# Midgap states in doped Mott insulators in infinite dimensions

Daniel S. Fisher

*Physics Department, Harvard University, Cambridge, Massachusetts 02138*

G. Kotliar and G. Moeller

*Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08855-0849*

Doping of Mott insulators is analyzed in the mean-field-like limit of large lattice coordination or high dimensions. In this limit, it is demonstrated analytically that doping a Mott insulator induces states in the Mott-Hubbard gap, resulting in a narrow peak in the spectral density well separated, for weak doping, from the Hubbard bands. The energy at which this feature appears—the critical chemical potential for doping—is calculated as a function of $U$. It is also shown that the criterion for linear instability of the insulating Mott phase is the equality of chemical potential and the band edge. The nonlinear instability analyzed here always occurs strictly *before* the chemical potential reaches the band edge.

The behavior of a Mott insulator as it is doped away from half filling is a long-standing open problem. It has received renewed theoretical and experimental attention motivated by attempts to understand the metallic state of the copper-oxide superconductors, which are obtained by doping Mott-insulating parent compounds.[1]

Exact results on this problem are very scarce. In one dimension, the exact solution of the Hubbard model yields that the jump in the chemical potential at half filling in going from electron to hole doping is the same as the value of the Mott Hubbard gap, defined as the lowest-energy excitation in the charge spectrum at half filling.[2] The main question on which we will focus, is whether this remains true in higher dimensions, or whether, in contrast, doping away from half filling will occur *before* the chemical potential reaches the edges of the Hubbard gap.

Numerical studies of the two-dimensional Hubbard model suggest that when the number of particles is slightly less than one per site, the chemical potential is again simply located at the top of the lower Hubbard band of the insulator. Correspondingly, when the density is slightly greater than one particle per site, the chemical potential jumps to the bottom of the upper Hubbard band.[3] Large $N$ studies of a model exhibiting a metal to charge-transfer-insulator transition reveal that upon doping the chemical potential also jumps from the bottom of the upper Hubbard band to the top of the lower Hubbard band.[4] Different results on this model have been obtained, however, via a different slave boson treatment of the same model.[5]

Our goal here is to make exact statements about this problem in the limit of large lattice coordination.[6] It has been recognized in the past few years that results obtained in this limit have a mean-field character, and this mean-field theory appears to account for many qualitatitve features, which are seen in transtion metal oxides. The quantitative agreement for some properties is also surprisingly good.[7] The hope is that this limit will also be useful in understanding weakly doped Mott insulators.

There are now several studies of the mean-field Hubbard model away from half filling, using the quantum Monte Carlo method.[8–10] In particular, quantum Monte Carlo and the maximum entropy technique have been used to analyze the spectral functions of the doped Mott insulator for very small values of doping.[9] These studies have been interpreted as indicating that the chemical potential jumps from the upper to the lower Hubbard band upon doping away from half filling.[11] Studies of the doped Mott insulator, using an exact diagonalization algorithm,[12] have also been performed.[13,14] As in the half-filled case,[15] this method gives the general features of the phase diagram correctly, but the spectral functions calculated with this technique lack the resolution necessary to address the questions posed in this paper.

It is apparent, from the numerical studies, that the behavior near to the Mott phase in infinite $d$ is generally characterized by the vanishing of the renormalized Fermi energy. The presence of this small energy scale makes it difficult to analyze the low-energy behavior numerically. To overcome this problem, we use, here, the projective self-consistent method, which was introduced in a previous publication[16] to study the Mott transition at half filling. We thereby establish analytically that, contrary to expectations, doping the Mott insulator in large dimensions induces states *inside* the Mott Hubbard gap for all $U$ above the Mott transition value $U_c$. The discontinuity in chemical potential is, therefore, strictly smaller than the gap. We calculate this discontinuity as a function of interaction strength $U$ and conclude that the shift of the chemical potential from the band edge is appreciable for intermediate values of the interaction. Furthermore, we show that the naive Mott-Hubbard criterion, equality of the chemical potential and the band edge, represents the

*spinodal* line, i.e., the linear instability condition for the metastable insulating phase (which is strictly metastable in mean-field theory).

The Hamiltonian of the Hubbard model with coordination number $z$ is given by

$$H = -\frac{t}{\sqrt{z}} \sum_{\langle ij \rangle \alpha} (f_{i\alpha}^\dagger f_{j\alpha} + f_{j\alpha}^\dagger f_{i\alpha})$$
$$+ U \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow} - \mu \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha}, \qquad (1)$$

where the hopping is scaled as $t_{ij} \to t/\sqrt{z}$ (Ref. 6) to yield a sensible $z \to \infty$ limit. In the limit of infinite dimensions, all local correlation functions of the Hubbard model can be calculated in terms of an Anderson impurity model,[17] which focuses on a single site

$$\mathcal{H}_{\mathrm{AM}} = \sum_{k\alpha} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} + \sum_{k\alpha} V_k (f_\alpha^\dagger c_{k\alpha} + \mathrm{H.c.})$$
$$+ \epsilon_f f_\alpha^\dagger f_\alpha + U n_{f\uparrow} n_{f\downarrow}, \qquad (2)$$

the "bath" $\{c_{k\alpha}\}$ representing the electrons on other sites. The energy levels, $\epsilon_k$, and the hybridization couplings $V_k$ of the bath must satisfy a self-consistency condition, which involves the Hilbert transform $D_0(z)$ of the density of states $\rho_0(\epsilon)$ of the noninteracting system.

The impurity Green's function $G[\epsilon_k, V_k](i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau f_\alpha(\tau) f_\alpha^\dagger(0) \rangle_{\mathcal{H}_{\mathrm{AM}}[\epsilon_k, V_k]}$ is a functional of the parameters $\epsilon_k, V_k$, which must be determined self-consistently. Introducing the hybridization function,

$$\Pi(i\omega_n) \equiv \sum_k \frac{V_k^2/t^2}{i\omega_n - \epsilon_k} , \qquad (3)$$

$G$ will be a functional of $\Pi$, and the self-consistency reads simply,

$$D_0[G^{-1}\{\Pi\} + t^2 \Pi] = G\{\Pi\}. \qquad (4)$$

The position of the $f$ level $\epsilon_f$ in $\mathcal{H}_{\mathrm{AM}}$ equals minus the chemical potential of the Hubbard model.[17]

In order to make better contact with physical systems in finite dimensions for which the bandwidth is finite, we will consider bounded bare densities of states, and view Eqs. (2–4) as mean-field equations to be used for a finite dimensional system. For definiteness, our numerical results were obtained for the case of a semicircular bare density of states, $\rho_0(\epsilon) = \sqrt{4t^2 - \epsilon^2}/2\pi t^2$; in this case, the self-consistency equation that determines the parameters of the Anderson impurity model has the simple form

$$G[\epsilon_k, V_k](i\omega_n) = \Pi(i\omega_n). \qquad (5)$$

In this paper, we will focus entirely on paramagnetic states that are likely to be realized at sufficiently large $U$ in strongly frustrated models at all but very low temperatures. Note that for the fully frustrated completely connected graph with $t_{ij}$ *random* in sign, the density of states is a semicircle, there is no antiferromagnetism, and our results become exact.[19,20]

The equations for the hybridization function $\Pi(i\omega_n)$

are strongly nonlinear. We will show that, for $U$ sufficiently large, there is a finite range of chemical potential for which two solutions coexist; a doped metal and an undoped insulator. We will discuss first the conditions for the appearance of the doped metal, and then later argue that the insulator is metastable, disappearing at a spinodal line. We will focus on hole doping; particle doping is equivalent from the particle-hole symmetry of the Hubbard model under $\mu \to U - \mu$.

From extensive work on the half-filled Hubbard model in infinite dimensions, it is known that as the Mott transition is approached from below, a narrow Kondo resonance appears at low energies with a spectral weight, $w$, and concomitant energy scale, $wt$, which goes to zero continuously at a critical $U$, $U_c$. Numerical and other approximate work suggests that similar behavior occurs as the electron density is raised towards half filling for $U > U_c$: i.e., that a narrow quasiparticle resonance appears at the Fermi energy with weight and width which disappear at some critical chemical potential $\mu_c^-(U)$, corresponding to the lower range of $\mu$ for exactly half filling.[8–10]

To analyze the disappearance of the metallic state as $\mu \nearrow \mu_c^-$, we assume that this general behavior occurs, and we use the projective self-consistent method developed earlier to handle the small energy scale near the Mott transition. The key idea is to separate the set $\{k\}$ of "bath" electrons into sets $k\epsilon H$ and $k\epsilon L$ with corresponding couplings $\{\epsilon_k^H, V_k^H\}$ and $\{\epsilon_k^L, V_k^L\}$ describing the high- and low-energy features. We then project out the high-energy degrees of freedom to obtain an effective self-consistent problem for the spectral density, involving the low-energy variables only.

The spectral function of the quasiparticle resonance is $\rho^L(\epsilon) = \sum_k (V_k^L)^2 \delta(\epsilon - \epsilon_k^L)$, where $V_k^L = V_k$ for $k\epsilon L$ and zero otherwise; for notational clarity, we also affix an $L$ to $\epsilon_k$ and $c_{k\alpha}$ for $k\epsilon L$. The weight of this quasiparticle resonance, $w = \int d\epsilon \rho^L(\epsilon)$, is the small parameter in our (singular) perturbation theory. (Note that there is a formal similarity between $w$ and the Bose expectation value representing the mean-field value of the quasiparticle residue in the slave boson technique of Ref. 18.)

The projective self-consistent method allows a detailed analysis of the low-energy behavior by projecting the system Eqs. (2–4) containing three energy scales $wt$, $t$, and $U$ onto a system in which only the smallest energy scale $wt$ appears. The projected self-consistency condition will require that the impurity low-energy Green's function $G_L$, calculated with an effective Hamiltonian $\mathcal{H}_L^{\mathrm{eff}}$, is related to the low-energy part of the hybridization function, $\Pi_L(i\omega_n) \equiv \sum_{\alpha, k \in L} \frac{(V_k^L)^2/t^2}{i\omega_n - \epsilon_k^L}$. For the semicircular bare density of states case, we simply have

$$G_L(i\omega_n, \{\Pi_L\}) = \Pi_L(i\omega_n), \qquad (6)$$

where the low-energy Green's function, $G_L$, is the time ordered Green's function under the low-energy Hamiltonian $\mathcal{H}_L^{\mathrm{eff}}$ of an operator $\sqrt{w} F_\alpha$, representing the action of the operator $f_\alpha$ of the original Anderson model $\mathcal{H}_{\mathrm{AM}}$ at low energies.

To construct the effective operators and the effective Hamiltonian to leading order in $w$, we first separate the impurity Hamiltonian Eq. (2) into three parts as

$$\mathcal{H}_{AM} = \mathcal{H}_a + \mathcal{H}_b + \mathcal{H}_m . \tag{7}$$

The high-energy ("atomiclike") part $\mathcal{H}_a$ is given by

$$
\mathcal{H}_a = U n_{f\uparrow} n_{f\downarrow} - \mu(n_{f\uparrow} + n_{f\downarrow})
$$
$$
+ \sum_{\alpha, k \in H} V_k^H (f_\alpha^\dagger c_{k\sigma}^H + \text{H.c.})
$$
$$
+ \sum_{\alpha, k \in H} \epsilon_k^H (c_{k\alpha}^H)^\dagger c_{k\alpha}^H . \tag{8}
$$

To zeroth order in $w$, this high-energy part will be the Hamiltonian of the half-filled Mott insulator. It thus has a spin doublet pair of ground states $|+\rangle_a$, $|-\rangle_a$. We define Hubbard operators $X_{\alpha\beta} = |\alpha\rangle_a \, _a\langle\beta|$ acting on this low-energy impurity doublet.

The low-energy spectrum of the impurity Hamiltonian consists of this doublet combined with excitations of the low-energy bath electrons, which have Hamiltonian

$$\mathcal{H}_b = \sum_{\alpha, k \in L} \epsilon_k^L (c^L{}_{k\alpha})^\dagger c^L{}_{k\alpha}. \tag{9}$$

These low-energy states are mixed with the high-energy excitations of $\mathcal{H}_a$, by

$$\mathcal{H}_m = \sum_{\alpha, k \in L} V_k^L (f_\alpha^\dagger c_{k\alpha}^L + \text{H.c.}) , \tag{10}$$

since $f_\alpha^\dagger$ or $f_\alpha$ acting on $|\pm\rangle_a$ create particle or hole states with energies increased by at least the particle or hole gap. It is convenient to define canonically normalized operators of the local low-energy bath electrons at the impurity site,

$$c_{L\alpha} \equiv \frac{1}{\sqrt{w}} \sum_{k \in L} V_k^L c_{k\alpha}^L ; \tag{11}$$

the mixing term is then simply

$$\mathcal{H}_m = \sqrt{w} t (f_\alpha^\dagger c_{L\alpha} + \text{H.c.}), \tag{12}$$

whose perturbative nature is manifest.

The effective Hamiltonian, $\mathcal{H}_{\text{eff}}^L$, of the low-energy Hilbert space, $|\pm\rangle_a \otimes \{k \in L\}$, can now be found by conventional perturbation theory in $\mathcal{H}_m$. The form of $\mathcal{H}_m$ and the intermediate excited states of $\mathcal{H}_a$ give rise to couplings in $\mathcal{H}_{\text{eff}}^L$ expressible in terms of Green's functions of $\mathcal{H}_a$. Defining at zero-temperature

$$
G_{\mu\nu,\alpha\beta}^a(i\omega, \mu) = -\int_{-\infty}^\infty d\tau \, _a\langle\mu|T_\tau f_\alpha(\tau) f_\beta^\dagger(0)|\nu\rangle_a e^{i\omega\tau}
$$
$$
= \left\langle \mu \left| f_\alpha \frac{1}{i\omega + E_g^a - \mathcal{H}_a} f_\beta^\dagger \right| \nu \right\rangle_a \tag{13}
$$
$$
- \left\langle \mu \left| f_\beta^\dagger \frac{1}{-i\omega + E_g^a - \mathcal{H}_a} f_\alpha \right| \nu \right\rangle_a , \tag{14}
$$

spin symmetry requires that

$$G_{\mu\nu,\alpha\beta}^a = \Lambda \delta_{\mu\nu}\delta_{\alpha\beta} + \Gamma(2\delta_{\alpha\nu}\delta_{\beta\mu} - \delta_{\mu\nu}\delta_{\alpha\beta}), \tag{15}$$

with $\Lambda = \frac{1}{2} \sum_\mu G_{\mu\mu,\uparrow\uparrow}^a$ the incoherent linear combination that enters the self-consistency condition Eq. (12) in the insulating phase.

Notice that the Green's functions appearing in Eq. (14) are functions of $\omega$, $\mu$, and $U$, but depend on $\mu$ and $\omega$ only via the combination $i\omega + \mu$, because the ground states of the insulator are independent of the value of the chemical potential. In the following discussion of the destruction of the metallic state, we will evaluate the Green's functions of Eq. (14) at zero frequency, and study their dependence on chemical potential, denoting $\Lambda(i\omega = 0)$ and $\Gamma(i\omega = 0)$ simply as $\Lambda$ and $\Gamma$.

The effective low-energy Hamiltonian is found to be

$$\mathcal{H}_{\text{eff}}^L = \mathcal{H}_b + J \vec{S}_a \cdot \vec{s}_L + K \sum_\alpha c_{L\alpha}^\dagger c_{L\alpha} + \text{const}, \tag{16}$$

with

$$\vec{S}_a = \frac{1}{2} \sum_{\alpha\beta} X_{\alpha\beta} \vec{\sigma}_{\alpha\beta} \quad \text{and} \quad \vec{s}_L = \frac{1}{2} \sum_{\alpha\beta} c_{L\alpha}^\dagger c_{L\beta} \vec{\sigma}_{\alpha\beta} \tag{17}$$

the effective spin operators acting on the ground states of $\mathcal{H}_a$ and on the low-energy local bath electrons, respectively. The spin and potential couplings are simply

$$J = 4wt^2\Gamma \tag{18}$$

and

$$K = wt^2\Lambda . \tag{19}$$

The effective operator which, acting on the ground state $|g_L\rangle$ of $\mathcal{H}_{\text{eff}}^L$, gives the low-energy part of the Green's function $G_L$, is

$$\sqrt{w} F_\alpha = -\sqrt{w} t \Lambda c_{L\alpha} - 2\sqrt{w} t \Gamma \sum_\beta c_{L\beta} X_{\beta\alpha} , \tag{20}$$

with

$$G_L(\tau) = -w\langle g_L | T_\tau F_\uparrow(\tau) F_\uparrow^\dagger(0) | g_L \rangle . \tag{21}$$

At frequencies high compared to the low-energy scale $wt$ but still small, the self-consistency condition for the semicircular case $\Pi_L = G_L$ reduces to $\langle \{F_\uparrow, F_\uparrow^\dagger\}\rangle_L = 1$, with $\langle\rangle_L$, denoting expectations in the ground state $|g_L\rangle$ of $\mathcal{H}_{\text{eff}}^L$. This yields the requirement that

$$t^2[\Lambda^2 + 3\Gamma^2 - 8\Gamma^2 \langle \vec{S}_a \cdot \vec{s}_L \rangle_L] = 1 \tag{22}$$

to leading order in $w$.

The condition Eq. (22) implies that for a self-consistent solution to exist in the limit of small $w$, $\Lambda$ and $\Gamma$ must be of order $1/t$, implying $J \sim K \sim wt$. The full low-energy self-consistency, which has the form $\Pi_L = G_L$ for the semicircular case, is more generally

$$G_a(0) + G_L = D_0\left[\frac{1}{G_a(0) + G_L} + t^2[\Pi_L + \Pi_a(0)]\right], \tag{23}$$

where $G_a(0) = \Lambda$, and $\Pi_a(i\omega = 0)$ satisfy the mean-field equations in the insulating phase $G_a(i\omega) = D_0[G_a(i\omega) +$

$t^2 \Pi_a(i\omega)$]. The $t^2$ in Eq. (22) is then replaced by $\Lambda^{-2} + dP_0(\Lambda)/d\Lambda$, with $P_0(\Lambda)$ the inverse of the Hilbert transform $D_0$. The solutions of the low-energy self-consistent problem are such that the $\{\epsilon_k^L\}$ are of order $wt$. This is to be expected: in infinite $d$, Fermi liquid theory implies that in a paramagnetic metal, the density of states at the Fermi level is unchanged by the interactions at fixed particle number, therefore for the low-energy spectral density to have weight $w$, it must have energy scale $wt$ even for large $U$.[21]

In the limit of small $w$, higher order corrections to $\mathcal{H}_{\rm eff}^L, F_\alpha$, and the high-energy parts of the self-consistency conditions are negligible. A (unique) self-consistent solution to the $w$-independent low-energy problem given by Eqs. (16), (20), and (23) can then be found only for a one parameter family of $\Lambda, \Gamma$. Since these are properties of the Mott-insulating state, depending smoothly on $U$ and $\mu$, a metallic solution with a narrow quasiparticle resonance with infinitesimal weight $w$ can occur for each $U > U_c$, only for a specific pair of values of chemical potential $\mu_c^{\pm}(U)$ corresponding to infinitesimal particle or hole doping. Note that particle-hole symmetry implies that $\mu_c^- = U - \mu_c^+$, it is thus convenient to define $\tilde{\mu} = \mu - \frac{U}{2}$, so that $\tilde{\mu}_c^- = -\tilde{\mu}_c^+$.

What is the physical significance of the critical $\mu_c^{\pm}(U)$? For $\mu \geq \mu_c^+$ or $\mu \leq \mu_c^-$, the numerical solution of the full self-consistent problem indicates that higher order terms in $w$ will stabilize the width of the narrow resonance. The form of these higher order terms, which can, in principle, be computed in detail, indicate that, for, e.g., hole doping, $w \sim \frac{\mu_c^- - \mu}{t}$. But a straightforward perturbative analysis shows that a continuation of the insulating solution will also persist beyond $\mu_c^{\pm}$. Thus, we must determine which solution has lower (free) energy $E(\tilde{\mu}, U)$ (at zero-temperature $F = E = \langle \mathcal{H} \rangle$ as we have incorporated $-\mu \hat{N}$ into $\mathcal{H}$). As discussed in Ref. 16, this can be determined by considering $-\frac{\partial F}{\partial U}|_{\tilde{\mu}}$, which is simply proportional to the fraction, $n_s$, of singly occupied sites. The metallic solution for small $w$ can readily be shown to sacrifice potential energy to gain kinetic energy by decreasing $n_s$ relative to the insulating solution by $O(w)$. Integration of $\frac{\partial F}{\partial U}|_{\tilde{\mu}}$ down from $U_c(\tilde{\mu})$ then yields that the weakly doped metallic phase has *lower* energy than the continuation of the insulating phase: $E_M \sim E_I - C(\mu - \mu_c)^2$. The insulator is thus *unstable* to the nonlinear formation of a large amplitude [the peak of $\rho^L(\epsilon)$ is of order $1/t$] narrow resonance at the Fermi level for $\mu$ just beyond $\mu_c$. We now turn to the computation of $\mu_c^{\pm}(U)$ and show that, as claimed, they are strictly inside the Mott gap of the insulator.

The determination of the critical $\mu_c^{\pm}(U)$ has, as described above, been reduced to two self-consistent problems, each with a single energy scale. The low-energy self-consistent effective Hamiltonian, $\mathcal{H}_{\rm eff}^L$, can be found rather well for any fixed ratio of $\Lambda/\Gamma$ by representing the bath plus the impurity approximately by a small cluster of sites. As discussed in Ref. 16, with judicious choice of the parametrization and means of approximating the self-consistency conditions, studies of clusters of size $N = 4, 6, 8$, and $10$ are found to have converged

by $N = 8$. For fixed $\Lambda/\Gamma$, the critical value of $\Gamma$ (and hence, $\Lambda$) is determined uniquely by the low-energy self-consistent solution, from Eq. (22). For $\Lambda/\Gamma = 0$, this reduces to the symmetric half-filled problem at $U = U_c$ and half filling, $\mu_c^{\pm} = \frac{U_c}{2}$.

In principle, the needed quantities from the high-energy parts, $\Gamma(\mu, U)$ and $\Lambda(\mu, U)$ can also be determined numerically by computing the self-consistent insulating solution. This works well for $U$ not too much larger than $U_c$, from which it is found that, $\tilde{\mu}_c^{\pm} \sim \pm\sqrt{U - U_c}$ for $U \geq U_c$, as expected from smoothness, with $\tilde{\mu}_c^{\pm}$ approaching nearer to the numerically determined upper (and lower) Hubbard band edges as $U$ increases. Unfortunately, for larger $U$, the proximity of $\mu_c$ to the band edges causes numerical problems; thus, an analytic method is needed.

In the limit $U \gg t$, the insulating solution becomes simple with spectral density consisting of an upper and lower Hubbard band with the two band centers separated by $U$. For the *semicircular case*, the Hubbard bands have the same shape as the bare density of states and the Green's function at zero energy for $\mu$ near the lower Hubbard band is simply

$$\Gamma \approx \Lambda \approx G^a(0) = \frac{1}{4t^2}\left(\mu - \sqrt{\mu^2 - 4t^2}\right). \quad (24)$$

The critical $\mu_c^-$ is then given by

$$\mu_c^- \approx 2t\left(\frac{1 - A_L}{\sqrt{1 - 2A_L}}\right), \quad (25)$$

where

$$A_L \equiv \langle \vec{S}_a \cdot \vec{S}_L \rangle_L . \quad (26)$$

We thus see that as long as $A_L$ is negative, which it must be because of the antiferromagnetic exchange in $\mathcal{H}_{\rm eff}^L$, $\mu_c^-$ will be *strictly* greater than the band edge at $2t$. Numerical solution of the low-energy problem yields, for $\Lambda/\Gamma = 1, A_L \approx -0.23$ (about half the value for the particle-hole symmetric case analyzed previously). We therefore obtain

$$\mu_c^- \approx 2.036t , \quad (27)$$

very close to, but still of order $t$ above, the lower Hubbard band edge at $2t$.

For intermediate values of $U$, the needed Green's functions $\Gamma$ and $\Lambda$ can be obtained either numerically or by a perturbation expansion in $t/U$;[22] the lowest nontrivial order in $t/U$, properly symmetrized, agrees with the numerics down to $U_c$. The full critical curve $\mu_c^-(U)$ for the semicircular bare density of states case can then be obtained by combining this with the numerical solution of the low-energy problem, the results are plotted in Fig. 1.

To show that, for general bare density of states, doping always creates states inside the Mott Hubbard gap, we must examine the conditions that determine the band edges of the insulator. For this purpose, we use techniques similar to the ones used to study the disappearance of the metal, with the part of the spectral density
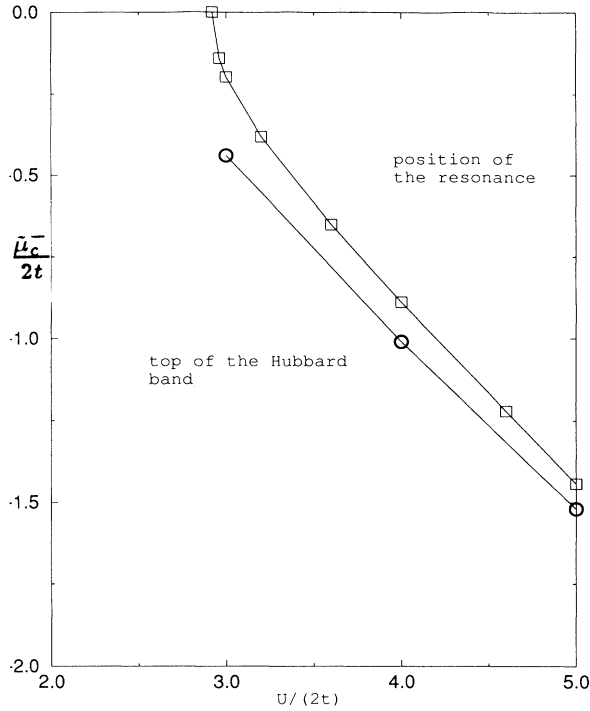
FIG. 1. Position of the quasiparticle resonance $\tilde{\mu}_{\bar{c}}$ for infinitesimal doping as a function of the interaction strength (squares). The circles indicate the top of the lower Hubbard band $\tilde{\mu}_s$ ($\tilde{\mu}_s = \mu_s - u/2$) measured with respect to the chemical potential at half filling. The results for $\tilde{\mu}_{\bar{c}}$ are accurate within 3% while the error bars in the determination of $\tilde{\mu}_s$ are three times as large, due to the finite-size effects near the band.

of the bath of conduction electrons near the band edge of the interacting theory, $\Pi^{\text{sing}}$, playing the role of the low-energy density of states $\Pi_L$ in the previous paragraphs. The problem is well posed only for a bare density of states $\rho_0(\epsilon)$, with *bounded* support. It can be shown that, in this case, the density of states of the "bath" electrons, $-\frac{1}{\pi}\text{Im}\Pi(\epsilon + i0)$, must vanish continuously at the band edge in the interacting system. This implies that the impurity will be only weakly coupled to the bath electrons near the band edge. In the following analysis, the Green's functions in Eq. (14) are evaluated as a function of $\omega$ with the chemical potential set equal to its half-full value $\mu = U/2$; generalization to other $\mu$ in the insulating phase is trivial.

The singular part of the impurity Green's function, $G$, near a band edge will be dominated by processes in which the impurity electron at some time hops into a near-band-edge bath state remains there for a long time, and then hops back. Other processes will involve integrals over intermediate energies and thus give rise to less singular contributions to $G$. The full amplitude for the impurity electron to hop into a near-band-edge bath state will be given in terms of the Green's functions of $f$ excluding the near-edge part of the bath. But since the bath spectral density is small near the edge, these will essentially be those of the full impurity-bath system. An explicit calculation in a controlled expansion of the near-edge parts

of the bath yields, for $i\omega$ near the band-edge energy, $b$,

$$G^{\text{sing}}_{\alpha\beta} \approx \frac{t^2}{2} \sum_{\mu\nu} G_{\mu\nu,\alpha\gamma}(b)\Pi^{\text{sing}}_{\gamma\delta}(i\omega)G_{\nu\mu,\delta\beta}(b), \quad (28)$$

with $\alpha, \beta, \gamma, \delta$ spin indices and $G_{\alpha\beta} = G\delta_{\alpha\beta}$ (and similarly for $\Pi_{\gamma\delta}$) from spin rotational invariance. Note that Eq. (28) includes the effects of the added electron exchanging spin with the spin of the ground state of the insulator [$|\nu\rangle_a$ to $|\mu = -\nu\rangle_a$] and creating a near-edge bath electron with the opposite spin.

From Eq. (28), we see that

$$G^{\text{sing}} \approx t^2[\Lambda^2(b) + 3\Gamma^2(b)]\Pi^{\text{sing}} , \quad (29)$$

where $\Lambda(b)$ and $\Gamma(b)$ are Green's functions of the insulating phase at the band edge; these are identical to those at zero frequency with the chemical potential corresponding to the band edge. For the semicircular case, the self-consistency condition simply implies that

$$\Lambda^2(b) + 3\Gamma^2(b) = 1/t^2 , \quad (30)$$

more generally, the condition will involve the derivative of the inverse $P_0$, of the Hilbert transform $D_0$:

$$\left[\Lambda^{-2} + \frac{dP_0}{d\Lambda}(\Lambda)\right](\Lambda^2 + 3\Gamma^2) = 1. \quad (31)$$

The condition Eq. (31) is seen to be exactly that for the instability of the insulator to a narrow resonance with the Fermi level at $b$—the generalization of Eq. (22)—but with the factor $A_L = 0$, i.e., no singlet developed. Because $\Lambda^2$ and $\Gamma^2$ increase as the energy moves away from a band edge into the gap, the nonlinear instability to the metal will always occur, since $A_L$ is strictly negative, for $\mu$ strictly inside the gap, as claimed. Note that the condition Eq. (31) corresponds to the condition for a *linear* instability of the insulating solution to a small spectral feature at the Fermi energy.

The insulating solution disappears when the system Eqs. (2–4) cannot be solved in the space of functions satisfying $\text{Im}G(i\omega_n) \to 0$ at low frequencies, i.e., insulating solutions. In this space, an insulating solution is extendable to a slightly changed $U$, provided that the matrix

$$M_{m,n} - \delta_{m,n} \equiv \frac{\delta G(i\omega_n)}{\delta\Pi(i\omega_m)} - \delta_{m,n} , \quad (32)$$

with $\omega_{m,n}$ Matsubara frequencies, is invertible. This ceases to occur when one of the eigenvalues of $M_{m,n}$ becomes equal to one; this corresponds to a spinodal line, and occurs at $\mu = \mu_s^{\pm}(U)$. The matrix $M_{m,n}$ is given by a connected correlation function of the impurity model;[23] it is closely connected to the matrix $\chi^L_{m,n}$, whose trace gives the compressibility (in the semicircular case), $\frac{dn}{d\mu} = \text{tr}[\chi^L_{m,n}]$, via $(\chi^L)^{-1} = t^2(I - M^{-1})$. The zero eigenvalue associated with the linear instability condition thus corresponds to an infinite eigenvalue in the compressibility matrix $\chi^L_{m,n}$. If the eigenvector corresponding to the first eigenvalue of $M$ to become unity involves spectral density in the gap, the analysis becomes

just like that used above to determine the band edge and similar to that for the metallic instability, but with $A_L = 0$. The important part of $M_{m,n}$ is $\delta_{mn}$ times the combination of $G$'s that relates $\Pi^{\mathrm{sing}}$ to $G^{\mathrm{sing}}$ in Eq. (28), here evaluated at $b = 0$ and viewed as a function of the chemical potential.

We thus see that, unless some other instability intervenes, the condition for the spinodal line $\mu_s^\pm(U)$ is that the chemical potential coincides with the band edge and that the phase transition occurs at $\mu_c^\pm$ with $|\mu_c^\pm| < |\mu_s^\pm|$. The same arguments show that at half filling the insulating solution becomes unstable at a value $U_s$ (called $U_{c1}$ in Refs. 10 and 20) strictly less than $U_c$.

In this paper we have shown that, contrary to dominant current views in the literature, the states induced in doping of the Mott-insulating phase of the Hubbard model on strongly frustrated lattices lie *within* the Mott Hubbard gap. The splitting of these states from the edge of the Hubbard band is of order $t$, but, in practice, may be appreciable only for values of $U$ close to the Mott transition.

For unfrustrated lattices, antiferromagnetism will certainly occur for intermediate $U$ at temperatures much greater than the energy scales involved in the weak-doping physics discussed here. Nevertheless, for large $U$ our results may still be informative. We consider bipartite lattices, such as the infinite coordination number Bethe lattice, which has a semicircular bare density of states. The simplest scenario involves only two phases: the undoped commensurate antiferromagnet, and a doped paramagnetic metal. For $U \gg t$, the energy of the antiferromagnetic solution at half filling will be lower than the paramagnetic solution by an amount of order $t^2/U$ (i.e., the Heisenberg exchange energy). But as the chemical potential is lowered through, say, $\mu_c^-$, the difference in energy will become

$$E_P - E_{AF} \approx C_A t^2/U - C_B(\mu_c^- - \mu)^2/t \qquad (33)$$

[with coefficients $C_A, C_B = O(1)$]. Thus, when $\mu < \mu_A$ with $\mu_c^- - \mu_A \approx \sqrt{\frac{C_A}{C_B}} \frac{t^{3/2}}{U^{1/2}}$, the paramagnetic metal will

have lower energy. For $U \gg t$, this will occur when the position of the narrow quasiparticle resonance is still of order $t$ above the main lower Hubbard band, but its width is only of order $t^{3/2}/U^{1/2}$. Thus, for doping $\delta$ less than some value $\delta_A$, the system will phase separate into an undoped antiferromagnet and a doped paramagnet with doping $\delta_A \sim \sqrt{t/U}$ and a narrow quasiparticle resonance with weight $w$ of order $\delta_A$. The effect of extra repulsive interactions, which suppress phase separation and can lead to regimes of doped antiferromagnet, will be discussed elsewhere.

We thus see that even in more realistic situations, it is still possible, within the infinite-$d$ mean-field theory, to get a regime of small doping with a narrow resonance at the Fermi surface. This results from the effects of strong correlations and makes the problem of doping the Mott insulator very different from the doping of an ordinary band insulator.

In finite dimensions the problem is still open. But a serious cautionary note is in order: the conventional wisdom on this problem is based on numerical calculations on small systems, or at rather high temperatures. When similar techniques are applied to the infinite dimensional Hubbard model, they *miss* the effects discussed here, yielding the erroneous result that doping creates states *within* the Hubbard bands.[11]

A crucial aspect of the mean-field theory of correlated Fermi systems is not understood: whether it shares with its classical counterpart a variational character. If this is the case, then our results could be used as the basis of calculations, which might provide a bound on the value of the chemical potential needed to dope a Mott insulator, at least in the limit of large $U$ where the effects of exchange are small. Resolving the subtle problem of weakly doped Mott insulators may have to wait for progress in this direction.

[1] For a review, see E. Dagotto, in Rev. Mod. Phys. **66**, 763 (1994).

[2] F. Woynarovich, J. Phys. C **15**, 85 (1982); **15**, 97 (1982).

[3] N. Bulut, D. J. Scalapino, and S. White, Phys. Rev. B **50**, 7215 (1994).

[4] C. Castellani, G. Kotliar, R. Raimondi, M. Grilli, Z. Wang, and M. Rozenberg, Phys. Rev. Lett. **69**, 2009 (1992).

[5] H. Jichu, T. Matsuura, and Y. Kuroda, J. Phys. Soc. Jpn. **58**, 4280 (1989); **59**, 2820 (1990).

[6] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).

[7] G. A. Thomas *et al.*, Phys. Rev. Lett. **73**, 1529 (1994); M. Rozenberg *et al.*, *ibid.* **75**, 105 (1995).

[8] M. Jarrell and T. Pruschke, Phys. Rev. B **49**, 1458 (1993); T. Pruschke, D. L. Cox, and M. Jarrell, Europhys. Lett. **21**, 593 (1993); Phys. Rev. B **47**, 3553 (1993).

[9] M. Jarrell and T. Pruschke, Z. Phys. B **90**, 187 (1993).

[10] M. J. Rozenberg, G. Kotliar, and X. Y. Zhang, Phys. Rev. B **49**, 10 181 (1994); G. Kotliar and M. Rozenberg, in *Proceedings of the Conference on the Mathematics and Physics of the Hubbard Model*, edited by D. Baeriswyl, D. Campbell; J. M. P. Carmelo, F. Guinea, and E. Louis (Plenum, New York, 1995).

[11] Th. Prushke, M. Jarrell, and J. Freericks, Adv. Phys. (to be published).

[12] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994).

[13] G. Moeller, Ph.D. thesis, Rutgers University, 1994.

[14] H. Kajueter, G. Kotliar, and G. Moeller (unpublished).

[15] M. Rozenberg, G. Moeller, and G. Kotliar, Mod. Phys. Lett. B **8**, 535 (1994).

[16] G. Moeller, Q. Si, G. Kotliar, M. Rozenberg, and D. Fisher,

Phys. Rev. Lett. **74**, 2082 (1995).

[17] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).

[18] G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).

[19] M. J. Rozenberg, X. Y. Zhang, and G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992).

[20] A. Georges, and W. Krauth, Phys. Rev. B **48**, 7167 (1993).

[21] E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989); **76**, 211 (1989).

[22] J. Ye and D. S. Fisher (unpublished).

[23] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg (unpublished).