Landau Theory of the Finite Temperature Mott Transition

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In the context of the dynamical mean-field theory of the Hubbard model, we identify microscopically an order parameter for the finite temperature Mott end point. We derive a Landau functional of the order parameter. We then use the order parameter theory to elucidate the singular behavior of various physical quantities which are experimentally accessible.

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When the strength of the electron-electron interaction U is increased compared to the bare bandwidth $2D$, a metal-insulator transition occurs [1]. This phenomenon, known as the Mott transition, can take place in the absence of magnetic long-range order, and is still an outstanding problem in condensed-matter physics. From a theoretical point of view, a difficulty is the absence of an obvious order parameter to systematize the critical behavior of the observable quantities when the metal-insulator transition is not accompanied by the onset of magnetic long-range order. These issues are experimentally relevant to systems such as V_2O_3 and $Ni(Se,S)_2$ and are the subject of intensive experimental study [2].

In recent years, great progress has been made by using the dynamical mean-field theory (DMFT) [3]. This framework describes both paramagnetic metallic and paramagnetic insulating phases. The U-T phase diagram (T is the temperature) of the frustrated Hubbard model in the limit of large lattice coordination is qualitatively similar to that of the V_2O_3 and $Ni(Se,S)_2$ systems: A first-order phase-transition line ends in a second-order critical point, henceforth referred to as the Mott critical point, which is the main focus of this Letter. We will use this framework to address the fundamental questions raised in the previous paragraph.

There are two earlier qualitative ideas as to what should be the order parameter to describe the physics around the finite temperature Mott point. One idea is to connect the order parameter to the notions of "metallicity" or coherence. It can be traced back to the early paper of Brinkman and Rice [4] and is captured in a slave boson formalism where the metallic state has a nonzero expectation value of a Bose field which describes the coherent propagation of one particle excitations [5]. In a very different picture, Castellani *et al.* viewed the metal as a liquid rich in doubly occupied sites, and the insulator as a liquid with few doubly occupied sites. The metal to insulator transition is viewed as a condensation of doubly occupied sites, and the order parameter is related to the Blume-Emery-Griffith model [6]. The Landau approach presented here provides a synthesis of these ideas. It bridges naturally between a picture based on one particle excitations and a picture based on local collective excitations (or double occupancies). In agreement with Castellani *et al.* we find that the Mott transition has indeed an Ising-like character. On the other hand, we obtain a complementary description in terms of the one particle spectral function reminiscent of the slave boson picture. A simple and clear description of the critical behavior near the critical point emerges. It allows us to systematically derive the critical behavior of any observable quantity and to relate its nonanalytic dependence on T and U to that of the order parameter. Our results should be also of help in resolving some controversies on the solution of the Hubbard model in infinite dimensions [7,8] by providing a theoretical framework in which to analyze numerical results on the finite temperature Mott transition. It can also be used to analyze results of photoemission and optical conductivity experiments.

For simplicity, we focus on the single-band Hubbard model at half filling:

$$\hat{H} = -\frac{t}{\sqrt{z}} \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} . \tag{1}$$

The first term describes the hopping between nearest neighbors on a lattice with coordination number z. The corresponding half bandwidth is our unit of energy, $D = 2t = 1$. The second term is an on-site interaction suppressing double occupancies by imposing an energy cost U on each one. In the limit of infinite dimensions, $z \to \infty$, this model can be mapped onto a single-impurity Anderson model (SIAM) supplemented by a self-consistency condition. We adopt a semicircular density of states, which is realized on the Bethe lattice. The dynamical mean-field equations can be obtained by differentiating the Landau functional,

$$F_{\text{LG}}[\Delta] = -T \sum_{n} \frac{\Delta(i\omega_n)^2}{t^2} + F_{\text{imp}}[\Delta], \tag{2}$$

with respect to the hybridization function $\Delta(i\omega_n)$ of the SIAM, which has the meaning of a Weiss field. $i\omega_n$ are fermionic Matsubara frequencies, while $F_{\text{imp}}[\Delta]$ is the free energy of the SIAM, given by the action $S_{\text{imp}} = S_{\text{loc}}[\Delta = 0] + \sum_{\sigma,n} f_{\sigma}^{+}(i\omega_n)\Delta(i\omega_n) f_{\sigma}(i\omega_n)$. Here, $S_{\text{loc}}[\Delta = 0]$ is

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the action of the local f level with the hybridization set to zero. The first term in Eq. (2) is the cost of forming the Weiss field $\Delta(i\omega_n)$ around a given site, while the second one is the free energy of an electron at this site in the presence of the Weiss field. Using the Green's function of the SIAM, $G(i\omega_n) = (1/2T)\delta F_{\rm imp}/\delta\Delta(i\omega_n)$, the mean-field equation reads

$$\frac{t^2}{2T}\frac{\delta F_{\rm LG}[\Delta]}{\delta\Delta(i\omega_n)} = t^2 G(i\omega_n)[\Delta,\alpha] - \Delta(i\omega_n) = 0. \quad (3)$$

Here, $\alpha = (U,T)$ comprises the control parameters. This Landau approach was used to describe the energetics of the Mott transition at zero temperature [9]. We will show that, near the finite temperature Mott point, the Weiss field has a singular dependence which can be parametrized by a single number which assumes the role of an effective order parameter for this transition.

As in Landau theory, we *assume* that a finite temperature transition exists, and *derive* a complete description of the critical behavior near the transition as follows: First, we expand the mean-field equation (3) around the critical point, $\alpha_c = (U_c, T_c)$, up to third order in the deviation of the hybridization function from its value at the critical point, $\delta\Delta = \Delta(\alpha_c + \delta\alpha) - \Delta(\alpha_c)$, and to first order in $\delta\alpha = (U - U_c, T - T_c)$. This expansion is well-behaved because the impurity model *at finite temperatures* depends smoothly on α and $\delta\Delta(i\omega_n)$. In order to carry out this expansion it is convenient to define a fluctuation matrix:

$$M_{nm} = \frac{t^2}{2T}\frac{\delta^2 F_{\rm LG}[\Delta]}{\delta\Delta(i\omega_n)\delta\Delta(i\omega_m)}\bigg|_{\rm critical\ point}. \quad (4)$$

M_{nm} has the form $-\delta_{nm} + K_{nm}$, where K_{nm} is the Fourier transform of a kernel $K(\tau,\tau')$ which is proportional to the connected correlation function of an operator $O(\tau) = \int_0^\beta du\, f^+(u+\tau)f(u)$, $\langle O(\tau)O(\tau')\rangle - \langle O(\tau)\rangle\langle O(\tau')\rangle$, where the average $\langle\rangle$ is calculated with the action of an Anderson impurity model. It is well known that the correlation functions of the Anderson impurity model are *bounded*, and therefore the kernel K is square integrable $\int_0^\beta\int_0^\beta d\tau\, d\tau'\, |K(\tau,\tau')|^2 < \infty$. Therefore it K_{nm} is a Fredholm operator and has a *discrete* spectrum of eigenvalues which we labeled by the index l [10].

At half filling, particle-hole symmetry guarantees that the order parameter $\Delta(i\omega)$ is odd and wholly imaginary. Accordingly, the fluctuation matrix is real and symmetric and has real eigenvalues m_l belonging to eigenvectors $\phi_l(i\omega_n)$ which can be chosen to be purely imaginary and to form an orthonormal basis. The critical point, in this description of the problem, is signaled by the appearance of a single zero eigenvalue, $m_0 = 0$, which indicates the occurrence of a simple bifurcation.

Next, we represent $\delta\Delta$ in the eigenbasis of the matrix (4), $\delta\Delta(i\omega_n) = \sum_l \eta_l\phi_l(i\omega_n)$, where all η_l are real. By projecting the mean-field equation (3) onto the eigenbasis ϕ_l, we obtain an equation of the form

$$m_l\eta_l + F_l^{(0)}[\{\eta_{j\neq 0}\}] + F_l^{(1)}[\{\eta_{j\neq 0}\}]\eta_0 + F_l^{(2)}[\{\eta_{j\neq 0}\}]\eta_0^2 + F_l^{(3)}\eta_0^3 = 0, \quad (5)$$

which holds for all l. $F_l^{(0)}$ is of order $\delta\alpha$. $F_l^{(1)}$ and $F_l^{(2)}$ have Taylor expansions in the $\eta_{j\neq 0}$, where $F_l^{(1)}$ starts with the linear order. We solve Eq. (5) iteratively for all $\eta_{l\neq 0}$ to obtain $\eta_{l\neq 0} = a_l + c_l\eta_0^2 + d_l\eta_0^3$. Here, a_l is of first order in $\delta\alpha$, (which assures us that the leading singular dependence of the spectral function is proportional to ϕ_0); further corrections have the form $b_l\eta_0$ with b_l also of order $\delta\alpha$. By inserting this expression into the $l = 0$ case of Eq. (5), we derive an effective equation for the zero-mode amplitude η_0. We can think of η_0 as the soft mode near the transition and $\eta_{l\neq 0}$ as massive modes. The elimination of the massive modes renormalizes the coefficients of the effective action for the soft mode. In the resulting cubic equation for η_0, we eliminate the quadratic term by shifting η_0 by an appropriately chosen linear function in $\delta\alpha$, $\eta = \eta_0 + {\rm const}_1 \times (T - T_c) + {\rm const}_2 \times (U - U_c)$. Close to the critical point, η and η_0 are dominated by nonanalytic terms and are therefore essentially equal. We thus obtain an equation of state without a quadratic term in η:

$$p\eta + c\eta^3 = h. \quad (6)$$

Here, all quantities are real.

As in Landau theory, a microscopic calculation of the Landau coefficients (p,c,h) is difficult. However, we can extract exact information about the critical behavior from the knowledge that they are smooth functions of the control parameters: i.e., c is finite at the critical point, whereas p and h are linear functions of $\delta\alpha$, $h = h_1(U - U_c) + h_2(T - T_c)$, and $p = p_1(U - U_c) + p_2(T - T_c)$. As a consequence, η has a singular dependence on U and T near the critical point. At $U = U_c$, and for T near T_c,

$$\eta(U_c,T) \simeq {\rm sgn}(h_2/c)\,{\rm sgn}(T - T_c)\,|T - T_c|^{1/3}. \quad (7)$$

The mean-field equation (6) describes the Mott transition close to the critical point in terms of the order parameter η. In this form, the analogy with the liquid gas transition is evident. The Mott transition takes place on the line in the U-T plane where h vanishes and the system has full Ising symmetry. The critical point, (U_c, T_c), divides this line into two half-lines. On the half-line where $T < T_c$, there are two solutions, $\eta = \pm\sqrt{|p/c|}$. We will see later that η parametrizes the strength of the quasiparticle resonance of the single-particle spectrum [see Fig. 2 (below)]. A positive or negative "field" h increases or decreases this component of the spectral function, respectively. The field h decreases when U or T is increased, because either increase eliminates the metallic coherence and thus reduces the value of η. We have used the sign convention whereby ${\rm Im}\phi_0(\omega - i0^+)/\pi$ is positive.

We now turn to various consequences of our construction. From Eq. (6), we can obtain the *shape* of the coexistence region near the critical point, where two solutions of the mean-field equations coexist. It is centered symmetrically about the $h = 0$ line, and its width along $T = \text{const}$ lines, ΔU, scales with $(T_c - T)^{3/2}$. The constant of proportionality is given by $(4/\sqrt{c}\,|h_1|)[(p_2 - p_1 h_2/h_1)/3]^{3/2}$.

An important quantity which is measured in numerical simulations is the double occupancy. It is connected to our order parameter η as follows: $\langle d \rangle = (T/U)\sum_n \{[(i\omega_n + \mu)G(i\omega_n) - 1]e^{i\omega_n 0^+} - t^2 G(i\omega_n)^2\} = \langle d \rangle_c + c_1^{(d)}\eta + c_2^{(d)}\eta^2$. In this expansion about the critical point, we have retained only the leading and next to leading nonanalytic terms responsible for the critical behavior. The susceptibility $\chi = \partial\langle d \rangle/\partial U$ diverges at the critical point. For example,

$$\chi(U, T_c) \simeq (c_1^{(d)}/3)\,\text{sgn}(h_1/c)\,|h_1/c|^{1/3}|U - U_c|^{-2/3}. \tag{8}$$

The double occupancy is related to the magnetization by the identity $\langle (n_\uparrow - n_\downarrow)^2 \rangle = 1 - 2\langle d \rangle$. The magnetic response will therefore also exhibit nonanalytic dependences on the control parameters.

There have been several numerical studies of the finite temperature Mott transition in this model. The Landau approach predicts the functional dependence of various quantities near the transition, and therefore the expressions derived in this paper are useful for interpreting the numerical work. To illustrate how our approach sheds new light on previously obtained numerical data, we compare in Fig. 1 the results for the double occupancy $\langle d \rangle$ obtained within the iterated perturbation theory (IPT) and quantum Monte Carlo (QMC) calculations with $\Delta\tau = 0.5/D$, after carrying out the shifts and the rescaling described in the figure caption. Within the statistical errors of the QMC calculation, the agreement is excellent. This surprising result is consistent with the Landau theory: different approximations for the solution of the impurity model reduce to the same Landau theory near the critical point, but with different values of the Landau coefficients. Therefore, with a suitable rescaling, the results near the critical point should agree with each other, and with a fit based on the Landau theory which is shown in the line in Fig. 1.

Small changes in the values of $\Delta\tau$ result in shifts of U_c, T_c, and $\langle d \rangle$ at criticality, but do not change the form of the critical behavior. We also note that the critical slowing down which has been observed in the iterative solutions of the mean-field equations are a direct consequence of the presence of the soft mode η described in the Landau approach.

From our construction, it is clear that η provides the leading nonanalytic behavior of the Weiss field. In order to get a better feeling for its physical significance, we have to understand how it can be probed experimentally. Since the order parameter is closely related to the amplitude of the quasiparticle peak, photoemission is an ideal tool to probe the temperature and pressure dependence of the order parameter near the critical point. This experimental technique, in the angle integrated mode, would also measure the convolution of the Fermi function with the analytically continued eigenfunction of the zero mode, $\text{Im}\phi_0(i\omega_n = \omega - i\delta)$. To visualize the shape of the spectral function near the critical point, we must resort to calculations based on analytic methods such as IPT.

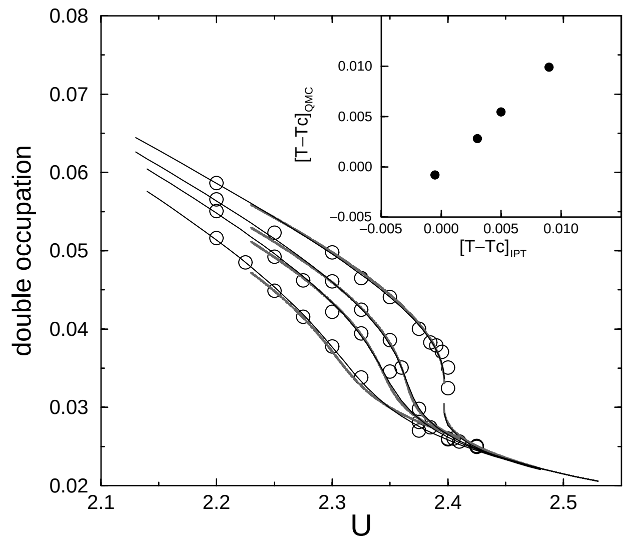

FIG. 1. Double occupation $\langle d \rangle$ as a function of U for different temperatures. The thin lines denote IPT results for $T_{\text{IPT}} = 0.0469, 0.05, 0.052, 0.056$ (top to bottom). The thick lines are a fit to the IPT data using the LG theory. The circles are QMC data obtained at $T_{\text{QMC}} = 1/40, 1/35, 1/32, 1/25$ [8]. The IPT results where shifted by a constant -0.07 along the U axis and by -0.003 along the $\langle d \rangle$ axis. The curves for the three larger temperatures are above T_c and the lowest temperature ones (two branches) are just below. The inset shows the scaling of the *reduced* temperatures $[T - T_c]_{\text{QMC}}$ versus $[T - T_c]_{\text{IPT}}$.

The inset of Fig. 2 shows the spectral function very near the critical point, computed within the IPT.

It illustrates how the compromise between metallic and insulating features is realized. A finite η, depending on its sign, adds or subtracts spectral weight to the coherent low-energy feature immersed in a constant background in between the Hubbard bands. The zero mode is seen to affect mainly the low-energy part of the spectrum, which determines whether the system is metallic or insulating. The strong temperature dependence has been noticed in previous theoretical and experimental studies [12]. Its origin and connection to an order-parameter description of the Mott transition, however, had not been recognized until now. In the main panel of Fig. 2 we display the height of the quasiparticle peak $A_0 = i\Delta(i0^+)/\pi t^2$, for $U \simeq U_c$, as a function of temperature in the vicinity of T_c. The rapid variation seen in the figure is consistent with the form $A_0 = A_{0c} + c_1^{(A)}\eta + c_2^{(A)}\eta^2$ with coefficients $c_i^{(A)}$ independent of U and temperature.

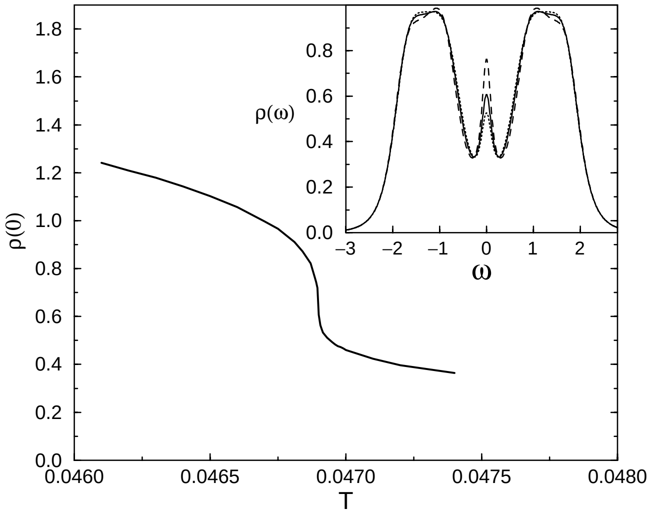

FIG. 2. The density of states at the Fermi energy $\rho(0) \equiv A_0$ as a function of temperature in the critical region ($U = 2.463\,16 \approx U_c$). The singular behavior of the slope at $T_c \approx 0.046\,897$ can be clearly appreciated. The inset shows the variation of the spectral function for $U \simeq U_c$ in the vicinity of T_c: dashed line for $T - T_c/T_c = -0.000\,25$, solid line for $T - T_c/T_c = 0.000\,06$, and dotted line for $T - T_c/T_c = 0.000\,49$ [11].

Optical techniques are probably the best tool available to test the predictions of our theory. For instance, one may consider the integral of the optical conductivity up to some cutoff, $N_{\rm eff}(T)$. Since the optical conductivity in infinite dimensions is directly expressed in terms of the single-particle Green's function, $N_{\rm eff}(T)$ must also exhibit the singular temperature dependence near the transition. We would therefore expect the temperature variation of this quantity to be most visible for a relatively small cutoff, displaying a rapid variation with T similarly as for A_0. Since the singular dependence arises from the order parameter η, it should be possible to fit the Drude weight by $N_{\rm eff}(T) = N_{\rm eff}(T_c) + c_1^{(N)}\eta(T) + c_2^{(N)}\eta^2(T)$. $N_{\rm eff}(T)$ has recently been measured in $NiS_{2-x}Se_x$ [13]; the observed strong temperature dependence of the effective number of carriers is consistent with our predictions.

In summary, we derived an order parameter description of the Mott transition near its critical point in the U-T plane. We showed that the critical behavior in proximity to this point is governed by an Ising-like Landau functional and is present in a large number of observable quantities. We predict that any physical quantity which is sensitive to the single-particle spectrum exhibits singular dependences on the control parameters close to the finite-temperature Mott point. The leading nonanalytic behavior of other physical quantities can be obtained along similar lines, i.e., by recognizing their coupling to the order parameter. This involves a few coefficients (i.e., the $c^{(A)}$'s) which depend on the observable (and on the approximation method) and, as in Landau theory, should be taken as parameters. The dependence on temperature and on pressure is completely determined from the temperature or pressure dependence of the order parameter that follows from Eq. (6).

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[10] This is true only at finite temperatures, which ensures that the limit of integration β is finite. At zero temperature the spectrum of fluctuations is continuous and the transition at a point denoted U_{c2} has a very different character and was described in Ref. [9].

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