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A. A. Ovchinnikov I. I. Ukrainskii (Eds.)

Electron-Electron Correlation Effects in

Low-Dimensional Conductors and Superconductors

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Preface

Advances in the physics and chemistry of low–dimensional systems have been really magnificent in the last few decades. Hundreds of quasi–one–dimensional and quasi–two–dimensional systems have been synthesized and studied.

The most popular representatives of quasi–one–dimensional materials are polyacethylenes CH_x [1] and conducting donor–acceptor molecular crystals TTF–TCNQ. Examples of quasi–two–dimensional systems are high temperature superconductors (HTSC) based on copper oxides LA_2CuO_4, $YBa_2Cu_3O_{6+y}$ and organic superconductors based on BEDT–TTF molecules.

The properties of such one– and two–dimensional materials are not yet fully understood. On the one hand, the equations of motion of one–dimensional systems are rather simple, which facilitates rigorous solutions of model problems. On the other hand, manifestations of various interactions in one–dimensional systems are rather peculiar. This refers, in particular, to electron–electron and electron–phonon interactions. Even within the limit of a weak coupling constant electron–electron correlations produce an energy gap in the spectrum of one–dimensional metals implying a Mott transition from metal to semiconductor state.

In all these cases perturbation theory is inapplicable. Which is one of the main difficulties on the way towards a comprehensive theory of quasi–one–dimensional systems. – This meeting held at the Institute for Theoretical Physics in Kiev May 15-18 1990 was devoted to related problems. The papers selected for this volume are grouped into three sections.

Section 1 contains papers dealing with electron correlation problems. Applications to 2–d superconductors, a connection between 1–d Hubbard and Luttinger models, a treatment of correlations in high–T_c superconductors, the 2–d Peierls–Hubbard model giving rise to kink–antikink pairs with superconducting condensation and the optical spectra of superconducting copper–oxides are discussed. *Section 2* provides information on progress in the understanding of Mott–Peierls semiconductor polymers, on the way in which electron–electron correlations affect the properties of polymers and a description of a new approach to the study of electron–electron correlations in large molecules and polymers. *Section 3* deals with correlation effects in magnetization and kinetics including some features of the 2–d Hubbard model.

Kiev,
December 1990

A.A. Ovchinnikov
I.I. Ukrainskii

V. E. Zakharov (Ed.)

What is Integrability?

With the contributions by numerous experts

1991. XIV, 321 pp. 1 fig. (Springer Series in Nonlinear Dynamics) Hardcover
ISBN 3-540-51964-5

This monograph deals with integrable dynamic systems with an infinite number of degrees of freedom. Leading scientists were invited to discuss the notion of integrability with two main points in mind:

1. a presentation of the various recently elaborated methods for determining whether a given system is integrable or not;
2. to understand the increasingly more important role of integrable systems in modern applied mathematics and theoretical physics.

Topics dealt with include: the applicability and integrability of "universal" nonlinear wave models (Calogero); perturbation theory for translational invariant nonlinear Hamiltonian systems (in 2+1d) with an additional integral of motion (Zakharov, Schulman); the role of the Painlevé test for ordinary (Ercolani, Siggia) and partial differential (Newell, Tabor) equations; the theory of integrable maps in a plane (Veselov); and the theory of the KdV equation with non-vanishing boundary conditions at infinity (Marchenko).

A. Hasegawa

Optical Solitons in Fibers

2nd enl. ed. 1990. XII, 79 pp. 25 figs. Softcover ISBN 3-540-51747-2

Already after six months high demand made a new edition of this textbook necessary. The most recent developments associated with two topical and very important theoretical and practical subjects are combined: **Solitons** as analytical solutions of nonlinear partial differential equations and as lossless signals in dielectric **fibers.** The practical implications point towards technological advances allowing for an economic and undistorted propagation of signals revolutionizing telecommunications. Starting from an elementary level readily accessible to undergraduates, this pioneer in the field provides a clear and up-to-date exposition of the prominent aspects of the theoretical background and most recent experimental results in this new and rapidly evolving branch of science. This well-written book makes not just easy reading for the researcher but also for the interested physicist, mathematician, and engineer. It is well suited for undergraduate or graduate lecture courses.

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B. N. Zakhariev, A. A. Suzko

Direct and Inverse Problems

Potentials in Quantum Scattering

1990. XIII, 223 pp. 42 figs. Softcover ISBN 3-540-52484-3

This textbook can almost be viewed as a "how-to" manual for solving quantum inverse problems, that is, for deriving the potential from spectra and/or scattering data. The formal exposition of inverse methods is paralleled by a discussion of the direct problem.
In part differential and finite-difference equations are presented side by side. A variety of solution methods is presented. Their common features and (dis)advantages are analyzed. To foster a better understanding, the physical meaning of the mathematical quantities are discussed in detail.
Wave confinement in continuum bound states, resonance and collective tunneling, and the spectral and phase equivalence of various interactions are some of the physical problems covered.

V. B. Matveev, M. A. Salle

Darboux Transformations and Solitons

1991. IX, 120 pp. 12 figs. (Springer Series in Nonlinear Dynamics)
Hardcover ISBN 3-540-50660-8

In 1882 Darboux proposed a systematic algebraic approach to the solution of the linear Sturm-Liouville problem. In this book, the authors develop Darboux's idea to solve linear and nonlinear partial differential equations arising in soliton theory: the nonstationary linear Schrödinger equation, Korteweg-de Vries and Kadomtsev-Petviashvili equations, the Davey-Stewartson system, Sine-Gordon and nonlinear Schrödinger equation, 1+1 and 2+1 Toda lattice equations, and many others.
By using the Darboux transformation one can construct and examine the asymptotic behavior of multisoliton solutions interacting with an arbitrary background. In particular, the approach is useful in systems where an analysis based on the inverse scattering transform is more difficult.
The approach involves rather elementary tools of analysis and linear algebra so that it will be useful not only for experimentalists and specialists in soliton theory, but also for beginners with a grasp of these subjects.

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Introduction

A.A. Ovchinnikov[1] *and I.I. Ukrainskii*[2]

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Advances in physics and chemistry of low–dimensional systems have been really magnificent in the last few decades. Hundreds of quasi–one–dimensional and quasi–two–dimensional systems have been synthesized and studied. The Properties of those materials attracted physicists, chemists and engineers.

The most popular representatives of quasi–one–dimensional materials are polyacethylenes CH_x [1] and conducting donor–acceptor molecular crystals TTF–TCNQ [2].

One of the promising families relates to quasi–two–dimensional systems are new high temperature superconductors (HTSC) based on copper oxides LA_2CuO_4, $YBa_2Cu_3O_{6+y}$ [3] and organic superconductors based on BEDT–TTF molecules [4].

Quantum processes in low–dimensional systems are characterized by a number of peculiarities. This fact results in the development of special methods of theoretical studies in low–dimensional phenomena. We describe this problem now for one–dimensional (1–d) systems. In one–dimensional physics and chemistry there is a number of certain difficulties and some of them are far from being overcome. On the one hand, motion equations in one–dimensional systems are much simpler. This facilitates rigorous solution of a model problem which is often impeded by a large number of dimensions. On the other hand manifestations of various interactions in one–dimensional systems are rather peculiar. This refers, in particular, to electron–electron and electron–phonon interactions. The perturbation theory is inapplicable in both cases. Thus, electron–phonon interaction leads to field localization of electron excitation in one–dimensional system which results in soliton excitations and Peierls deformation. Calculations of soliton excitation can not be done by decomposition in the series of electron–phonon coupling constant.

Electron–electron interactions, even within the limit of a weak coupling constant, produces an energy gap in the spectrum of one–dimensional metal which means the Mott transition from metal to semiconductor state. And in this case the perturbation theory is inapplicable.

Similar situation occurs in one–dimension with respect to electron–impurity interactions. Started by Mott and Twose theoretical studies of this problem show that all one–electron states in 1–d disordered system are localized and, hence, cannot be calculated using the perturbation theory. State localization turns the direct current conductivity into zero.

Inapplicability of the perturbation theory is one of the main difficulties on the way to accomplish the theory of quasi–one–dimensional systems.

These difficulties were being surpassed in different ways.

Regarding electron–phonon interaction the most fruitful method is is to reduce the set of equations into a completely integrable system which can be the nonlinear Schrödinger equation, the sine–Gordon equation and others.

Advances in description with respect to electron–electron interactions turned out to be less pronounced however more yielding regarding the physics of 1–d systems. The major reason for it lies in well–known complications of the many–electron theory for systems with an infinitely number of electrons.

Quantum chemistry and, in particular, the theory of many–electron systems are based upon the Hartree–Fock approximation. Making a joke theoreticians often rephrase the saying "the word came first" into "the Hartree–Fock approximation came first".Then various many–electron theories appeared where the wave function must be represented not by one Slater determinant but an infinite series of these determinants. And if the number of particles in the system grows as $N(N \to \infty)$ then the number of terms in this infinite series must increase at least as e^{an}, where a is a constant $(a \approx 1)$. This particular infinite complication of the theory is the main hindrance for its wide application in calculations. One of the objectives of the present book is to show , however that very often these difficulties are being considerably exaggerated. As a rule, having analyzed the Hamiltonian of the system under study using the many–electron theory one can reduce the problem to a simpler Hamiltonian or, or without any loss in quality construct multiconfigurational wave function of the system which can be factorized into an antisymmetrized product of one– or two–electron wave functions. As approximations for a wave function, besides the extended Hartree–Fock approximation (EHF) described in details in [1], the spinless fermion approximation in case of strong interactions and the variable localized geminals approximation (VLG) can be mentioned [5].

In the EHF and spinless fermion approximations a many–electron wave function is finally factorized into the product of single–particle functions (orbitals), and in the VLG approximation the factorization into the product of two–particle functions (geminals) is done.

Now we draw the reader's attention to another aspect of the theory of quasi–one–dimensional systems. Real systems with one–dimensional anisotropy are, in fact, three–dimensional. In case of a theoretical study it is expedient to mentally separate a 1–d subsystem out of the real system using its specific features.

The separation of a quasi–one–dimensional subsystem goes naturally through analysis of the total Hamiltonian represented by the sum

$$\widehat{\mathcal{H}} = \sum_{n} \widehat{\mathcal{H}}_{n} + \frac{1}{2} \sum_{n,m} \widehat{V}_{n,m} \, , \tag{1}$$

where $\widehat{\mathcal{H}}_{n,m}$ is the Hamiltonian of a $\boldsymbol{n}$-th quasi–one–dimensional substructure (filaments needles, chains or stacks), and operators $\widehat{V}_{n,m}$ describe its interactions with other quasi–one–dimensional subsystems.

Further we assume that the interaction operators include no terms responsible for electron exchange between separate quasi–one–dimensional subsystems. And this predetermines the subdivision of the Hamiltonian into the sum (1). This approximation provides satisfactory description of polyacethylenes, donor–acceptor molecular conducting crystals and many other quasi–one–dimensional systems.

Before we start to consider particular expressions for the Hamiltonians of electron–phonon systems under study it is worthwhile to note the following.

Most processes of interest in quasi–one–dimensional systems are determined by the energy spectrum and the nature of elementary excitations of these systems. The low–energy region of the spectrum is mainly related to a small part of the total number of the system electrons. This facilitates a rigorous enough description of electron processes occurring in these systems. Say, most interesting properties of polyacethylenes originate from the π–electrons number equals the number of carbon atoms and essentially less than the total number of electrons in the system.

Studying most significant properties of donor–acceptor molecular conducting crystals it suffices to consider one electron only per a donor–acceptor pair. For a TTF–TCNQ crystal it means that only one electron out of 208 is to be considered.

A similar situation occurs in other quasi–one–dimensional systems.

A reduced number of the degrees of freedom of the system requires a model Hamiltonian parameters of such a Hamiltonian are to be obtained from experiments on related systems.

In terms of quantum chemistry we should use semi–empirical methods.

Coming back to close similarity in the quantum chemistry and the theory of conjugated molecules and polymers, we write down a well known Hückel–Pople (HP) Hamiltonian [1]

$$\begin{aligned} \mathcal{H} = {} & \sum_{mm'\sigma} \beta_{mm'} c^{+}_{m\sigma} c_{m'\sigma} + \sum_{m} \alpha_{m} c^{+}_{m\sigma} c_{m\sigma} + \\ & \frac{1}{2} \sum_{mm'\sigma} \gamma_{mm'} c^{+}_{m\sigma} c_{m\sigma} c^{+}_{m'\sigma} c_{m'\sigma} \, , \end{aligned} \tag{2}$$

where $c^+_{m\sigma}$ is an electron creation operator on the m–th site with the spin σ. The HP Hamiltonian allowed to study most interesting properties of molecules with conjugated bonds.

As a rule, in (2) it suffices to consider electron hopping (a resonance term) for adjacent atoms only, that is

$$\beta_{mm'} = \beta(R_{m,m'})\delta_{m',m+1} \ , \tag{3}$$

where $R_{m,m'}$ is the distance between m-th and m'-th atoms. To obtain a qualitatively correct description of most effects one can use in the electron interaction operator (the second term in (2)) only first several terms. A most frequently used approximation is that of Hubbard–Anderson (HA)

$$\gamma_{mn} = \gamma_0\delta_{mn} \ . \tag{4}$$

Sometimes it is of importance to consider electron interactions of the neighboring atoms, that is, to assume

$$\gamma_{mn} = \begin{cases} \gamma_0\delta_{mn} \ , \\ \gamma_1\delta_{m\pm1,n} \ . \end{cases} \tag{5}$$

The values of a resonance integral (3) is a function of the distance between the m–th and $(m+1)$–th sites. In conjugated molecules it is sufficient to use the first term of this function expansion in the vicinity of $R = R_0 = 1.397$ Åcorresponding to the c–c bond length in benzene

$$\beta(R) = \beta_0 - (R - R_0)\beta' \ . \tag{6}$$

The approximations (3)–(6) suffice to study a great number of experiments except for dynamic (and kinetic) properties of quantum–one–dimensional systems to explicitly account for vibrational degrees of freedom. This is done by adding to the Hamiltonian (2) the phonon Hamiltonian

$$\mathcal{H}_{\text{ph}} = \sum_{ki} \hbar\Omega_{ki}(b^+_{ki}b_{ki} + \frac{1}{2}) \ , \tag{7}$$

where b^+_{ki} is a phonon creation operator of the i–th mode with a quasi–momentum k.

Starting from (6), the operator of electron–phonon subsystem interactions is chosen like that suggested by Fröhlich

$$\mathcal{H}_{\text{e-ph}} = \sum_{kq} \lambda_{qi}(b^+_{q,i} - b_{-q,i})a^+_{k,\sigma}a_{k+q,\sigma} \ , \tag{8}$$

where a constant λ_{ki} is proportional to the β derivative with respect to R, that is β' in (6).

Like other cases, for quasi–one–dimensional systems it is often sufficient to use only the classical form of the phonon part of the Hamiltonian