

## Metal-to-Nonmetal Transitions

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## 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  $10^6 \Omega^{-1} \text{m}^{-1}$  for typical metals down to  $10^{-20} \Omega^{-1} \text{m}^{-1}$  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  $3.8 \times 10^{18} \text{cm}^{-3}$  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 lose 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  $n^{1/3}a_B = 0.2$ . 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. Egdel (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

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