possess the same symmetry properties as the Riemann tensor R of a Levi-Civita connection ∇. The vector space of all algebraic curvature tensors $\mathfrak{R}$ can be generated by every of the following types of tensors

$$y_t^*(S \otimes S) \quad , \quad y_t^*(A \otimes A) \quad , \quad y_t^*(U \otimes w)\,, \tag{1}$$

where S and A are symmetric or alternating tensors of order 2, w is a tensor of order 1 and U is a tensor of order 3 which belongs to an irreducible $(2\,1)$-symmetry class. y_t denotes the Young symmetrizer of the Young tableau

$$t \;:=\; \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array}\,. \tag{2}$$

In differential geometry examples of curvature tensors are well-known which are formed by (differentiable) expressions of type $y_t^*(S\otimes S)$ and $y_t^*(A\otimes A)$. In particular, expressions of type $y_t^*(S \otimes S)$ arise in applications of the Nash embedding theorem.

We show that (differentiable) expressions of all three types (1) occur in certain curvature formulas for stationary space-times of general relativity. In these formulas the tensors U are given by the $[2\,1]$-part of the tensor field

$$\tau_i \tau_{[j;k]}\,, \tag{3}$$

where τ^i is the unit vector field proportional to the timelike Killing field ξ^i of the stationary space-time. (The symmetry class of (3) is characterized by the Littlewood-Richardson product $[1^2][1] \sim [2\,1] + [1^3]$.)

In the infinite set of irreducible $(2\,1)$-symmetry classes the symmetry class of the U induced by (3) belongs to the finite subset of $(2\,1)$-symmetry classes which allow a maximal reduction of the length of $y_t^*(U \otimes w)$. A stationary space-time is static iff the $[1^3]$-part of (3) vanishes.

Geometry and rigged strings in Bethe Ansatz

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The main purpose of this report is the thorough analysis of completeness of the solutions of the one-dimensional Heisenberg Hamiltonian through the hypothesis of strings. A somehow astonishing conclusion emerges from studying of the structure of the classical configuration space of this system. Namely, all allowed information concerning quantum states, which are exact solutions of the Bethe equations, encoded in quantum numbers, are predictable via a bijection between the set of the magnetic configurations and the string configurations. This startling and beautiful observation constitutes the proof of the completeness of the eigenstates of the Heisenberg Hamiltonian, deduced in a purely combinatorial way. We interpret the set of all magnetic configurations with a fixed number r of spin deviations as the classical configuration space of a hypothetic system of r Bethe pseudoparticles, which move, in a stroboscopic manner, on the magnetic ring. The geometry of this configuration space, induced by the action of Heisenberg Hamiltonian and the translation symmetry group of the ring, implies the structure of a locally r-dimensional hypercubic lattice, with well defined F-dimensional boundaries, $1 \leq F \leq r$. We demonstrate that rigged string configurations originate from these boundaries, depending upon the island structure of spin deviations. We show that a relatively simple combinatoric definition of rigged strings reproduces completely exact results of Bethe Ansatz. It is expressed in terms of a combined bijection: Robinson-Schensted with Kerov-Kirillov-Reshetikhin (RSKKR), which produces a geography of exact Bethe Ansatz solutions on the classical configuration space.

The duality of Weyl and linear extension of Kostka matrices

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Application of the Robinson-Schensted algorithm to the basis of magnetic configurations of the one dimensional Heisenberg magnet with an arbitrary spin gives an efficient way for a classification of the irreducible basis of the Weyl duality. The plactic monoid is shown to be an adequate tool for describing this irreducible basis in a way consistent with the Schensted insertion procedure, i.e. the creation of a new single-particle state (a letter of the single-node spin) in already constructed Young and Weyl tableaux. Schensted insertion is interpreted in terms of Gelfand triangles - combinatoric analogues of Weyl tableaux, with exposed occupation numbers, consistent with canonical chains of subgroups of both symmetric and unitary group. A transition matrix between these two bases should exist due to the linear structure of the Hilbert space. This matrix can be looked at as the linear extension of the famous Kostka matrix. We show how to obtain this matrix and give an interpretation of its elements as coefficients of certain wave packet with exactly defined symmetry. We also shown that the outcome of the Robinson-Schensted algorithm can be adequately decribed in terms of double Gelfand triangles, presented by Prof. Louck in SSPCM.

On the convolution the and product of distributions as irregular operations

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The product and the convolution of L. Schwartz's distributions can be defined by means of delta-sequences and unit-sequences. The results on the existence of the convolution and the product of distributions and tempered distributions as well as on the Fourier transform exchange formula $F(f * g) = F(f) \cdot F(g)$ for tempered distributions are presented together with applications to the formulas for the products of distributions which are applicable in physics.

Charge transport in thin layers of organic crystals

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Organic conductors have been studied since a long time (e.g. anthrancene since 1950s , TTF-TCNQ since 1970s, C60 since 1990s). Recently, the pentacene thin layers have been studied widely due to theirs best properties for application in field-efect transistors . The layers of this material grown under special growth conditions in the shape of layered semiconductors in which the molecular planes are parallel to a substrate. The charge transport in such structures is far from full understanding . The dominated molecular orbital overlap mechanism needs further studies . In this paper we survey types of carriers transport in molecular crystals. The main ideas were adapted to the epitaxial thin layers. The layers of pentacene are studied particulary as an example.

The role of point symmetry in electron(ic) bound states on defects in magnetic semiconductors

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While acknowleging the extraordinary influence and profound implications of symmetry methods in physics, we argue that these methods have a broader setting in enumerative combinatorics. This is illustrated in several ways by explicit results.

Quasimomenta of string configurations

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We develop a reciprocal space analogue of the combinatorial bijection of Robinson-Schensted and Kerov-Kirillov-Reshetikhin (RSKKR) between magnetic configurations - the initial basis for quantum calculations of the eigenproblem of the Heisenberg Hamiltonian for a one-dim finite Heisenberg chain, and rigged string configurations - the exact results of Bethe Ansatz. Existence of such a bijection implies an interpretation of the exact quantum numbers of riggings as quasimomenta of l-strings. The extended size of an l-string results in selection rules for these quasimomenta, and thus in a division of the Brillouin zone into compact subzones of forbidden and allowed states of the system of coupled Bethe pseudoparticles. The forbidden Brillouin subzone for a particular l-string is evidently the effect of kinematical restrictions for motions of constituent Bethe pseudoparticles. These restrictions can be easily predicted in a combinatorialy unique way due to completness of the RSKKR bijection.

Equivariant functions and operators in topological quantum mechanics

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We consider here two cases of t.q.m. (topological quantum mechanics). In the first one the configuration space is a plane with one point removed. The second case is quantum mechanics of anyons. We show that the space of states in t.q.m. depends on choice of Hamiltonian of the system.

Combinatorics of boson strings: Sheffer-type polynomials and monomiality.

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We consider the sequences of integers which appear in the process of normal ordering of powers of strings of boson operators as well as of powers of certain linear combinations of different strings. We show that these sequences are generalizations of standard Stirling and Bell numbers . We apply the methods of combinatorial analysis in order to investigate many properties of these sequences like recurrence relations, generating functions and closed form expressions (generalized Dobinski formulas) . This enables one to obtain coherent state expectation values of exponentiated boson strings which turn out to be generating functions of fundamental family of Sheffer-type polynomials. On the other hand we demonstrate that many formulas for normal ordering may be derived by an alternative method called the monomiality principle (Dattoli et al.) which is related to the umbral calculus. We apply our formalism to the problems of condensed matter physics (superfluidity) and quantum optics (Kerr hamiltonians) as well as to enumerative problems of Quantum Field Theory.

Operations on distributions: regular and irregular

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In the frame of the Mikusiński sequential theory of L. Schwartz distributions, elements of the theory of regular and irregular operations is presented with application to some formulas which may be of interest to physisists, e.g.:

$$\sqrt{}(\delta) = 0, \sqrt{}(1+\delta^2) = 1+\delta, log(1+\delta) = 0, sin\delta = 0.$$

Part C

Geometric aspects in nanophysics

Exact calculations for the ground state properties of the frustrated 2-dimensional Ising model

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The 2D Ising model is one of the most widely studied systems in statistical physics largely because it is one of the few non-trivial models that admit an exact solution. The original method of Onsager [1] based on Lie algebras was superseded by a combinatorial approach [2,3] in which the partition function is expressed in terms of a determinant. One can alternatively express the formalism in terms of non-interacting fermions or Grassmann variables. Although the early formulation considered specifically the perfect Ising lattice, problems of disordered systems can also be addressed using the technique.

Perhaps the most studied disordered system is the so-called spin-glass problem [4] in which the key element is frustration. This is characterized by conflicts in the spin configurations needed to minimize the energy. Frustration can arise from the geometry of the lattice or from a quenched random distribution of positive (ferromagnetic) and negative (antiferromagnetic) bonds. One of the canonical models of frustrated systems is the 2-dimensional J Ising model.

We showed [5] a number of years ago how certain features of the 2D $\pm$J Ising model are particularly transparent when expressed within the determinantal formalism [3], and we developed a technique for the exact calculation of the ground state energy and entropy of this system and applied it to the square [6,7] and triangular [8] lattices. Recently we have extended these ideas to evaluate the ground state correlation functions [9]. The talk will review the methodology and discuss the latest results.

1. L. Onsager, *Phys. Rev. 65*, 117 (1944).
2. M. Kac and J.C. Ward, *Phys. Rev. 88*, 1332 (1952).
3. H.S. Green and C.A. Hurst, *Order-Disorder Phenomena* (Interscience, London, 1964).
4. S.F. Edwards and P.W. Anderson, *J. Phys. F: Met. Phys.* 5, 965 (1975).
5. J.A. Blackman, *Phys. Rev. B* 26, 4987 (1982).
6. J.A. Blackman and J. Poulter, *Phys. Rev. B* 44, 4374 (1991).
7. J.A. Blackman, J.R. Gonçalves and J. Poulter, *Phys. Rev. E* 58, 1502 (1998).
8. J. Poulter and J.A. Blackman, *J. Phys. A: Maths. Gen.* 34, 7527 (2001).
9. J. Poulter and J.A. Blackman, *Phys. Rev. B* (2005) to be published.

EPR properties of Chromium in CdTe single crystals

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We have studied single CdTe monocrystals with relatively high concentration of Chromium. EPR measurements were studied in room temperature. The angular dependence of spectrum has been obtained. The spectrum in liquid nitrogen shows the different kind of EPR centers. The changing of the valence is addresed. Simulations of spectrum performed using program EPR-NMR.

Persistent currents in the presence of equilibrium and non-equlibrium noise

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We study dynamical and steady state properties of magnetic fluxes and currents in a mesoscopic cylinders formed by a stack of rings using semi-phenomenological model based on the Langevin equations. We discuss equilibrium and non-equilibrium systems. One of the forms of the fluctuation-dissipation theorem is reviewed in this context. We emphasize the influence of noise on the self-sustaining currents which are predicted to flow in the system in the steady state.

Symmetry and structural properties of carbon nanotube quantum dots and superlattices

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The electronic structure and quantum conductance of metallic carbon nanotube quantum dots and superlattices are investigated. We work within the tight-binding model and pi-electron nearest-neighbors approximation. In particular, we study systems built of (12,0)/(6,6), (12,0)/(9,3) and (8,2)/(5,5) double and multiple junctions. We show that the rotational symmetry of carbon nanotubes and structural properties of the nanotube junctions play a crucial role in determining of the transport properties of the investigated systems.

Effect of time reversal symmetry on states of quasiparticles in crystals

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States of quasiparticles in crystals with a well established translational symmetry such as: electrons, holes, excitons, phonons, etc., are classified according to irreducible representations (irrps) of the corresponding factor groups $G^{\mathbf{k}}/T$. The wave vector $\mathbf{k}$ runs over the entire first Brillouin Zone (BZ). When the irrps are complex, the time reversal symmetry (TRS) must be taken into account. Using Wigner criterion adopted to space groups, we have investigated irrps $D_j^{\mathbf{k}}$ of high symmetry point and lines in BZ of some hexagonal crystals with the space group C_{6v}^4 - $P6_3/mc$. We have found that many irrps $D_j^{\mathbf{k}}$ are complex. Therefore, the state of " .. - ons" (electrons, phonons, etc.) in these crystals will be classified according to the "joint" irrps $D_j^{\mathbf{k}} \oplus (D_j^{\mathbf{k}})^*$. Consequently, an extra degeneracy of those states follows. In general, in presence of the TRS in crystals all group theoretical calculations such as classification of vibrational modes from those the dynamical matrices can be computed, selection rules involved in the optical transitions, electronic band structures, and so on, must take into account the joint irrps $D_j^{\mathbf{k}} \oplus (D_j^{\mathbf{k}})^*$ of time reversal influenced states.

We provide a detailed analysis based on experimental data of phonon's classification and optical transitions in terms of the TRS in some wurtzite crystals ZnO, GaN and others.

The role of point symmetry in electron(ic) bound states on defects in magnetic semiconductors

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We analyze elecrically active defects (such as the vacancies V_A created by missing ions A) in the magnetic semiconductors. The defects cannot be considered shallow or hydrogenic impurities. There is ample empirical evidence that they can influence strongly both the charge transfer in the affected system and the latter's magnetic properties. In order to interpret the empirical data, we find single-electron eigen-states of appropriate ionic clusters with and without missing atoms. The point symmetry of the clusters is essentially employed in a determination of the electron eigen-states.

Duality of Weyl and electron states in acene

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Organic materials have been recently the object of the intense studies due to their opto-electronic properties. They follow from the states of the outer-shell electrons which take part in molecule bonding. The symmetry of molecules provides the classification of energy states according to the group theory method. We apply Weyl Duality scheme for energy structure classification of selected acenes.

Symmetric and asymmetric dispersion relation for carbon nanotubes

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The standard tight-binding dispersion relation for graphene and carbon nanotubes has an electron-hole symmetry. This symmetry has not been observed experimentally until recently. Moreover, if the overlap between pi-orbitals on neighbouring carbon atoms is taken into accout, the dispersion relation is indeed asymmetric. We estimate the observable effects of this asymmetry on the DOS, seen in conductivity measurements and explain the symmetry found in the experiment. The amount of the overlap influences also the dependence of CN's magnetic susceptibility on the temperature.

Monte Carlo Study of Background Field Ising Model and the Yang Lee Singularity

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A method is presented for performing Monte Carlo simulations on spin models having background fields. The method is used to study a critical point at a nonzero value of the magnetic field. In particular, the method is used to study the Yang Lee edge singularity of the Ising model.

Unexpected magnetism in low dimensional systems: the role of symmetry

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The geometric structure and the underlying symmetry of a solid are probably their most fundamental characteristics, because understanding the physical properties of almost any state of matter usually requires a detailed knowledge of the relative positions of atoms. In fact, pure geometrical arguments are encountered in almost any analysis of Condensed Matter Physics. When dimensionality is reduced, the role of geometry and symmetry might be crucial and can give rise to new phenomena. In this talk we will show that low dimensional systems, as carbon nanotubes or surfaces of non-magnetic ionic insulators, present a magnetic ground state.

Carbon nanotubes constitute a new class of 1D systems, in which physical properties are intimately related to geometry. They can be metals or semiconductors depending on their diameter and chirality. Further, chiral tubes present spin-splitting at the Fermi level in the absence of a magnetic field, whereas achiral tubes preserve spin degeneracy, as evidenced by tight-binding electronic structure calculations with the inclusion of spin-orbit interaction. These remarkably different behaviors of chiral and nonchiral nanotubes have a symmetry origin.

On the other hand, the occurence of spin-polarization at ZrO_2, Al_2O_3 and MgO surfaces is proved by means of *ab-initio* calculations within the density functional theory. Large spin moments, as high as 1.56 μ_B, develop at O-ended polar terminations, transforming the non-magnetic insulator into a half-metal. The magnetic moments mainly reside in the surface oxygen atoms and their origin is related to the existence of $2p$ holes of well-defined spin polarization at the valence band of the ionic oxide. The direct relation between magnetization and local loss of donor charge shows that the magnetization is a direct consequence of the loss of coordination of Oxygen atoms rooted in the lower symmetry of the surface.

Rapid Magnon Relaxation

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The standard procedure for calculating life-times of magnons is to construct equations of motion for magnon occupancy numbers and to solve them for a state of a weak departure from equilibrium. In the last decade a number of experiments used pulse techniques to study dynamics of magnetization after very short pulses bringing magnetic systems out of equilibrium. Therefore a relevant question is how magnons relax after a short strong pulse of magnetic field. The three- and four-magnon relaxation processes are discussed. It is shown that the inverse relaxation time ia a short interval after a strong perturbation is enhanced by a temperature independent contribution , depending on the strength of the perturbation.

On LCAO Positron Wavefunctions in Crystals

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In this work we deal with the construction of delocalized positron wavefunctions in crystalline solids within the linear combination of atomic orbitals (LCAO) scheme.

The present method leads to an accurate wavefunction of a positron, both in the core and in the interstitial region of a crystal. Furthermore, its representation by a superposition of atomic orbitals is simple enough for the application to calculations of expectation values, like e.g. of accurate electron-positron annihilation rates (high momentum components).

The representation of the positron wavefunction can be optimized with respect to the two points of view: Firstly, the number of orbitals in the LCAO ansatz can be minimized (e.g. within the localized spherical orbitals (LSO) method) and, secondly, the orbitals can be chosen to be very localized around their atoms and vanishing near all others: This leads to the computational advantage, that no three- or multicenter integrals have to be evaluated during the numerical calculations. The one- and two-center integrals, on the other hand, can be treated using standard numerical techniques in spherical polar or elliptic coordinates. The transformation from the first into the second representation can be performed via a "fuzzy" cellular partitioning of the crystal volume via an analytically continuous shape-function.

Finally we demonstrate our method in the case of a positron in lithium.

Symmetry of the pentacene molecule studied in the frame of the group action on a set

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Pentacen is very important material in the application of polymers in electronic. The pentacene molecule can be treated as a chain of benzen rings or as two conjugated polyethylene chains. In both cases the whole symmetry is described by L2/mcm line group. In the paper we determine strata, epikernels, and related terms which adress the whole geometrical properties of the molecule.

Noether's theorem and low symmetry aspects concerning the crystal (ligand) field Hamiltonians and spin Hamiltonians

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This review consists of two parts. The first part deals with the applications of Noether's theorem to the crystal/ligand field (CF/LF) Hamiltonians and spin Hamiltonians invariant under continuous rotational symmetry, i.e. hexagonal II, tetragonal II, trigonal II, monoclinic, and triclinic ones. Interrelationships and deeper meaning of the following concepts: (i) Noether's theorems, (ii) the algebraic symmetry of Hamiltonians, and (iii) the rotational invariants and moments of CF Hamiltonians, are considered. An important theorem and a conjecture on the conserved quantities stipulated by Noether's theorem for the Hamiltonians in question are formulated. Geometrical meaning of the second-order conserved quantities suggests feasibility of derivation of a conservation law encompassing all the conserved quantities identified. The existence of the conserved quantities has profound implications for interpretation of experimental CF parameter datasets, which are encapsulated in five corollaries. Our considerations reveal that various aspects, which have not been fully realized in the literature as yet, require reinterpretation. This includes, e.g., (i) the feasibility of determination of CF parameters from fitting experimental spectra, and (ii) the reduction of the existing higher-order rotational invariants for hexagonal type II symmetry and cubic symmetry to combinations of primary lower-order invariants. Our novel approach enables adoption of better fitting strategies utilizing the well-defined conserved quantities, which are invariant under continuous rotational symmetry, as well as clarification of the inconsistencies between the crystal-field parameter (CFP) datasets reported in literature for various low symmetry transition-ion host systems. The second part deals with the fundamental intricate aspects, hitherto not fully understood, concerning the Hamiltonians for the 'low symmetry' cases, including the continuous rotational symmetry cases, as defined above, as well as orthorhombic ones. This includes: (1) selection of the axis systems, (2) types of CF parameters and their properties, (3) introduction of a new notion of a nominal axis system for the fitted CFP datasets, (4) implications of the Noether's theorem and the algebraic symmetry of CF Hamiltonians, (5) correlation properties among CFP datasets, (6) the rotational degrees of freedom and the reduction of the number of independent CFP's, which are of special importance for triclinic symmetry cases, and (7) extension of the multiple correlated fitting tech-

nique, including a quantitative method for CFP datasets comparison. Clarification of these intricate aspects enables us to provide a general framework aimed at achieving an increased compatibility and reliability of CFP datasets for transition ions at low symmetry sites in crystals. This framework may be especially useful for trivalent lanthanides in technologically important low symmetry hosts for which only limited energy-level data are available.

Symmetry analysis of quadrupolar, structural and magnetic ordering in UPd3

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In the present analysis the ordering of electric quadrupole components and possible deformation of the ionic potentials in quadrupolar phase transitions in crystals are investigated by the symmetry analysis method. The components of quadrupole moment tensor (QMT) are usually defined as

$$Q_{ij} = \int (3x_i x_j - \rho^2 \delta_{ij}) q(\vec{\rho}) d^3x$$

where $q(\vec{\rho})$ is the charge density distribution. The matrix of QMT is symmetrical and traceless. The QMT matrix can be brought to principal axes ,which may be treated as symmetry-adapted local coordinate system. Then the matrix takes the simplest form: only three values on the diagonal are nonzero and only two of them are independent. For an initial spherical potential QMT defines its deviations from the spherical form, related to existence of nonzero quadrupole moment. The quadrupolar ordering concept is intended to characterize, at all atomic positions in the crystal, the spatial shape of the surface associated with the quadrupole potential contribution and the orientation of QMT principal axes in relation to the crystallographic system. The signs of QMT components characterize the type of deformation and their values characterize the deformation magnitudes. By the symmetry analysis method all types of quadrupolar ordering, possible for given parent structure, are calculated, together with their resulting final symmetry groups. An additional symmetry analysis is also carried out to determine the possible patterns of atomic displacements of the neighboring atoms, and the ordering of the magnetic moments, which are consistent with the symmetry imposed by the quadrupolar ordering. The symmetry analysis method derived from the theory of group and representations [Yu.A. Izyumov, and V.N. Syromyatnicov, "Phase transitions and Crystal Symmetry, (1990), Dordrecht: Kluwer] is based on the decomposition of full representation of the crystal space group, calculated for a given wave vector k, into its irreducible representations (IR). The final ordering pattern is composed as a linear combination of basis vectors (BV) of the irreducible representations. The investigation of quadrupolar ordering based on symmetry analysis and the output data from MODY-win program [W.Sikora at all. J.Appl. Cryst. 37, (2004), 1015] does not deliver absolute values of potential deformations, since the coefficients received from the program define the QMT matrix except for an arbitrary multiplication

factor. The essential results of the symmetry analysis are the signs and ratios of QMT matrix coefficients for the considered atomic site and other sites related by the symmetry, what finally leads to the pattern of quadrupolar ordering. In the presented work the method is applied to quadrupolar and magnetic moment ordering of U atoms and possible patterns of atomic displacements of the neighboring Pd atoms in the hexagonal UPd3 compound. All possible types of quadrupolar ordering are calculated, together with their resulting final symmetry groups. The possible patterns of atomic displacements of the neighboring Pd atoms, and the ordering of the U magnetic moments, which are consistent with the symmetry imposed by the quadrupolar ordering, are also calculated. The models of ordered structure and discussion of corresponding sets of free parameters resulting from symmetry considerations are compared with the results of experimental investigations [D.F. McMorrow at all.,Phys.Rev.Lett, 87, (2001), 057201-1-4].

Quantum critical phenomena on an example: Localization of fermions in correlated electron systems

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I will discuss briefly the localization of electrons in the Mott-Hubbard and the Kondo-lattice systems by referring to what the experimental data show. Such an approach is enforced by the circumstance that no microscopic theory exits so far for those strongly correlated fermionic systems.

Persistent Currents in Carbon Nanotubes

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Persistent currents driven by a static magnetic flux parallel to the carbon nanotube (CN) axis are investigated. Owing to the hexagonal symmetry of graphene the Fermi contour expected for a 2D lattice reduces to two points. However, the electron or hole doping shifts the Fermi energy upwards or downwards and, as a result, the shape of the Fermi surface changes. We show that the shift of the Fermi energy changes dramatically the persistent currents and the electronic structure for zigzag as well as armchair nanotubes [1]. Persistent currents in multiwalled carbon nanotubes (MWNT's) are also investigated. The geometrical structure and possibility of the existence of MWNT's with shells in various chiral configurations are explored. The currents are calculated considering a possible Fermi energy shift by hole doping. The influence of self-inductance of different shells is taken into account. The optimal chiralities for the maximal current are found. The optimal hole doped configurations are shown to exhibit spontaneous currents in Kelvin temperatures. In the optimal diamagnetic configuration a Meissner-type effect, i.e., partial flux expulsion can occur [2]. The application of magnetic field B parallel to the tube axis can change the conducting properties of the CN from metallic to semiconducting and vice versa. Apart from that B induces (via the Bohm-Aharonov effect) orbital magnetic moments (OMM) in the nanotube. These moments are studied both in pure and hole- or electron-doped CNs, isolated or in a circuit. Remarkably, OMM in pure CNs depends uniquely on their original conducting properties, length, and temperature but it does not depend on the nanotube radius or the particular chirality. In doped nanotubes the magnetic moments can be strongly altered and depend on the radius and chirality. Temperature can even change their character from diamagnetic at low T to paramagnetic at high T. A general electron-hole asymmetry increasing with the doping is also found [3].

[1] Phys. Lett. A **299** (2002) 593-600
[2] Phys. Rev. B **70**, (2004) 075406
[3] Phys. Rev. B **72**, 1 (2005)

Symmetry and asymptotic conditions of the direct mapping and of the External potential to the Optimized Effective pottential (Applications to the eigenstates of molecules)

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In this paper, general symmetry properties of physical systems are used in order to produce a mapping of the external potential of a many electron system to its optimized effective potential OEP). The so derived effective potential is used to calculate the OEP spin orbitals. Applications are made both to open and closed shell atoms and molecules and the results are compared to those of the exact Hartree-Fock approximation. The relative deviations from the exact HF theory (E/?) are of the order of 10-4. Further there is a strong overlap between the Optimized effective potential and the Hartree-Fock many-electron wave functions. Because of the symmetry constraint imposed on the OEP potential, the many electron wave functions derived by the present method, transform according to the irreducible representations of the exact states. The Moeller Plesset perturbation theory is applied in order to calculate the correlation energy and the results found are compared with those derived by using other methods.

Effects of symmetry lowering of spin systems and comparison with experiment

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The Heisenberg Hamiltonian is a highly symmetric Hamiltonian where group theory is very effective for the qualitative as well as the quantitative study of its eigenstates. For this matter, a system of nested algebras was developed. Recently, experimental facts on magnetic materials showed that interactions lowering symmetry like the Dzialoshinski term are necessary for their interpretation. A perturbation theory is developed for such Hamiltonians and applied to experimental data with very good agreement between theory and experiment.

Magnetic translation group and classification of states of itinerant electron

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We consider an itinerant electron on two-dimensional finite square lattice in a magnetic field. A magnetic translation group (MTG) for this system with the periodic Born-Karman conditions has been introduced. The irreducible representation of MTG is used for classification of energy levels of electron states for this model.

Longitudinal normals for piezoelectric elastic media.

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We show that the problem of finding of components of longitudinal normals for all piezoelectric classes is equivalent to the problem of solving two sets of two polynomial equations up to 6th degree. It is proved that the number of longitudinal normals for triclinic media cannot exceed 36. If the number of longitudinal normals contained in any plane is finite, then it cannot be larger than 6. Directions of longitudinal normals are found for quartz, $LiNbO_3$, $LiGaO_2$, and $Ba_2NaNb_5O_{15}$. For these compounds, we numerically studied how piezoelectric terms of the propagation matrix influences the number and directions of the longitudinal normals.

Numerical Measurements of Finite-Size Scaling at Yang-Lee Singularities of 2D Spin Models

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The Hamiltonian limit of two dimensional statistical Ising and 3-state Potts models in complex magnetic field is studied numerically. The Phenomenological Renormalisation Group approach is used to locate the critical field value at Yang-Lee singularity (YLS). The low lying part of the spectrum is calculated. The pattern of the calculated energy levels and their degeneracies is compared to the predictions of the ADE classification of the Conformal Field Theory for non-unitary minimal models. We obtain a convincing identification of the YLS of the 3-state Potts model with the with the (A4, A1) minimal CFT. We also study the YLS in Ising model by similar methods confirming the identification for the YLS of that model.

The influence of entangled photons on distant persistent currents

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Two mesoscopic rings which are far from each other are considered. A source of two mode nonclassical microwaves irradiates the rings with correlated photons. Classically correlated (separable) and quantum mechanically correlated (entangled) microwaves are considered, and their effect on persistent currents is quantified by studying the correlation function of currents from distant rings.It is shown that classical or quantum mechanical photon correlations are inherited by the currents.