Critical Behavior near the Mott Transition in the Hubbard Model

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(Received 10 January 1994; revised manuscript received 29 June 1994)

We introduce a systematic approach to analyze the low-energy behavior of strongly correlated electron systems in infinite dimensions, and apply it to the metal-insulator transition in the half-filled Hubbard model. We determine the low-energy scaling functions of the metallic state, including the single-particle Green function and dynamical spin susceptibility, as well as thermodynamic properties. Comparisons are made with experimental data on transition metal oxides.

PACS numbers: 71.27.+a, 71.28.+d, 74.20.Mn

The interaction-driven metal-insulator transition is a fundamental problem in condensed matter physics which is fascinating because of its nonperturbative nature and the emergence of new low-energy scales. Early ideas of Mott [1], Hubbard [2], Brinkman and Rice [3] have recently been put on a more quantitative footing by a mean-field approach which is exact in the limit of large lattice coordination [4]. In infinite dimensions it is possible to construct models which do not order magnetically down to zero temperature irrespective of the proximity to the transition (see below). Such a treatment is relevant to systems close to the interaction-driven metal-insulator transition but have not ordered magnetically. The approach to the Mott transition was found to be characterized by the vanishing of the renormalized Fermi energy [5]. This small energy scale makes it difficult to analyze the critical behavior.

In this Letter, we introduce a new projective self-consistent approach for correlated electrons in large dimensions. Using the separation of energy scales, we obtain exact low-energy information about the critical behavior on the metallic side of the Mott transition in infinite dimensions. The divergent linear specific heat coefficient γ, the local susceptibility $\chi_{\rm loc}(\omega)$, and the single-particle spectral function, relevant for photoemission, are calculated. The ratio of the static $\chi_{\rm loc}(0)$ to γ is found to approach a constant, yielding a generalized Wilson ratio, while the low frequency $\chi''_{\rm loc}(\omega)/\omega$, relevant for NMR and neutron scattering, is $O(\gamma^2)$. Finally, the coefficient of the ω^2 term in the imaginary part of the self-energy diverges as γ^2; this is related to the observed T^2 resistivity in the $LaTiO_3$ system [6–8].

The Hamiltonian of the half-filled Hubbard model is given by $\mathcal{H} = -(t/\sqrt{d})\sum_{\langle ij\rangle\sigma} f^\dagger_{i\sigma} f_{j\sigma} + U\sum_i (f^\dagger_{i\uparrow} f_{i\uparrow} - \frac{1}{2})(f^\dagger_{i\downarrow} f_{i\downarrow} - \frac{1}{2})$ where the hopping is scaled as $t_{ij} \to t/\sqrt{d}$ [4]. In the limit of infinite dimensions, all local correlation functions of the lattice model can be calculated in terms of an Anderson impurity model [9] $\mathcal{H}_{\rm AM} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} V_k (f^\dagger_\sigma c_{k\sigma} + \text{H.c.}) + U(n_{f\uparrow} - \frac{1}{2})(n_{f\downarrow} - \frac{1}{2})$ provided that the bath dispersion ϵ_k and the hybridization coupling V_k satisfy a self-consistency condition which involves the density of states $\rho_0(\epsilon)$ of the noninteracting system. In order to make better contact with physical systems in finite dimensions, for which the bandwidth is finite, we consider the case of a semicircular bare density of states, $\rho_0(\epsilon) = (2/\pi D)\sqrt{1 - (\epsilon/D)^2}$ for which the self-consistency equation has the simple form

$$G(i\omega_n) = \Pi(i\omega_n) \equiv \sum_k \frac{4V_k^2/D^2}{i\omega_n - \epsilon_k}. \qquad (1)$$

Here, $G[\epsilon_k, V_k](i\omega_n) = -\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle T_\tau f_\sigma(\tau) \times f^\dagger_\sigma(0)\rangle_{H_{\rm AM}[\epsilon_k, V_k]}$ is the impurity Green function which is a functional of the parameters ϵ_k, V_k to be determined self-consistently. We are interested in highly frustrated lattices that have any magnetic transitions that might occur suppressed to low temperatures; we thus study only paramagnetic solutions. 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 magnetic order, and our results become exact [10,11].

Numerical and other approximate solutions [5,10–12] of the self-consistent Anderson model have shown that as the interaction strength U increases, the self-consistent single-particle density of states, $\rho(\epsilon) = -\frac{1}{\pi}\,\mathrm{Im}G(\epsilon + i0)$, develops a narrow peak about zero energy separated by regions of low spectral density from peaks near $\pm U/2$ as shown in Fig. 1. At a critical value of U, U_c, the narrow peak appears to vanish [5], leaving a paramagnetic insulating solution with a finite gap. Just below U_c there is a separation of energy scales such that $\rho(\epsilon)$ and the one-particle Green function can be decomposed into a sum of a low- and a high-energy part as $\rho(\epsilon) = \rho^L(\epsilon) + \rho^H(\epsilon)$ and $G = G_L + G_H$. $\rho^L(\epsilon)$ contains all states up to a cutoff intermediate between the low-energy bandwidth, D^L, and U with spectral weight $w = \int d\omega\, \rho^L(\omega)$. The upper and lower Hubbard bands, with energies near $\pm U/2$, are represented by ρ^H. The self-consistent equation (1) implies that the parameters $\{\epsilon_k, V_k\}$ can be separated into a low-energy set $k \in L$ and a high-energy set $k \in H$; these we denote by $\{\epsilon^L_k, V^L_k\}$ and $\{\epsilon^H_k, V^H_k\}$. This separation allows us to divide the set of

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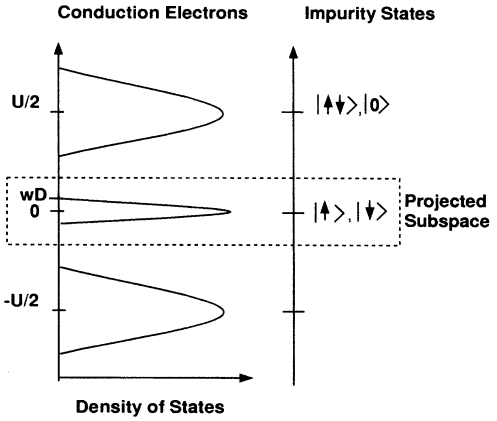

FIG. 1. Schematic plot of the spectral functions of the conduction electrons and the impurity configurations, illustrating the narrow low-energy and broad high-energy parts.

operators c_k into a low-energy set, those having $k \in L$, and a high-energy set, those having $k \in H$; we call them $c^L_{k\sigma}$ and $c^H_{k\sigma}$, respectively. It should be noted that, here, "k" is a dummy variable labeling the states in the bath of conduction electrons of the Anderson model; it should not be confused with the Bloch wave vector quantum number of electrons in the original Hubbard model.

Just below U_c, w is small and $D^L \sim wD \ll U$, making the problem numerically intractable. Our main idea is to project out the high-energy states to obtain a low-energy effective problem involving ρ^L only and hence only one energy scale. This is in the same spirit as Landau theory: The focus is on the low-energy degrees of freedom represented conventionally by an order parameter and here by ρ^L, while the effects of the high-energy degrees of freedom are contained in a few coefficients. In our case, both these coefficients and the minimization over the "direction" of the order parameter—i.e., the shape of $\rho^L(\epsilon)$—must be obtained numerically.

We first separate the impurity Hamiltonian into three parts as $\mathcal{H}_{\rm AM} = \mathcal{H}_a + \mathcal{H}_b + \mathcal{H}_m$ with

$$\mathcal{H}_a = \frac{U}{2}\left(n_{f\uparrow} - \frac{1}{2}\right)\left(n_{f\downarrow} - \frac{1}{2}\right) + \sum_{\sigma,k}^{H} V^H_k (c^\dagger_{k\sigma} f_\sigma + \text{H.c.}) + \sum_{\sigma,k}^{H} \epsilon^H_k c^\dagger_{k\sigma} c_{k\sigma}\,, \tag{2}$$

analogous to the Hamiltonian of an Anderson impurity in a semiconductor. $\mathcal{H}_b = \sum^L_{k,\sigma} wD\tilde{\epsilon}_k c^\dagger_{k\sigma} c_{k\sigma}$ is the low-energy conduction electron kinetic energy in terms of rescaled variables $\tilde{\epsilon}_k = \epsilon^L_k/wD$. The hybridization with the low-energy electrons is $\mathcal{H}_m = \sqrt{w}\, D \sum_\sigma (c^\dagger_{L\sigma} f_\sigma +$ H.c.) with $c_{L\sigma} \equiv \sum^L_k 2\tilde{V}_k c^L_{k\sigma}$ the local low-energy operators with $\{c_{L\sigma}, c^\dagger_{L\sigma}\} = 1$ and $\tilde{V}_k = V^L_k/\sqrt{w}\, D$ showing explicitly the perturbative nature of the hybridization with the low-energy band.

The ground states of $\mathcal{H}_a$ are a spin doublet $|\sigma\rangle_a$ with energy E^a_g separated by a gap of order U from the excited states. We can therefore perform a canonical transformation to project out the excited states of $\mathcal{H}_a$ and derive an effective Hamiltonian, $\mathcal{H}^{\rm eff}_L$, which acts on the low-energy Hilbert space $\{|\sigma\rangle_a\} \otimes \{$states of the $c^L_{k\sigma}\}$. If the excited states were only the empty and the doubly occupied site, this would be a Schrieffer-Wolff canonical transformation [13]. To lowest order in w,

$$\mathcal{H}^{\rm eff}_L = \mathcal{H}_b - \frac{wD^2}{4}\sum_{\sigma\sigma'} c^\dagger_{L\sigma} c_{L\sigma'} X_{\sigma'\sigma} \times \left({}_a\langle\sigma'|f_\sigma \frac{1}{H_a - E^a_g} f^\dagger_{\sigma'}|\sigma\rangle_a - {}_a\langle\sigma'|f^\dagger_{\sigma'} \frac{1}{H_a - E^a_g} f_\sigma|\sigma\rangle_a \right) + \text{const}, \tag{3}$$

where $X_{\sigma\sigma'} \equiv |\sigma\rangle_{aa}\langle\sigma'|$ project onto the ground states of $\mathcal{H}_a$. To the needed accuracy, the $\{V^H_k, \epsilon^H_k\}$ are those of the *insulating* solution of the infinite d Hubbard model [14,15] at U_c, which can be readily obtained numerically as the insulator has only one energy scale.

Because of rotational invariance, the matrix elements in Eq. (3) reduce to a single number, $\Gamma \equiv {}_a\langle\uparrow|f_\downarrow \frac{1}{H_a - E^a_g} f^\dagger_\uparrow \times |\downarrow\rangle_a$. We then have an intermediate coupling Kondo problem with a single energy scale wD, exchange $J = -wD^2\Gamma + O(w^2)$, and Hamiltonian

$$\mathcal{H}^{\rm eff}_L = J\{\vec{S}\}_a \cdot \{\vec{S}\}_L + \mathcal{H}_b + \text{const} + O(w^2)\,, \tag{4}$$

with $\vec{S}_a = \frac{1}{2}\sum_{\sigma\sigma'} X_{\sigma\sigma'}\vec{\sigma}_{\sigma\sigma'}$ acting on the $\{|\sigma\rangle_a\}$ and $\{\vec{S}\}_L = \frac{1}{2}\sum_{\alpha\beta} c^\dagger_{L\alpha}\vec{\sigma}_{\alpha\beta} c_{L\beta}$ the local spin operator of the low-energy "conduction electrons."

The low-energy part of the impurity Green function G_L is now the time ordered Green function under $\mathcal{H}^{\rm eff}_L$ of the canonically transformed f_σ operators of the original Anderson model $\mathcal{H}_{\rm AM}$; to lowest order in S, these are $\sqrt{w}$ times the effective low-energy operators

$$F_\sigma = \frac{D\Gamma}{2}[(X_{-\sigma-\sigma} - X_{\sigma\sigma})c_{L\sigma} - 2X_{-\sigma\sigma}c_{L-\sigma}]. \tag{5}$$

The self-consistency condition requires that the Green function of F under $\mathcal{H}^{\rm eff}, G_L$, equals that of c_L under $\mathcal{H}_b, \Pi_L$. In terms of rescaled frequencies $i\tilde{\omega}_n = i\omega_n/wD$, w drops out and

$$\tilde{\Pi}_L(i\tilde{\omega}_n) \equiv \sum^L_{k,\sigma} \frac{4\tilde{V}^2_k}{i\tilde{\omega}_n - \tilde{\epsilon}_k} = \tilde{G}_L(i\tilde{\omega}_n)[\tilde{\epsilon}_k, \tilde{V}_k], \tag{6}$$

yielding a closed set of Eqs. (4)–(6) for low energies from which the parameters $\{\tilde{\epsilon}_k\}$ and $\{\tilde{V}_k\}$ have to be determined self-consistently. These equations reduce the full problem into a self-consistent problem for the low-energy sector only; we call such a reduction procedure a projective self-consistent approach. These self-consistent equations are solved iteratively at zero temperature [14,16]. The

Green functions and $\mathcal{H}_L^{\rm eff}$ are approximated in terms of a *finite* set of $N-1$ conduction electron orbitals $c_{i\sigma}^{\dagger}$, with energy levels $\tilde{\epsilon}_i$ and hybridization $\tilde{V}_i$. The ground state of $\mathcal{H}_L^{\rm eff}$ on the resulting N-site cluster is obtained using the Lanczos technique. The local Green function as well as correlation functions are calculated using a continued fraction expansion [16]. The projected self-consistency condition can be best approximated by a χ^2 fitting of the Matsubara Green function $\chi^2 = \sum_{\tilde{\omega}_n=\Omega_{\rm min}}^{\Omega_{\rm max}} |\tilde{G}_L(i\tilde{\omega}_n) - \tilde{\Pi}_L(i\tilde{\omega}_n)|^2$ where $\Omega_{\rm min}$ and $\Omega_{\rm max}$ are low and high frequency cutoffs [14]. Here $\Omega_{\rm min}$ is determined by the smallest pole of the continued fraction expansion of $\tilde{G}_L$ and is reduced as N increases, while $\Omega_{\rm max}$ is chosen to be large enough that the results do not significantly depend on it.

We analyze the behavior to leading order in w. The "high" frequency limit of $\tilde{G}_L = \tilde{\Pi}_L$ yields the condition $1 = \langle\{F, F^{\dagger}\}\rangle = 2\Gamma^2 D^2(3/8 - \langle\vec{S}_a \cdot \vec{S}_L\rangle_L) + O(w)$ in the self-consistent ground state of $\mathcal{H}_L^{\rm eff}$. This can be satisfied for only one particular value of ΓD and thus of U, thereby yielding an exact condition for U_c.

We have analyzed the low-energy problem defined by the projective self-consistent equations (4)–(6) for clusters of $N = 4$, 6, 8, and 10 sites. We find that the results have converged by $N = 8$. We determine $A_L \equiv \langle\vec{S}_a \cdot \vec{S}_L\rangle_L \approx -0.46$, characterizing the intermediate Kondo coupling nature at the critical point. From a self-consistent numerical solution of the insulating state, we determined $\Gamma(U)$. A low-order expansion for Γ in powers D/U [17] is also found to be good down to U_c. Both methods, when combined with A_L, yield $U_c \approx 2.9$. Just below U_c, the energy of the metal E_g^M can be shown to be lower than that of the insulator E_g^I by noting that $dE_g/dU = \langle n_{f\uparrow} n_{f\downarrow}\rangle$. Integrating this equation between U_c and U one finds that $E_{gs}^I - E_{gs}^M > 0$ since the metal has a greater double occupancy. This analytic argument then establishes that U_c is indeed the physical transition at $T = 0$, and that the metal-insulator transition at zero temperature is second order in agreement with earlier numerical findings [15].

To obtain $w(U)$, higher order terms in w must be retained. An approximate calculation yields $w \propto U_c - U$ and also $E_g^I - E_g^M \sim (U_c - U)^2$. More generally, all that is needed for this scenario to be correct is for a certain coefficient—analogous to the coefficient of ϕ^4 in Landau theory—to be positive as $U \to U_c$. This is borne out by a direct calculation, and is consistent with all the earlier work on this problem.

Here we focus on *ratios* of physical quantities as $U \longrightarrow U_c^-$ for which only the lowest order in w is needed. In the inset of Fig. 2 we show the single-particle spectral function for $N = 10$. The Green functions as functions of the scaled Matsubara frequency $\tilde{\omega}_n$ for $N = 6$, 8, and 10 are shown in Fig. 2, along with the rescaled noninteracting Green function. The low frequency part of the Green function improves systematically and remains

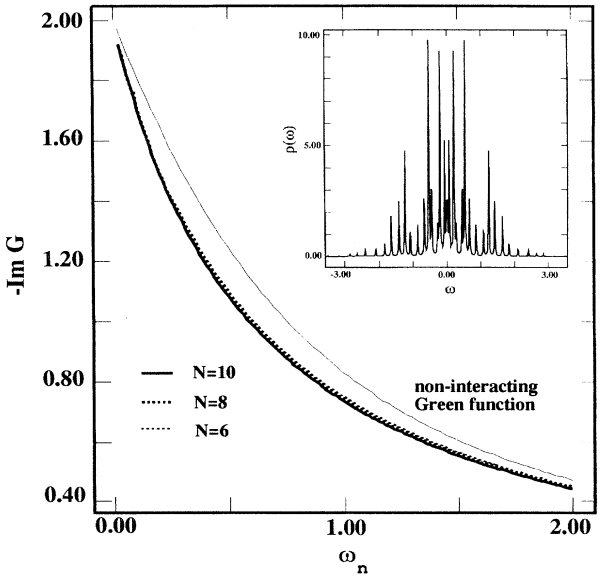

FIG. 2. Imaginary part of the scaled low frequency Green function $\tilde{G}_L$ versus the scaled Matsubara frequency $\tilde{\omega}_n$ for system sizes $N = 6, 8, 10$ and for the noninteracting system with a semicircular density of states. Inset: The single-particle spectral function for $N = 10$ as function of $\tilde{\omega}$ with a broadening $\delta = 0.01$.

essentially unchanged for $N = 8$ and 10. At $\tilde{\omega}_n = 0^+$, the value of the scaled Green function at zero frequency is determined by the low-energy self-consistency equation and is the same as that of the noninteracting Green function, $\mathrm{Im}G(0^+) = -2/D$, unchanged by the interactions as expected from Fermi liquid theory [4]. This is a nontrivial check of the numerics. The scaled self-energy $\tilde{\Sigma}_L(i\tilde{\omega}_n)$ is obtained by extracting from $\Sigma(i\omega_n) = i\omega_n - (D/2)^2 G(i\omega_n) - G^{-1}(i\omega_n)$ the terms with a singular dependence on w. For small $\tilde{\omega}_n$, i.e., $\omega_n \ll wD$,

$$\tilde{\Sigma}_L(i\tilde{\omega}_n) \approx \mathrm{sgn}(\tilde{\omega}_n)[-1.7i|\tilde{\omega}_n| - i1.2(i\tilde{\omega}_n)^2 + O(\tilde{\omega}_n^3)]. \tag{7}$$

The term of the self-energy linear in $i\tilde{\omega}_n$ implies a quasiparticle residue $Z \equiv (1 - \partial\Sigma/\partial i\omega_n)^{-1} \approx w/1.7$ which vanishes as the critical point is approached. Similarly, the low frequency imaginary part of the analytically continued self-energy diverges as $\mathrm{Im}\Sigma(\omega + i0^+) \approx -1.2\omega^2/w^2 D + O(\omega^3/D^2 w^3)$. This leads to a quasiparticle mass $m^*/m = 1/Z \approx 1.7/w$, and a linear specific heat coefficient

$$\gamma \approx (2\pi k_B^2/3)1.7/Dw\,, \tag{8}$$

which diverge as $(U_c - U)^{-1}$ at the critical point. This divergence is consistent with the Brinkman-Rice scenario of the Mott transition [3], as well as the infinite d second order perturbative result [18,19].

The low frequency *local* dynamical spin susceptibility is $\chi_{\rm loc}(i\omega_n) \approx (g\mu_B)^2 \int_0^{\beta} d\tau\, e^{i\omega_n\tau}\langle T_\tau \tilde{S}_z(\tau)\tilde{S}_z(0)\rangle_{H_{\rm eff}}$,

where $\tilde{S}_z \approx B^2(X_{\uparrow\uparrow} - X_{\downarrow\downarrow})/2$, with $B = {}_a\langle\uparrow|f_\uparrow^\dagger f_\uparrow|\uparrow\rangle_a \approx 0.97$; it can also be calculated from a continued fraction expansion. At low frequencies, $\chi_{\rm loc}(i\tilde{\omega}_n)$ can be fitted by

$$\chi_{\rm loc}(i\tilde{\omega}_n) \approx (g\mu_B/2)^2[8 - 36|\tilde{\omega}_n| + O(\tilde{\omega}_n^2)]/wD\,. \quad (9)$$

From Eq. (8) and the static limit of Eq. (9), a generalized Wilson ratio is found near the critical point,

$$R \equiv \frac{\chi_{\rm loc}(0)/\chi_{\rm loc}^{\rm free}(0)}{\gamma/\gamma^{\rm free}} \approx 2.8\,, \quad (10)$$

where $\chi_{\rm loc}^{\rm free}(0)$ and $\gamma^{\rm free}$ are the values in the absence of interactions. Compared to the value for the infinite bandwidth Anderson impurity model [20], $R_{\rm AM} = 2$, the critical value of R is enhanced as a result of the finite bandwidth of the electron bath. We note that the usual definition of the Wilson ratio is in terms of the $\mathbf{q} = 0$ component of $\chi(\mathbf{q}, \omega = 0)$. In large dimensions for generic $\mathbf{q} \neq 0, \chi(\mathbf{q}) \approx \chi_{\rm loc}$, while $\chi(\mathbf{q} = 0)$ is controlled by the magnetic exchange. We have therefore used the more characteristic $\chi_{\rm loc}$ in the definition of the generalized Wilson ratio. The enhancement of R is similar to that found in the Gutzwiller approximation [3] which also ignores the magnetic exchange.

The term of $\chi_{\rm loc}(i\tilde{\omega}_n)$ linear in $|\tilde{\omega}_n|$ leads to an imaginary part of the local dynamical spin susceptibility of the form $\lim_{\omega\to 0}\chi''_{\rm loc}(\omega + i0^+)/\omega \approx 36(g\mu_B/2)^2/(Dw)^2$. This implies a generalized Korringa ratio, $\lim_{\omega\to 0}\chi''_{\rm loc}(\omega + i0^+)/\omega\chi'_{\rm loc}(0)^2$ which is *finite* at the critical point, but again modified from the value for the infinite bandwidth Anderson model [21].

Finally, the temperature dependence of the resistivity induced by electron-electron scatterings can be estimated based on the quadratic in the $\tilde{\omega}_n$ term in the self-energy. Specifically, we convert the ω^2 in $\Sigma(\omega)$ at zero temperature to $(\pi T)^2$ at zero frequency and assume that the self-energy is a good approximation for a three-dimensional cubic lattice with lattice spacing a [22]. Using the Kubo formula, we find a resistivity $\rho(T) = AT^2$ where $A = (3\sqrt{2\pi}\,\pi^2\hbar a/e^2D)\partial^2 i\Sigma(i\omega_n)/\partial(i\omega_n)^2$, giving rise to a finite ratio

$$\frac{A}{\gamma^2} \approx (2.3a) \times 10^{-12}\ \Omega\,{\rm cm\,(mole\,K/mJ)^2}, \quad (11)$$

where a is the lattice constant in units of Å. Photoemission experiments [6] have indicated that $LaTiO_3$ is very close to the Mott transition point. Equation (11) yields $A/\gamma^2 \approx 1.5 \times 10^{-11}\ \Omega$ cm (mole K/mJ)^2 using $a = 6.3$ Å [7]. This is close to the measured value for $x = 0.1$, $A/\gamma^2 = 1.0 \times 10^{-11}\ \Omega$ cm (mole K/mJ)^2 [8]. While it is not clear *a priori* that the critical value for A/γ^2 when the Mott transition point U_c is approached at half filling should be the same as that when approached away from half filling, it will be shown elsewhere that doping a Mott insulator near U_c introduces a low-energy scale analogous to wD and that our analysis can be extended to the doping induced Mott transition. We also notice that in NiS_xSe_{2-x} where a metal-insulator transition is approached without changing the number of carriers the A/γ^2 close to the transition [23] is very close to the value quoted for the $Sr_xLa_{1-x}TiO_3$ system.

In summary, we have introduced a projective self-consistent approach to strongly correlated electron systems. Our method can be generalized to deal with other problems, in which the separation of energy scales can be exploited [24]; for example, the proposed breakdown of Fermi liquid theory [25], and superconductivity in models with repulsive interactions [14,26], both of which have been recently analyzed in large d.

We thank V. Dobrosavljević, A. Georges, A. E. Ruckenstein, and X. Y. Zhang for useful discussions. D. S. F. also thanks the Ecole Normale Supérieure for hospitality during the time this work was begun. This work was supported by the NSF under Grants No. DMR 9224000 and No. DMR 9106237, and (for D. S. F.) the A.P. Sloan Foundation.

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