PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

The Mott transition

D. E. Logan and P. NoziÈres

Phil. Trans. R. Soc. Lond. A 1998 **356**, 249-259
doi: 10.1098/rsta.1998.0160

The Mott transition

By D. E. Logan[1] and P. Nozières[2]

[1] *Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, UK*

[2] *Theory Group, Institut Laue-Langevin, Avenue des Martyrs, BP 156X, 38042 Grenoble Cedex 9, France*

Current understanding of the Mott transition in the infinite-dimensional Hubbard model is reviewed. It is argued that the problem remains open, but is likely to hinge on a proper understanding of the role of exhaustion.

Keywords: Mott transition; Hubbard model; exhaustion; electron interactions

1. Introduction

Of the various possible metal–insulator transitions, one of the most persistent and challenging is that driven by electron interactions: the Mott transition (Mott 1990), named after the great pioneer who devoted nearly half a century to its understanding and implications.

From a theoretical viewpoint, the problem is captured at nominally its simplest level by the one-band Hubbard model in the half-filled sector of one electron per site. The Hubbard model itself has been studied extensively in the 35 or so years since its formal inception (Hubbard 1963; Gutzwiller 1963; Kanamori 1963), but, save for the $d = 1$ dimensional limit, a thorough understanding of it is still lacking.

In recent years, however, considerable progress has occurred in understanding the Hubbard model in the opposite extreme: of large spatial dimensions, strictly the infinite-d limit, the importance of which was first pointed out only eight years ago by Metzner & Vollhardt (1989). Intense study of the infinite-d Hubbard model, in particular at half-filling on bipartite lattices, has since ensued (detailed reviews are given, for example, in Vollhardt 1993; Georges *et al.* 1996; Pruschke *et al.* 1995; Gebhard 1997). In suppressing spatial fluctuations, the intrinsically many-body problem simplifies considerably in infinite d, reducing in effect to a dynamical single-site mean-field theory, and mapping exactly onto an effective self-consistent single impurity Anderson model. The motivation for studying this limit resides in the expectation—or at least the hope—that an understanding of it will serve as a starting point for the investigation of finite dimensions; together with the knowledge that at least some important vestiges of finite-d behaviour remain inherent in the infinite-d limit.

One highlight of this many-faceted work has been the emergence of detailed predictions for the Mott transition by Kotliar *et al.* (1996), whose iterated perturbation theory (IPT) approach (Georges & Kotliar 1992; Zhang *et al.* 1993; Rozenberg *et al.* 1994*a*; Georges & Krauth 1993), in particular, provides perhaps the most comprehensive and self-contained description.

In this paper we argue that the resultant scenario for the Mott transition is controversial. In § 2, we begin with a brief summary of the qualitative results arising

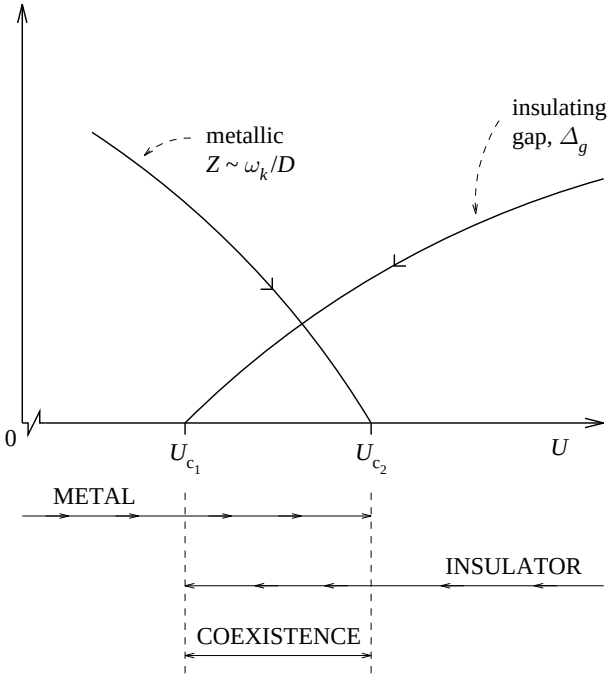

Figure 1. Coexistence of metallic and insulating solutions for $U_{c1} < U < U_{c2}$, as arises within IPT (for which $(U_{c2} - U_{c1}) \sim D$).

from IPT, before asking whether the picture emerging from it is convincingly corroborated by other approaches. Simple physical arguments are then developed that lead to two quite distinct scenarios for the Mott transition. One of these is just the picture emerging from IPT, and suggests a physical explanation for it; the other leads to a more conventional scenario for the transition as a single zero-temperature quantum critical point. The two scenarios are discriminated by whether or not the exhaustion problem of Nozières (1985) is relevant, and a further understanding of which is, we believe, crucial to the Mott transition. At present, however, we conclude that a qualitative understanding of the transition remains elusive.

2. Review

We first review briefly the salient qualitative features of the iterated perturbation theory approach of Kotliar and co-workers (details are given in the original papers (Georges & Kotliar 1992; Zhang *et al.* 1993; Rozenberg *et al.* 1994*a*; Georges & Krauth 1993), and the review (Georges *et al.* 1996)). The approach itself is directly analogous to second-order perturbation theory in the interaction strength U, much studied in the context of the single-impurity Anderson model itself (see, for example, Hewson 1993). The key difference, of course, is that when applied to the Hubbard model the problem must of necessity be solved self-consistently: hence *iterated* perturbation theory.

The essential feature of IPT is that, at zero temperature in particular, *two* solutions—one metallic, and one insulating—are found to coexist over a finite range of the interaction strength, as illustrated schematically in figure 1. To be specific, and starting from the non-interacting limit $U = 0$, a metallic Fermi-liquid solution

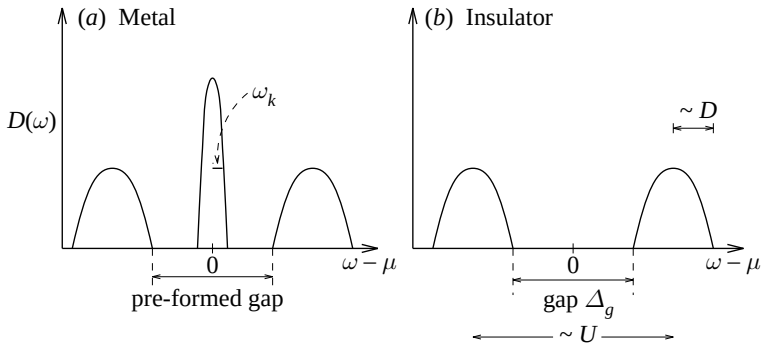

Figure 2. Schematic illustration of typical single-particle spectra for (*a*) metallic phase close to U_{c2} and (*b*) insulating phase.

is found to exist up to (but no further than) a critical interaction strength, U_{c2}. A typical single-particle spectrum for the metallic phase close to U_{c2} is sketched in figure 2*a* (from particle-hole symmetry it is symmetric about the Fermi level $\mu = \frac{1}{2}U$). It consists of upper and lower Mott–Hubbard bands, together with the important Kondo-like many-body resonance centred on the Fermi level, with its characteristsic low-energy Kondo scale, ω_K; and as the critical interaction strength U_{c2} is approached from below, the quasi-particle weight $Z \propto \omega_K$ vanishes continuously, as illustrated in figure 1. Alternatively, starting instead from the large-U regime of the Mott insulator where the spectrum consists solely of lower and upper Mott–Hubbard bands separated by the insulating gap Δ_g (see figure 2*b*), an insulating solution is found to persist down to a critical interaction strength $U_{c1} < U_{c2}$, below which insulating solutions no longer occur.

For $U_{c1} < U < U_{c2}$, metallic and insulating solutions thus coexist. The magnitude $(U_{c2} - U_{c1})$ of the coexistence interval is rather large, on the order of the non-interacting bandwidth, D (for the d^∞ Bethe lattice, $U_{c2} \sim 3.4D$ and $U_{c1} \sim 2.6D$ (Georges *et al.* 1996)). Further, and importantly, the metallic solution is found to have a lower energy than the insulator in the coexistence interval and is thus the ground state. The Mott transition itself thus occurs at the critical interaction strength U_{c2}.

At finite temperatures an analogous situation is found to occur (Georges *et al.* 1996), as schematized in figure 3: for any $T < T_2$, a metallic-like solution exists for $U < U_{c2}(T)$, while an insulating solution exists for $U > U_{c1}(T)$ with $U_{c1}(T) \leqslant U_{c2}(T)$ for all $T \leqslant T_2$. Coexistence of the two types of solution thus again occurs, and a conventional free-energy construction leads to the actual first-order transition line shown in figure 3 as $U_c(T)$. The IPT phase diagram thus consists of a line of first-order metal–insulator transitions terminating in a second-order critical point at T_2—analogously to a liquid–gas transition, such that below the critical temperature there is a first-order transition between the two phases, while a continuous transition from one to the other is possible by circumventing the critical point.

Strictly speaking, of course, the above considerations are irrelevant to the *true* ground state of the half-filled Hubbard model, where for all $U > 0$ the local moments order antiferromagnetically and the ground state is an antiferromagnetic insulator. Magnetic long-ranged order is destroyed thermally at the Néel temperature $T_N(U)$; since $T_N > T_2$, it swamps, so to speak, the MIT. Thus, as studied extensively by Jarrell & Pruschke (Jarrell 1992; Jarrell & Pruschke 1993) in particular—via quantum Monte Carlo—the true ground state phase diagram consists, as illustrated in

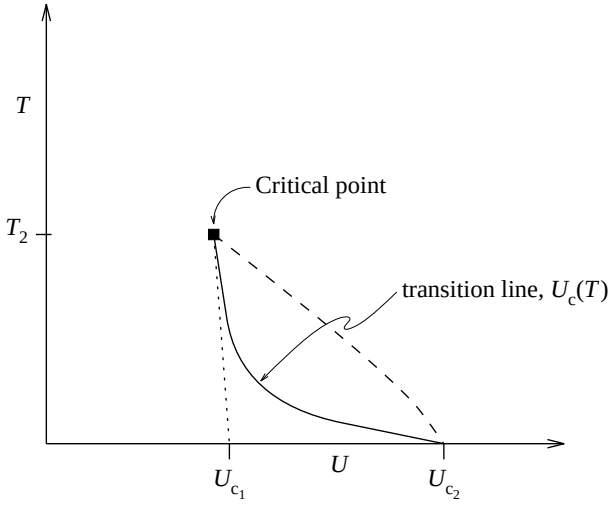

Figure 3. Schematic IPT phase diagram with the line of first-order metal–insulator transitions denoted by $U_c(T)$; the lines $U_{c1}(T)$ and $U_{c2}(T)$ are shown dotted and dashed, respectively.

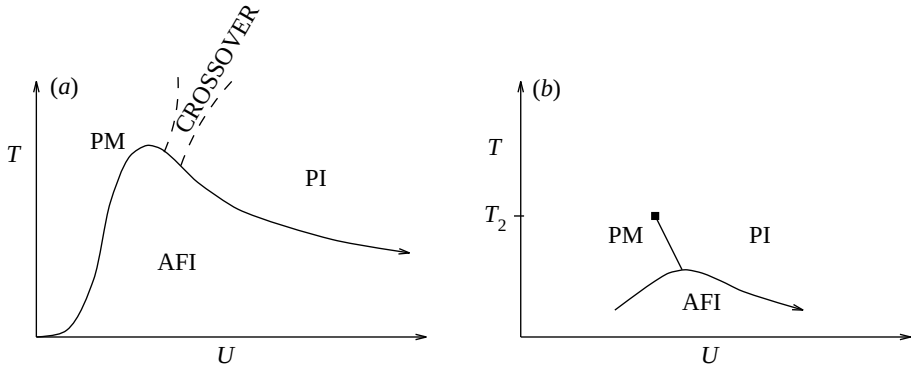

Figure 4. Schematic of (*a*) true ground state phase diagram; (*b*) phase diagram with partial frustration: AFI: antiferromagnetic insulator; PI: paramagnetic insulator; PM: paramagnetic metal.

figure 4*a*, of an antiferromagnetic insulating phase for $T < T_N$. Above the Néel temperature, at moderate to large interaction strengths, occurs a thermal paramagnetic insulating phase—with local moments but no long-ranged order thereof—while at lower U, a paramagnetic metallic phase occurs. When U is varied, the transition between the paramagnetic metallic and insulating-like phases is smooth.

Magnetic ordering can, however, be frustrated, via, for example, the introduction of random nearest and next-nearest neighbour hopping (Georges *et al.* 1996) which, in frustrating simply the ordering of the local moments, suppresses the Néel temperature and thus 'exposes' the line of first-order metal–insulator transitions (as shown schematically in figure 4*b*). The resultant phase diagram is, in fact, strikingly similar to that for V_2O_3 under pressure, containing as it does a paramagnetic insulator separated from a paramagnetic metal by a line of first-order transitions terminating in a second-order critical point. Of course, an infinite-dimensional one-band model that contains no coupling to lattice degrees of freedom does scant justice to the chemical complexities of transition metal oxides. But the qualitative similarity between the

phase diagrams has engendered the belief that, with extension to include, for example, orbital degeneracy, realistic connection to real materials can be made; and much work in this direction has ensued (see, for example, Georges *et al.* 1996).

Finally, in the limit of *full* frustration, magnetic ordering is entirely suppressed, and the phase diagram of figure 3 is again recovered. It is appropriate either to the fully frustrated Hubbard model or, equivalently, to the entirely unfrustrated case when AFLRO is ignored.

(*a*) *Critique*

The first-order transition described above stems directly from the existence of two characteristic energies in the vicinity of U_{c2}, namely the width ω_K of the Kondo resonance and the Mott gap Δ_g. The latter is finite when ω_K goes to zero at the transition: the Kondo resonance vanishes in the middle of a large *preformed gap* (figure 2*a*). The metallic and insulating states are thus well separated. At $T = 0$, the metallic state is always lower in energy when it exists, but at any finite temperature the insulating state is a local minimum due to the spin entropy of a disordered paramagnetic phase. As a result, both phases are locally stable and a first-order transition ensues. This contrasts sharply with a simple band crossing picture in which free carriers would disappear when the gap opens, resulting in a single zero-temperature quantum critical point.

The presence of a preformed gap being crucial, we must carefully assess the evidence for it. That evidence is based on several different aproaches. The simplest method is IPT, which is supposed to interpolate between weak and strong coupling. Appealing though it is, IPT is not entirely uncontroversial and has been challenged in particular by Macarie & d'Ambrumenil (1995). In any event, it is an approximation—as of necessity is any essentially analytical approach—and one probably best suited to describe the metallic phase: its originators point out (Georges *et al.* 1996) that it is unlikely to give a sound description of the collapse of the Mott insulator as U tends to U_{c1}; and it is known to be largely unable to describe the antiferromagnetic phase, missing as it does essential low-energy spin-flip scales there (Logan *et al.* 1996). Clearly, as is well appreciated, one should not rely on IPT alone.

What then of Quantum Monte Carlo (QMC) simulations? QMC is exact in principle, and although unable in practice to access the $T = 0$ limit of particular interest, one should be able to glean firm evidence for coexisting metallic and insulating-like solutions by QMC studies at accessible finite temperatures below the putative second-order critical temperature T_2. Rozenberg, Kotliar and Zhang (Zhang *et al.* 1993; Rozenberg *et al.* 1994*a*) have indeed reported such QMC evidence, consistent with the predictions of IPT. What was actually found (Rozenberg 1996, personal communication), however, was an oscillation between two apparent solutions—one metallic-like, the other insulating-like—and *each* of which was then assumed to be a stable QMC solution. Such behaviour was also observed by Pruschke (1995, and personal communication), but was found to be a numerical artifact that disappeared upon improving the simulation code, whereupon one or other but not both of the metallic and insulating-like solutions was truly stabilized. QMC studies to date are thus not mutually consistent and do not as yet appear to resolve the matter.

A similar situation arises with so-called exact diagonalization methods (Caffarel & Krauth 1994; Rozenberg *et al.* 1994*b*) whereby, exploiting the analogy of the d^∞ Hubbard model to a self-consistent single impurity Anderson model, the self-consistent 'bath' to which a nominal 'impurity' site is coupled is modelled by a finite number

n_s of orbitals, with $n_s \lesssim 10$ typically. Further approximations are required, involving judicious choices both of bath parametrization and means of approximating the self-consistency equations. According to the specific approximations chosen, differing conclusions arise regarding the question of coexistence between metallic and insulating solutions (Caffarel & Krauth 1994; Rozenberg *et al.* 1994*b*); although it is doubtful whether the low energy scales of such dominance in the problem can in practice ever be satisfactorily resolved by such methods.

Other approaches likewise yield conflicting perspectives. The non-crossing approximation—with well-understood limitations, being confined to finite T and unable to describe properly Fermi liquid behaviour as $T \to 0$—does not appear to provide corroborating evidence at finite temperature for coexistence of metallic and insulating-like solutions (Pruschke *et al.* 1993). In contrast, the self-consistent projective method (Moeller *et al.* 1995) supports the basic picture arising from IPT—with the *a priori* assumption of well-separated energy scales. We will argue below that such an assumption raises problems. The resulting picture is, however, very transparent and sheds much light on the underlying mechanisms: we therefore examine it in more detail. The idea is to focus on the low energy states near the Fermi level, in much the same way as one goes from an Anderson model to a Kondo Hamiltonian, eliminating charge fluctuations of the impurity via a Schrieffer–Wolf transformation (see, for example, Hewson 1993). Here, the starting point is a self-consistent Anderson 'impurity' model in which a given site with interaction U is hybridized to a fictitious continuum that accounts for excursions into the outside world. That 'bath' is calculated self-consistently. Compared to a usual Anderson impurity, the novelty resides in the separation of the bath into a narrow resonance near the Fermi level, and two broad Mott sidebands. Projecting onto low-energy states means in effect eliminating both the $n_0 = 0$, 2 states of the central site *and* the Mott sidebands of the spectrum. The algebra is more involved, but the final result within second-order perturbation theory is unmodified: a spin-$\frac{1}{2}$ Kondo 'impurity' is coupled to a narrow fermion band of width $\omega_K \sim ZD$, containing NZ states altogether (D is the original bandwidth, to which all energies are referred). That coupling has both scalar and exchange terms. The scalar coupling is zero for the electron-hole symmetric case (otherwise it probably fixes the position of the resonance inside the gap). The exchange coupling yields a Kondo temperature T_K, which is found to be of order ω_K (the effective bandwidth). The exchange coupling is thus intermediate, as befits the universal regime expected when ω_K is much smaller than any other energy scale in the problem. The physics of free carriers is ultimately reduced to a Kondo problem: the magnetic entropy $N \log 2$ of the paramagnetic Mott sidebands is quenched by exchange with free carriers lying in the central resonance, resulting in a steep specific heat $C_v(T)$. Such 'heavy fermion' behaviour is common to all theories, including the most naive ones such as the Gutzwiller approximation.

Such a picture offers a very appealing interpretation of the first-order Mott transition, as shown in Moeller *et al.* (1995). Assume we start from an insulating state with gap Δ_g; we then transfer NZ states from the Mott sidebands to a resonance near the Fermi level. We clearly pay a cost in kinetic energy:

$$E_c \sim NZ\Delta_g, \tag{2.1}$$

but these 'freed' electrons are eligible to produce a Kondo effect: at $T = 0$, the ground state energy will be lowered due to the occurrence of singlet screening. Let E_g be that energy gain. If $E_g > E_c$, the balance is favourable, and free carriers appear

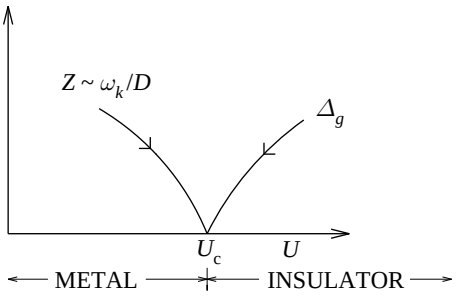

Figure 5. Situation arising if exhaustion is salient: the Mott transition as a single zero-temperature quantum critical point.

spontaneously. If $E_g < E_c$, the system remains insulating. Note further the presence of a built in saturation mechanism: if Z grows, the central states repel the Mott sidebands, the gap Δ_g thereby increases and the balance ceases to be favourable. As noticed in Moeller *et al.* (1995), a simple 'Landau theory' ensues, very similar to that found in the Gutzwiller approach. Even more interesting is the temperature dependence: when T exceeds T_K, the gain in exchange energy disappears, parallel and antiparallel spin configurations being equally populated in contrast to the singlet ground state. Only the cost in kinetic energy remains: the resonance disappears instead of broadening, the weight Z vanishing without noticeable change in width. The whole physical picture is thus clear: what is needed is an estimate of the Kondo energy E_g.

3. The problem of exhaustion

While for a *single* Kondo impurity, E_g is roughly the Kondo temperature $\sim ZD$, a difficulty arises for the whole system: one is attempting to screen a large number of spins, N, with a small number of electrons in the central resonance, NZ. Clearly screening cannot be an individual process in which each spin traps a partner: hence the 'exhaustion problem' raised long ago (Nozières 1985). Collective singlet formation is a definite possibility: each electron visits in sequence many impurities and magnetic entropy is quenched when precession has averaged all spin orientations. It is very likely that direct RKKY coupling between spins also plays an important role. Granted that the issue remains unclear: the relevant energy scales for quenching the spin entropy, as well as the position of the Fermi surface, are matters of debate. But we shall reduce the controversy to a single question: *does one gain the Kondo energy* ω_K *once per spin, or once per electron in the resonance*? The picture of an electron visiting spins in succession would imply the latter choice. We leave this question open, and confine ourselves to the corresponding scenarios for the Mott transition.

Scenario 1. The Kondo energy is gained once for each spin in the sidebands, i.e. $E_g = N\omega_K \sim NZD$. It follows trivially that the energy balance becomes favourable when $\Delta_g \sim D$: the Kondo resonance thus appears in the middle of a large preformed gap of order D, and the picture of IPT ensues.

Scenario 2. The Kondo energy is gained once for each electron in the resonance, i.e. $E_g = NZ\omega_K \sim NZ^2D$. Then the balance becomes favourable when the gap Δ_g is of order $ZD \sim \omega_K$. In such a case there is no preformed gap, the Mott transition being governed solely by a single energy scale: as shown in in figure 5, the resonance

width and insulating gap are slaved to each other in the critical regime, and each vanishes at the transition. In other words, the Mott transition in this case is a single zero-temperature quantum critical point, as referred to in § 2.

The arguments sketched above lead then to two physically very distinct scenarios for the $T = 0$ Mott transition. On the one hand, if the screening physics is in essence that of independent Kondo impurities, one has a two energy-scale transition accompanied by a pre-formed spectral gap, as indeed arises tangibly within IPT; on the other, if exhaustion is salient, one has instead a Mott transition characterized by a single energy scale. In consequence, the finite temperature behaviours likewise differ radically, with first-order transitions arising in the former case, but smooth crossovers only in the latter.

Of course, the simple physical arguments given above do not by themselves tell us which of the two scenarios is correct, although we do not understand how exhaustion could be avoided. But we certainly believe the issue is crucial in understanding the Mott transition: at minimum, if exhaustion is to be circumvented—as in the scenario arising from IPT—we need to understand how; and, if so, whether it is a feature peculiar to the infinite-dimensional limit.

In summary, and despite considerable progress in recent years, our contention is that even a qualitative understanding of the Mott transition still eludes us: we have tried to reduce it to a simple physical question—which should receive a simple physical answer.

References

Caffarel, M. & Krauth, W. 1994 *Phys. Rev. Lett.* **72**, 1545.

Gebhard, F. 1997 *The Mott metal–insulator transition*. Berlin: Springer.

Georges, A. & Kotliar, G. 1992 *Phys. Rev.* B **45**, 6479.

Georges, A. & Krauth, W. 1993 *Phys. Rev.* **48**, 7167.

Georges, A., Kotliar, G., Krauth, W. & Rozenberg, M. J. 1996 *Rev. Mod. Phys.* **68**, 13.

Gutzwiller, M. C. 1963 *Phys. Rev. Lett.* **10**, 59.

Hewson, A. 1993 *The Kondo problem to heavy fermions*. Cambridge University Press.

Hubbard, J. 1963 *Proc. R. Soc. Lond.* A **276**, 238.

Jarrell, M. 1992 *Phys. Rev. Lett.* **69**, 168.

Jarrell, M. & Pruschke, T. 1993 *Z. Phys.* B **90**, 187.

Kanamori, J. 1963 *Prog. Theor. Phys.* **30**, 275.

Logan, D. E., Eastwood, M. P. & Tusch, M. A. 1996 *Phys. Rev. Lett.* **76**, 4785.

Macarie, L. S. & d'Ambrumenil, N. 1995 *J. Phys. Cond. Matt.* **7**, 3237.

Metzner, W. & Vollhardt, D. 1989 *Phys. Rev. Lett.* **62**, 324.

Moeller, G., Si, Q., Kotliar, G., Rozenberg, M. J. & Fisher, D. S. 1995 *Phys. Rev. Lett.* **74**, 2082.

Mott, N. F. 1990 *Metal–insulator transitions*. London: Taylor and Francis.

Nozières, P. 1985 *A. Phys.* **10**, 19.

Pruschke, T. 1995 Habilitation thesis, University of Regensburg.

Pruschke, T., Cox, D. L. & Jarrell, M. 1993 *Phys. Rev.* B **47**, 3553.

Pruschke, T., Jarrell, M. & Freericks, M. 1995 *Adv. Phys.* **44**, 187.

Rozenberg, M. J., Kotliar, G. & Zhang, X. Y. 1994*a* *Phys. Rev.* B **49**, 10 181.

Rozenberg, M. J., Moeller, G. & Kotliar, G. 1994*b* *Mod. Phys. Lett.* **8**, 535.

Vollhardt, D. 1993 In *Correlated electron systems* (ed. V. J. Emery). Singapore: World Scientific.

Zhang, X. Y., Rozenberg, M. J. & Kotliar, G. 1993 *Phys. Rev. Lett.* **70**, 1666.

Discussion

G. Kotliar (*Serin Physics Laboratory, Rutgers University, NJ, USA*). The phase diagram of the Hubbard model is strongly dependent on the nature of the lattice, which determines the type of magnetic order. Mott emphasized that the metal–insulator transition is an issue somewhat separate from the issue of magnetic order. The phase diagram of the one-band Hubbard model on the square lattice (which is not frustrated) is not, in my opinion, relevant to the metal–insulator transistion in systems such as the titanates or vanadium oxide. To describe these systems we need models where the magnetic order is suppressed. Within a one-band model, magnetism can only be suppressed by introducing additional hopping matrix elements in the kinetic energy. To my knowledge, this observation in the context of dynamical mean-field theory was made independently by Rozenberg *et al.* (1992) and Georges & Krauth (1993). The role of magnetic order in the phase diagram was discussed even earlier in Georges *et al.* (1992), where the dynamical mean-field equations in the presence of magnetically broken symmetry were first derived. The first numerical determination of the phase diagram in the (unfrustated) square lattice was first carried out by Jarrell (1992). The phase diagram in the *unfrustrated Bethe lattice* was obtained in Rozenberg *et al.* (1994) and Ulmke *et al.* (1995).

Titanates have a perovskite structure (simple cubic lattice) which is not frustrated, while V_2O_3 has a corundum structure which is not frustrated either. The source of frustration in realistic oxides has to be found in their orbital degenerancy rather than their lattice structure. This important observation due to Castellani *et al.* and Khomski is essential for the understanding of V_2O_3 (Rice 1995). The role of orbital degeneracy in the context of the dynamical mean-field equations, and the extent to which it justifies the use of the paramagnetic solution, was recently discussed in Rozenberg (1996), Kotliar & Kajueter (1996) and Kajeuter & Kotliar (1997), where more realistic calculations were carried out.

I am pleased to hear that our work on the nature of the Mott transition in the frustrated Bethe lattice is interesting. I must disagree, however, with Dr Logan's statement that our conclusions (as to the topology of the phase diagram of the fully frustrated Hubbard model) are *solely based* on iterated perturbation theory. I should mention the exact diagonalization studies using exact diagonalization techniques (Rozenberg *et al.* 1994) which lead to the same qualitative picture (and to more accurate values for U_{c1} and U_{c2}). Furthermore, the development of the more accurate projective self-consistent method, allowed a precise determination of the critical behaviour near the Mott transition and provided a rigorous proof that the qualitative scenario obtained within IPT is a genuine property of the Hubbard model in the limit of infinite dimensions (Moeller *et al.* 1995; Fisher *et al.* 1995).

Dr Logan stated in his talk that Monte Carlo calculations and other approximate calculations by Prushke and his group reached the opposite conclusion, i.e. only one critical U at zero temperature and no coexistence at finite temperature. It is important to settle this issue. The differences concerning the *finite temperature transition* could be clarified by a careful comparison of the results produced by different computer codes (a Monte Carlo code would lead to finite temperature coexistence written by Krauth is available in the internet address described in our review (Georges *et al.* 1996)). I suggest to study with the methods in question the orbitally degenerate model. Analytic, as well as numeric, calculations (Rozenberg 1996; Kotliar & Kajeuter 1996; Kajeuter & Kotliar 1997) indicate that the difference between U_{c1}

and U_{c2} is amplified by higher occupation and higher orbital degeneracy. This will facilitate the numerical study.

Finally, I would like to point out that while I am completely certain that we obtained the correct solution of the Hubbard model in the limit of infinite lattice coordination, it is by no means clear that the results describe nature quantitatively very close to the transition. This is, in my view, the real challenge for the future. There are several reasons to suspect that in *finite dimensions* a closing of a gap will occur at the same time that the central resonances appear: (i) this is the scenario predicted by a finite d large N calculation (Castellani *et al.* 1992); (ii) there are no clear indications that the $1/d$ corrections near the Mott transition are singular perturbations (Georges, work in progress); (iii) gap closing is the scenario suggested by slave bosons calculations (Castellani *et al.* 1992).

I am optimistic that in our next meeting we will have a much better handle on if (and how) finite dimensionality corrections modify the large d predictions. By then, some realistic dynamical mean-field calculations will have been performed and compared with three-dimensional compounds. Then we will be able to assess how well we understand the classic problem formulated by Sir Nevill Mott.

F. Gebhard (*Institut Laue-Langevin, Grenoble, France*). In reply to Professor Kotliar's comments, the projective self-consistent method uses the *assumption* that the high and low energy scales can be separated completely in the vicinity of the Mott–Hubbard metal–insulator transition in the infinite-dimensional Hubbard model. At best, the method allows one to prove that this assumption is self-consistently fulfilled. If this assumption was true, the Mott–Hubbard transition would be discontinuous because the Mott–Hubbard gap would jump to its finite pre-formed value when the matallic state ceases to exist. However, I doubt that the prerequisite of energy-scale separation is indeed fulfilled. Hence, there is no evidence against the (more likely) scenario of the Mott–Hubbard transition as a continuous zero-temperature quantum phase transition where the quasi-particle weight in the metallic Fermi liquid vanishes at the same critical interaction strength where the Mott–Hubbard gap opens.

D. E. Logan. I have three brief comments to make in reply to Professor Kotliar.

(i) The distinction between frustrated and unfrustrated lattices is, of course, essential to real finite-dimensional systems, but is rather a red herring in the infinite-dimensional limit under discussion. Here, as we know, the phase diagram of the half-filled Hubbard model on the fully frustrated Bethe lattice is identical to that arising for the unfrustrated case when magnetic ordering is simply ignored.

(ii) It was neither stated nor implied that Professor Kotliar's conclusions regarding the Mott transition in the infinite-d Hubbard model are based solely on iterated perturbation theory (IPT). They are not, although IPT does provide probably the most self-contained description. What I did point out, and would reiterate, is that complimentary studies by different groups—using quantum Monte Carlo (QMC), exact diagonalization and other theoretical approaches—yield conflicting results; and therefore that the scenario arising from IPT is not as yet convincingly corroborated. I do, however, agree with him that, as far as QMC is concerned, it is probably feasible, and certainly important, to sort the matter out.

(iii) I agree with Professor Kotliar entirely that an important challenge for the future is, as it has been for nearly half a century, to understand the Mott transition in finite-dimensional systems. But it remains my contention that, even in the simplifying limit of infinite d, a qualitative understanding of the problem remains elusive.

Additional references

Castellani, C., Kotliar, G., Raimondi, R., Grilli, M., Wang, Z. & Rozenberg, M. 1992 *Phys. Rev. Lett.* **69**, 2009.

Fisher, D., Kotliar, G., Krauth, W. & Rozenberg, M. 1996 *Phys. Rev.* B **52**, 17 112–17 118.

Georges, A. & Krauth, W. 1993 *Phys. Rev. Lett.* B **48**, 7167.

Georges, A., Kotliar, G. & Si, Q. 1992 *Int. J. Mod. Phys.* B **6**, 705.

Georges, A., Kotliar, G., Krauth, W. & Rozenberg, M. 1996 *Rev. Mod. Phys.* **68**, 13–125.

Jarrell, M. 1992 *Phys. Rev. Lett.* **69**, 168.

Kajeuter, H. & Kotliar, G. 1997 *Int. J. Mod. Phys.* B **11**, 729.

Kotliar, G. & Kajeuter, H. 1996 *Phys. Rev.* B **54**, 14 221.

Moeller, G., Si, Q., Kotliar, G., Rozenberg, M. & Fisher, D. S. 1995 *Phys. Rev. Lett.* **74**, 2082–2085.

Rice, T. M. 1995 In *Spectrosopy of Mott insulators and correlated metals* (ed. A. Fujimori & Y. Tokura). Berlin: Springer.

Rozenberg, M. 1996 Preprint.

Rozenberg, M., Zhang, X. Y. & Kotliar, G. 1992 *Phys. Rev. Lett.* **69**, 1236.

Rozenberg, M. J., Kotliar, G. & Zhang, X. Y. 1994 *Phys. Rev.* B **49**, 10 181.

Ulmke, M., Janiš, V. & Vollhardt, D. 1995 *Phys. Rev.* B **51**, 10 411.

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES