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Metal-to-Nonmetal Transitions

With 76 Figures

Springer

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Springer Series in Materials Science ISSN 0933-033X
ISBN 978-3-642-03952-2 e-ISBN 978-3-642-03953-9
DOI 10.1007/978-3-642-03953-9
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2009943834

Cover design: SPi Publisher Services

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

Materials can be divided into metals and nonmetals. The characteristic feature of metals like copper and aluminum is a high electrical and thermal conductivity, while nonmetals such as phosphor and sulfur are insulators. The electrical conductivity varies over many orders of magnitude, from $10^6\,\Omega^{-1}\,\mathrm{m}^{-1}$ for typical metals down to $10^{-20}\,\Omega^{-1}\,\mathrm{m}^{-1}$ for almost ideal insulators. However, a sharp separation between metals and insulators is in general not possible. For instance, semiconducting materials such as silicon and germanium fill the conductivity domain between metals and insulators. Their electrical conductivity is dependent on temperature and, in addition, can be varied strongly by doping the material with donor or acceptor atoms. A famous example is the sharp insulator-to-metal transition measured in Si:P at temperatures below 0.1 K and donor concentrations of about $3.8 \times 10^{18}\,\mathrm{cm}^{-3}$ phosphor atoms [1].

Furthermore, materials may exist in both states: carbon is metallic as graphite and insulating as diamond. A fascinating quantum effect is observed at low temperatures: some materials even loose their electrical resistivity and become superconductors. Therefore, the questions *What is a metal?* and *When does a metal transform into a nonmetal?* are of fundamental interest and related to many aspects of modern physics and chemistry. We refer the interested reader to the very nice introduction into this diverse topic given by Edwards [2].

This book offers a collection of reviews on nonmetal-to-metal (or metal–insulators or Mott transitions) in very different physical systems, from solids with a regular periodic structure via disordered fluids and plasmas, finite metal clusters up to exotic nuclear and quark matter. The surprising similarity in the behaviour of these very diverse systems is due to the complex many-body nature of the respective interactions, which drives the transition and entails a non-perturbative treatment. Therefore, the Mott transition can be regarded as a prominent test case for methods of non-perturbative many-body physics. This book aims to give an overview on the current status of the theoretical treatment of Mott transitions and new experimental progress and findings in these fields as well.

In his original work, Mott [3] initiated the detailed discussion of metal–insulator transitions with an analysis of the critical screening length required to trap an electron around a positive ion in a solid from which he derived the relation $n^{1/3}a_{\mathrm{B}} = 0.2$. This famous Mott criterion has been very successful in describing metal–insulator transitions in various ordered systems, for example solids and doped semiconductors. Then Hubbard [4] introduced his today well-known and intensively studied model such that interactions between electrons are accounted for only when they are on the same site – via the repulsive Hubbard U term. Considering disordered systems, Anderson [5] could show that at a certain degree of disorder all electrons will be localized and the system becomes non-conducting.

These basic models contain important physical effects such as screening, repulsive on-site electron–electron interactions and disorder in a clear conceptual way and were, therefore, studied extensively. Details can be found in earlier reviews on this topic [6–9]. In real physical systems, we have to treat *all* relevant correlation and quantum effects to account for finite temperatures and thus thermal excitations and, where applicable, to include the influence of disorder as well. The simultaneous occurrence of correlations and disorder and their mutual interplay is of major importance in this context as has long been stressed by Mott. The construction and evaluation of respective Mott–Hubbard–Anderson-type models is one of the most challenging problems of many-body physics, see for example [10, 11].

The transition from a non-conducting to a conducting state in, for example electron–ion systems is connected with a change in the electronic wave function from being localized on a single atom or at few sites to a delocalized state. Landau and Zeldovich proposed already in 1943 that this electronic transition could introduce additional lines of first-order transitions in the phase diagram of the fluid state [12]. Their prediction has stimulated precise measurements of the liquid–vapour phase transition in metallic fluids such as mercury up to the critical point, see [13]. A new interpretation of data for the combined liquid–vapour and metal-to-nonmetal transition in mercury is given in Chap. 2. Furthermore, this electronic transition may have a strong impact on the high-pressure phase diagram of, for example hydrogen as the simplest and most abundant element [14, 15]. Extreme states of matter, that is pressures of several megabar and temperatures of many thousand Kelvin, occur in the interior of giant planets in our solar system as well as in extrasolar giant planets, which have been detected in great number. A better understanding of their formation processes, their current structure and evolution is intimately related to the high-pressure equation of state and the location of phase transition lines in fluid hydrogen–helium mixtures, see also Chap. 4.

It is obvious that the energy spectrum of electron–ion states, which contains in general a series of bound states at discrete, negative energies as well as a continuum of scattering states at positive energies, plays a central role for the understanding of the metal–nonmetal transition. The energy spectrum can be calculated by solving effective two-particle Schrödinger or

Bethe–Salpeter equations, which contain the correlation and quantum effects in a strongly coupled system via a perturbative treatment, or within improved self-consistent schemas such as the GW approximation, see [16–18]. In particular, the properties of *bound states* (formation, life time and dissolution) have been studied extensively in partially ionized plasmas as function of density and temperature.

Bound states in Coulomb systems are atoms (excitons) in electron–ion (electron–hole) plasmas and fluids. This concept can be generalized to nuclear matter where deuterons or alpha particles as found in neutron stars or in heavy ion collisions are bound states composed of nucleons that interact via effective nucleon–nucleon potentials. Bound states occur also in quark matter as diquark (e.g. pi-meson) or three-quark states (nucleons). The transition to a quark–gluon plasma can then be interpreted as the dissolution of all respective multi-quark states, similar to the transition from a partially to a fully ionized electron–ion or electron–hole plasma. Driving force is in all cases an increase in pressure or density. Thus, the original concept of Mott has found wide applications beyond traditional Coulomb systems, and the respective Mott transition is intensively studied.

In the following chapters, we present reviews on the Mott transition in these various systems, which will address the specific questions as well as the general problems. We start in Chap. 1 with a description of quantum phase transitions in strongly correlated one-dimensional electron–phonon systems and a detailed discussion of the models of Luttinger, Peierls and Mott. A new inspection of the metal–nonmetal transition in fluid mercury is given in Chap. 2, which has revealed a non-congruent nature for the first time. This might have consequences also for other predicted first-order phase transitions such as the hypothetical plasma phase transition in warm dense matter (see Chaps. 3 and 4), various phase separations in dusty plasmas, or the exotic phase transitions in neutron stars (see Chaps. 6 and 7). Various aspects of the Mott effect in dense fluids and plasmas have been treated up to now, but Pauli blocking as a direct quantum statistical effect is a novel topic and will be discussed in Chap. 3 within a chemical model. The metal–insulator transition in dense hydrogen is of primary importance for modeling interiors of Jupiter-like giant planets. A confrontation of advanced chemical models with quantum molecular dynamics simulations within a strict physical picture is performed in Chap. 4. The so far hypothetical plasma phase transition is discussed both in Chap. 3 and in Chap. 4. Metal–insulator transitions can also be induced in small metal clusters by irradiation with intense and short laser pulses. The highly effective energy deposition by resonance absorption, the various ionization processes (tunnel, field, impact) and the subsequent Coulomb-driven cluster explosion process are described in Chap. 5. The Mott effect in nuclear matter is reviewed in Chap. 6 within a cluster mean-field approximation. For instance, the formation of a two-nucleon quantum condensate is observed. The properties of the condensate are strongly influenced by the bound states immersed in the dense medium, that is by the Mott

effect. A quantum field theory for the understanding of the phase diagram of exotic quark matter is outlined in Chap. 7. The crossover between Bose–Einstein condensation of diquark bound states and condensation of diquark resonances is discussed in close relation to the usual Mott effect.

At this point, we express our greatest respect to the enormous and pioneering work of Sir Nevil Mott. Without his outstanding contributions, our knowledge of fundamental interaction and correlation effects in various fields of physics would be much poorer today. His work has inspired many physicists worldwide, among them also theory groups in Germany, especially in Rostock, Greifswald and Berlin, who have developed new concepts based on Mott's ideas for the metal–insulator transition in fluids and plasmas as well as in nuclear and quark matter. Therefore, it was self-evident to celebrate Mott's 100th birthday on 30 September 2005 at the University of Rostock by dedicating an International Workshop to the subject of *Nonmetal–Insulator Transitions in Solids, Liquids and Plasmas*; participants of the meeting are shown in Fig. 1. The contributions to this book are mainly based on lectures given on that occasion or were invited afterwards:

Fig. 1. Participants of the International Workshop in Rostock on the occasion of Mott's 100th birthday on 30 September 2005 (from *left* to *right*): F. Hensel, B. Holst, D. Semkat, N. Nettelmann, A. Kietzmann, A. Kleibert, J. Adams, A. Bechler, M. French, T. Fennel, R. Egdell, K.-H. Meiwes-Broer, T. Döppner, W. Ebeling, J. Berdermann, T. Bornath, H. Reinholz, W.-D. Kraeft, V. Schwarz, H. Stolz, R. Ludwig, G. Röpke, R. Redmer, A. Weiße and D. Kremp.

- P.P. Edwards (Oxford): Phase Separation in Metal–Ammonia Solutions: Was Mott, or was Ogg Correct?
- R. Egdell (Oxford): Electron Spectroscopy and Metal-to-Nonmetal Transitions in Oxides
- H. Stolz (Rostock): Mott Effect and Bose–Einstein Condensation in Dense Exciton Systems
- G. Röpke (Rostock): Mott Effect in Nuclear Matter: Formation of Deuterons at Finite Temperature and Density
- W. Ebeling (Berlin): On Coulombic Phase Transitions
- F. Hensel (Marburg): Electronic Transitions in Liquid Metals
- K.-H. Meiwes-Broer (Rostock): Metal–Insulator Transitions in Expanding Clusters
- R. Redmer (Rostock): Metal–Nonmetal Transition in Dense Plasmas

We thank all contributors to this book for the careful preparation of their manuscripts. Finally, the project could be finished successfully and we thank all authors for their patience and for staying tuned to the project until the end. We thank Peter Edwards for his interest and the continuing support.

We thank the Deutsche Forschungsgemeinschaft (DFG) for support within the SFB 652, especially for the organization of the Workshop in 2005. Finally, we thank the Spinger-Verlag for supporting our project and, especially, Mr. Balamurugan Elumalai for the excellent mentoring of the edition of this book.

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Rostock
February 2010

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1

Luttinger, Peierls or Mott? Quantum Phase Transitions in Strongly Correlated 1D Electron–Phonon Systems

Holger Fehske and Georg Hager

Abstract. We analyse the complex interplay of charge, spin, and lattice degrees of freedom in one–dimensional electron systems coupled to quantum phonons. To this end, we study generic model Hamiltonians, such as the Holstein models of spinless fermions, the Holstein–Hubbard model and a Heisenberg spin-chain model with magneto-elastic interaction, by means of an unbiased numerical density–matrix renormalisation group technique. Thereby particular emphasis is placed on the Luttinger–liquid charge–density-wave, Peierls–insulator Mott-insulator, and spin–Peierls quantum phase transitions.

1.1 Introduction

The way a material evolves from a metallic to an insulating state is one of the most fundamental problems in solid state physics. Apart from band structure and disorder effects, electron–electron and electron–phonon interactions are the driving forces behind metal–insulator transitions in the majority of cases. While the so-called Mott–Hubbard transition [1] is caused by strong Coulomb correlations, the Peierls transition [2] is triggered by the coupling to vibrational excitations of the crystal. Both scenarios compete in a subtle way. As a result, quantum phase transitions (QPT) between insulating phases become possible. Most notably this applies to quasi one-dimensional (1D) materials like conjugated polymers, organic charge transfer salts, ferroelectric perovskites, or halogen-bridged transition metal complexes, which exhibit a remarkably wide range of strengths of competing forces [3, 4]. Moreover, 1D systems are known to be very susceptible to structural distortions.

The challenge of understanding such a kind of metal–insulator or insulator–insulator QPT has stimulated intense work on generic microscopic models of interacting electrons and phonons. In this respect, the 1D Holstein–Hubbard model is particularly rewarding to study [5–10]. It accounts for a tight-binding electron band, a local coupling of the charge carriers to optical phonons, the energy of the phonon subsystem in harmonic approximation, and an intra-site Coulomb repulsion between electrons of opposite spin:

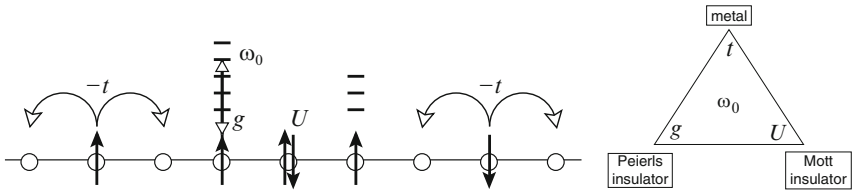

Fig. 1.1. The 1D Holstein–Hubbard model (*left panel*) and the competing ground states for the half-filled band case (*right panel*)

$$H = -t \sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} - g\omega_0 \sum_{i\sigma} (b^\dagger_i + b_i) n_{i\sigma} + \omega_0 \sum_i b^\dagger_i b_i + U \sum_i n_{i\uparrow} n_{i\downarrow} \,. \quad (1.1)$$

Here $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) a spin-σ electron at Wannier site i of a 1D lattice with N sites, and $b^\dagger_i$ (b_i) are the corresponding bosonic operators for a dispersionsless phonon with frequency ω_0.

The physics of the Holstein[1]–Hubbard[2] model is governed by three competing effects: the itinerancy of the electrons ($\propto t$), their on-site Coulomb repulsion ($\propto U$), and the local electron–phonon (EP) coupling ($\propto g$). As the EP interaction is retarded, the phonon frequency (ω_0) defines a further relevant energy scale (see Fig. 1.1). This advises us to introduce besides the adiabaticity ratio, ω_0/t, two dimensionless coupling constants

$$u = U/4t \quad \text{and} \quad g^2 = \varepsilon_\mathrm{p}/\omega_0 \quad \text{or} \quad \lambda = \varepsilon_\mathrm{p}/2t \,. \quad (1.2)$$

Both Holstein and Hubbard interactions tend to immobilise the charge carriers. Therefore, Peierls insulator (PI) or Mott insulator (MI) states are expected to be favoured over the metallic state, at least for the half-filled band case ($\sum_{i,\sigma} n_{i\sigma} = N_\mathrm{el} = N$) and at zero temperature. Strictly speaking, this holds in the adiabatic limit ($\omega_0 = 0$) for 'U-only' (Hubbard model) and 'λ-only' (Peierls model) parameters. For the more general Holstein–Hubbard model, the situation is much less obvious. Clearly a large phonon frequency will act against any static ordering. If insulating phases exist nevertheless, their ground-state properties will depend on ω_0 and on the ratio of Coulomb and EP interactions u/λ. Likewise, the nature of the physical excitations is puzzling as well. While one expects 'normal' electron–hole excitations in the PI phase ($U = 0$), charge (spin) excitations are known to be massive (gapless) in the MI state of the Hubbard model ($\lambda = 0$). Thus, varying the

[1] The Holstein model [11] has been studied extensively as a paradigmatic model for polaron formation in the low-density limit. For commensurate band fillings, the coupling to the lattice supports charge ordering.

[2] The Hubbard model [12], originally designed to describe ferromagnetism of transition metals, has more recently been used as the probably most simple model to account for strong Coulomb correlation effects in the context of high-temperature superconductivity.

control parameter u/λ, a cross-over from standard quasi-particle behaviour to spin-charge separation might be observed in the more general 1D Holstein–Hubbard model.

The aim of this contribution is to affirm this physical picture and the anticipated phase diagram of the 1D Holstein–Hubbard model. For these purposes we adapt Lanczos exact diagonalisation (ED) [13], kernel polynomial (KPM) [14] and density-matrix renormalisation group (DMRG) [15] methods for EP problems (for an overview see [16, 17]). These numerical techniques allow us to obtain unbiased results for all interaction strengths with the full quantum dynamics of phonons taken into account.

1.2 Luttinger–Peierls Metal–Insulator Transition

To study the metal–insulator transition in 1D EP systems, we neglect, in a first step, the spin degrees of freedom in (1.1). Even so, the resulting 1D spinless fermion Holstein model,

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j - g\omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i, \tag{1.3}$$

is, despite its seeming simplicity, not exactly solvable. It is generally accepted, however, that the model exhibits a QPT from a metallic to an insulating phase at half-filling ($N_\mathrm{e} = N/2$) [18,19]. During the last two decades, a wide range of analytical and numerical methods have been applied to map out the ground-state phase diagram in the whole $g-\omega_0$ plane [18, 20–26], with significant differences, especially in the low-frequency intermediate EP coupling regime. In the adiabatic limit ($\omega_0 \to 0$), the critical coupling $\lambda_\mathrm{c}(\omega_0)$ vanishes. In the anti-adiabatic ($\omega_0 \to \infty$) strong EP coupling regime, the model can be transformed to the exactly solvable XXZ model [18,23], which shows a transition of Kosterlitz–Thouless type.

Before we determine the metal–insulator phase boundary, let us characterise the metallic and insulating phases themselves. According to Haldane's Luttinger liquid (LL) conjecture [27], an 1D gapless (metallic) system of interacting fermions should belong to the Tomonaga–Luttinger universality class [28,29]. As the Holstein model of spinless fermions is expected to be gapless at weak couplings g, the system is described by (non-universal) LL parameters u_ρ (charge velocity) and K_ρ (correlation exponent).

In the following, we try to determine u_ρ and K_ρ by large-scale DMRG calculations. To leading order, the charge velocity and the correlation exponent is related to the ground-state energy of a finite system with N sites

$$\frac{E_0(N)}{N} = \varepsilon_0(\infty) - \frac{\pi}{3}\frac{u_\rho}{2}\frac{1}{N^2} \tag{1.4}$$

($\varepsilon_0(\infty)$ denotes the bulk ground-state energy density) and the charge excitation gap

$$\Delta_{\rm c}(N) = E_0^{\pm}(N) - E_0(N) = \pi \frac{u_\rho}{2} \frac{1}{K_\rho} \frac{1}{N} \tag{1.5}$$

(here $E_0^{\pm}(N)$ is the ground-state energy with ± 1 fermion away from half-filling $n = N_{\rm el}/N = 0.5$). Note that the LL scaling relations (1.4) and (1.5) were derived for the pure electronic spinless fermion model only [30]. A careful finite-size analysis shows, however, that they also hold for the case that a finite EP is included [31]. Figure 1.2 shows the resulting LL parameters, exemplarily for two frequencies belonging to the adiabatic (upper left panel) and anti-adiabatic (upper right panel) regimes. Interestingly, the LL phase splits into two different regions: for small phonon frequencies, the effective fermion–fermion interaction is attractive ($K_\rho > 0$), while it is repulsive ($K_\rho < 0$) for large frequencies. In the latter region, the kinetic energy ($\propto u_\rho$) is strongly reduced and the charge carriers behave like (small) polarons. In between, there is a transition line $K_\rho = 1$, where the LL is made up of (almost) non-interacting particles. The LL scaling breaks down just at a critical coupling $g_{\rm c}(\omega_0/t)$, signalling the transition to the CDW (charge density wave) state. We find, for example $g_{\rm c}^2(\omega_0/t = 0.1) \simeq 7.84$ and $g_{\rm c}^2(\omega_0/t = 10) \simeq 4.41$.

The middle panels of Fig. 1.2 prove the existence of CDW long-range order above $g_{\rm c}$. Here the staggered charge structure factor

$$S_{\rm c}(\pi) = \frac{1}{N^2} \sum_{i,j} (-1)^j \langle (n_i - n)(n_{i+j} - n) \rangle \tag{1.6}$$

unambiguously scales to a finite value in the thermodynamic limit ($N \to \infty$). Simultaneously, $\Delta_{\rm c}(\infty)$ acquires a finite value. In contrast, we have $S_{\rm c}(\pi) \to 0$ in the metallic regime ($g < g_{\rm c}$). Note that such a finite-size scaling, including dynamical phonons, is definitely out of range for any ED calculation. The CDW at strong EP coupling is connected to a Peierls distortion of the lattice and can be classified as traditional band insulator and polaronic superlattice in the strong-coupling adiabatic and anti-adiabatic regimes, respectively.

The optical absorption spectra shown in the lower panels of Fig. 1.2 elucidate the different nature of the CDW for small and large adiabaticity ratios in more detail. The regular part of the optical conductivity,[3]

$$\sigma^{\rm reg}(\omega) = \sum_{m>0} \frac{|\langle \psi_0 | \hat{j} | \psi_m \rangle|^2}{E_m - E_0} \, \delta[\omega - (E_m - E_0)], \tag{1.7}$$

takes into account finite-frequency transitions from the ground state $|\psi_0\rangle$ to excited quasi-particle states $|\psi_m\rangle$ in the same particle sector.[4] Importantly, the current operator $\hat{j} = {\rm i}t \sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i)$ has finite matrix elements between

[3] The evaluation of dynamical correlation functions like $\sigma^{\rm reg}(\omega)$ can be carried out by means of the very efficient and numerically stable ED-KPM algorithm [14].

[4] In (1.7), $\sigma^{\rm reg}(\omega)$ is given in units of πe^2 and we have omitted an $1/N$ prefactor.

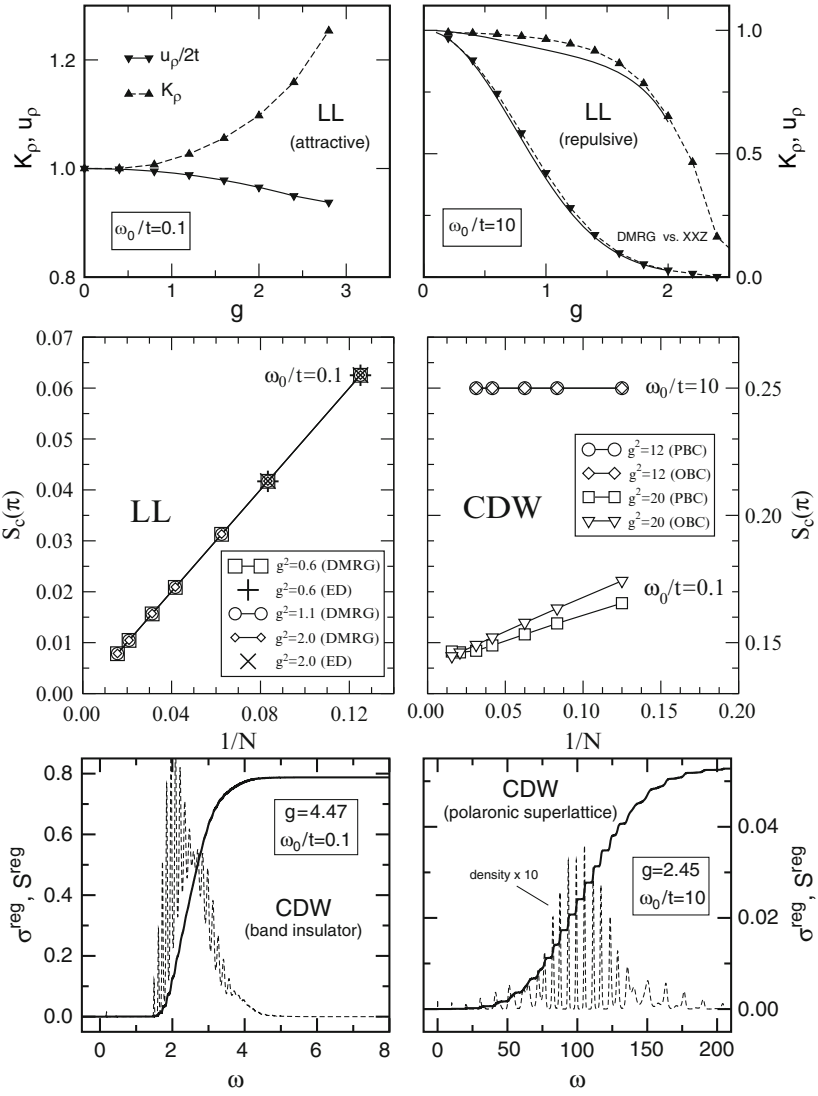

Fig. 1.2. Basic properties of the 1D half-filled spinless fermion Holstein model: Luttinger liquid parameters u_ρ and K_ρ in the metallic region (*top panels*; the *solid lines* in the right panel gives the asymptotic results for the XXZ model), finite-size scaling of the charge structure factor $S_c(\pi)$ below and above the metal–insulator transition (*middle panels*), and optical response $\sigma^{\rm reg}(\omega)$ in the CDW regime (*lower panels*). See text for further explanation

states of different site-parity only. In the adiabatic region, the most striking feature is the sharp absorption threshold and large spectral weight contained in the incoherent part of optical conductivity. In the anti-adiabatic regime,