Compressibility of the Two-Dimensional Infinite-U Hubbard Model

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(Received 16 April 1999)

We study the interactions between the coherent quasiparticles and the incoherent Mott-Hubbard excitations and their effects on the low-energy properties in the $U = \infty$ Hubbard model. Within the framework of a systematic large-N expansion, these effects first occur in the next-to-leading order in $1/N$. We calculate the scattering phase shift and the free energy, and determine the quasiparticle weight Z, mass renormalization, and the compressibility. It is found that the compressibility is strongly renormalized and diverges at a critical doping $\delta_c = 0.07 \pm 0.01$. We discuss the nature of this zero-temperature phase transition and its connection to phase separation and superconductivity.

PACS numbers: 74.25.Jb, 71.10.Fd, 71.27.+a

In recent years, there has been a growing interest in the physics of doped Mott insulators in connection with high-T_c superconductors. In the absence of a natural small parameter, relevant models of strong correlation have been extended and studied under large symmetry groups (large N) or large dimensions (large d). A generic feature of strong correlation is the coexistence of coherent quasiparticles [1] and the broad incoherent Mott-Hubbard excitations [2] that carry the main part of the spectral weight at small doping. It has been shown in the t-J model that the systematic large-N expansion in the slave boson formalism provides a transparent nonperturbative description of both the low-energy Fermi-liquid-like quasiparticles [3] already present in the large-N limit, and the incoherent Mott-Hubbard features at next-to-leading order in $1/N$ [4].

In this paper, we study corrections to the low-energy properties due to the effects of the interactions between quasiparticles and the incoherent Mott-Hubbard excitations by a complete calculation of the free energy and the single-particle Green's function to next-to-leading order in $1/N$. This has not been understood properly because of the difficulty involved in calculating the corrections to the mean-field parameters. For simplicity, we shall consider the $U = \infty$ Hubbard model with the spin symmetry group generalized from SU(2) to SU(N), although the physics discussed here pertains to models that include superexchange interactions such as the t-J model. This model has been solved for $N = \infty$. The ground state is a Fermi liquid at finite hole concentrations and exhibits a Brinkman-Rice transition at half filling [5]. We find that the interactions represented by the $1/N$ fluctuations are very strong near half filling, giving rise to a divergent compressibility at a finite critical doping $\delta_c = 0.07 \pm 0.01$ below which the Fermi liquid phase becomes unstable. In contrast to the Brinkman-Rice transition at half filling in the large-N limit, the quasiparticle residue Z and the mass renormalization are only weakly renormalized and remain finite at δ_c. These results suggest that the Landau Fermi liquid parameters are strongly renormalized. In particular, the instability is associated with $F_0^s \to -1$ as δ is reduced toward δ_c, signaling the onset of phase separation and/or superconductivity.

We begin with the slave boson representation of the Hubbard model. In the infinite-U limit, the model describes electrons with nearest-neighbor hopping, t, on a 2D square lattice, subject to the constraint that double occupancy on each site is prohibited. It is convenient to describe the projected Hilbert space in terms of a neutral spin-carrying fermion, $f_{i\sigma}^\dagger$, creating the singly occupied site and a spinless charge-e boson, b_i, keeping track of the empty site [5]. The electron creation operator becomes $c_{i\sigma}^\dagger = f_{i\sigma}^\dagger b_i$. In the SU($N$) generalization, the occupancy constraint thus translates into $f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = N/2$, where sum over repeated $\sigma = 1, \ldots N$ index is implied. The partition function in the coherent state path integral formulation is

$$Z = \int \mathcal{D}b^\dagger \mathcal{D}b \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}\lambda e^{-\int_0^\beta L(\tau)\,d\tau}, \quad (1)$$

where the Lagrangian is given by

$$\begin{aligned} L = & \sum_i [f_{i\sigma}^\dagger(\partial_\tau - \mu)f_{i\sigma} + b_i^\dagger \partial_\tau b_i] \\ & - \frac{t}{N}\sum_{\langle i,j\rangle}[f_{i\sigma}^\dagger f_{j\sigma} b_j^\dagger b_i + \text{H.c.}] \\ & + \sum_i i\lambda_i(f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - N/2). \end{aligned} \quad (2)$$

Here λ_i is a static Lagrange multiplier enforcing the local constraint and μ is the chemical potential fixing an average of δ holes or n particles per site, i.e., $\langle f_{i\sigma}^\dagger f_{i\sigma}\rangle = N(1-\delta)/2 \equiv n$. The Lagrangian in Eq. (2) has a U(1) gauge symmetry; it is invariant under local U(1) transformations: $b_i \to b_i e^{i\theta_i}$, $f_{i\sigma} \to f_{i\sigma}e^{i\theta_i}$, and $\lambda_i \to \lambda_i - \partial_\tau\theta_i$. We choose the radial gauge [6] where the boson fields $(b_i, b_i^\dagger)$ are replaced by a real amplitude field r_i while λ_i is

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promoted to a dynamical field $\lambda_i(\tau)$. In this gauge, the fermionic excitations can be identified with the Fermi liquid quasiparticles.

To enable a $1/N$ expansion to the next-to-leading order, we write the boson fields in terms of static mean-field and dynamic fluctuating parts,

$$r_i(\tau) = b[1 + \delta r_i(\tau)], \quad i\lambda_i(\tau) = \lambda + i\delta\lambda_i(\tau). \quad (3)$$

In the first part of the paper, we shall calculate b, λ, together with the chemical potential μ to the next-to-leading order. Using these results, we then analyze the single-particle Green's function, and determine the wave function renormalization Z and the quasiparticle mass renormalization and the compressibility.

Substituting Eq. (3) into Eq. (2), and integrating out the fermions and the boson fields $(\delta r, \delta\lambda)$ to quadratic order in Eq. (1), we obtain the free energy $F = -kT \ln Z$ to next-to-leading order in $1/N$,

$$F = -\frac{N}{\beta}\sum_{k,\omega_n}\ln(\epsilon_k - i\omega_n) + \lambda\left(b^2 - \frac{N}{2}\right) + F_{\rm bos}, \quad (4)$$

where ω_n is a fermion Matsubara frequency, $\epsilon_k = -\frac{2tb^2}{N}\gamma_k + \lambda - \mu$ with $\gamma_k = \cos k_x + \cos k_y$, and $F_{\rm bos}$ is the contribution due to boson fluctuations. The latter can be written in terms of the determinant of the inverse boson propagator matrix D^{-1},

$$F_{\rm bos} = \frac{1}{2\beta}\sum_{q,\nu_n}\ln {\rm Det}D^{-1}(q, i\nu_n), \quad (5)$$

where ν_n is a boson Matsubara frequency. Note that in order to properly regularize the theory in the radial gauge, ${\rm Det}D^{-1}$ should be evaluated on a discretized imaginary time mesh before taking the continuum limit in τ [7,8]. The opposite sequence of operations will lead to unphysical ultraviolet singularities. We find

$$\begin{aligned}{\rm Det}D^{-1}(q, i\nu_n) = {} & P_{\lambda\lambda}(q, i\nu_n)P_{rr}(q, i\nu_n) - P_{\lambda r}^2(q, i\nu_n) \\ & + 2b^2[\lambda - \epsilon_b(0)]S^- P_{\lambda r}(q, i\nu_n)/i\nu_n. \end{aligned} \quad (6)$$

Here $S^- = e^{-i\nu_n 0^-} - e^{i\nu_n 0^-}$ is a regularization factor and $\epsilon_b(q) = \lambda - 2t\sum \gamma_{k-q} n_f(\epsilon_k)$ with $n_f(\epsilon)$ the Fermi distribution function. $P_{\alpha\beta} = N(\Pi_{\alpha\beta} + B_{\alpha\beta})$ are the fermion polarizations given by $B_{rr} = 2b^2\epsilon_b(q)/N$, $B_{\lambda r} = B_{r\lambda} = 2b^2/N$, $B_{\lambda\lambda} = 0$, and

$$\Pi_{\alpha\beta} = \sum_k \frac{n_f(\epsilon_{k_+}) - n_f(\epsilon_{k_-})}{\epsilon_{k_+} - \epsilon_{k_-} - i\nu_n}\Lambda^\alpha(k,q)\Lambda^\beta(k,q), \quad (7)$$

where $k_\pm = k \pm q/2$ and $\Lambda = [-(2tb^2/N)(\gamma_{k_+} + \gamma_{k_-}), i]$ are the boson-fermion vertices.

The values of the parameters (b, λ, μ) are determined by minimizing the free energy in Eq. (4), leading to three self-consistent equations:

$$\frac{\partial F}{\partial b} = 0, \qquad \frac{\partial F}{\partial \lambda} = 0, \qquad \frac{\partial F}{\partial \mu} = -n. \quad (8)$$

Solving these equations to leading order in $1/N$, where only the fermion contribution enters Eq. (4), one recovers the results of Kotliar and Liu [5], namely, a boson condensate $b^2 = b_0^2 = N\delta/2$ and a chemical potential shift $\lambda = \lambda_0 = 2t\sum_k \gamma_k n_f(\epsilon_k)$. This corresponds to a Fermi liquid phase with a quasiparticle dispersion $\epsilon_k^0 = -(2tb_0^2/N)\gamma_k + \lambda_0 - \mu_0$ and a quasiparticle residue $Z = b_0^2 = N\delta/2 = m/m^*$. The compressibility $\kappa_0 = dn/d\mu = N\rho/(1 + 4t\rho|\epsilon_0|)$ where $\rho = \sum_k \delta(\epsilon_k^0)$ and $\rho\epsilon_0 = -\sum_k \gamma_k\delta(\epsilon_k^0)$. It diverges as $\delta \to 0$, together with $Z \to 0$ and $m^* \to \infty$, giving rise to a Brinkman-Rice metal-insulator transition [1].

The effects of interactions between the quasiparticles and the incoherent Mott-Hubbard excitations enter through $F_{\rm bos}$ in Eq. (4) at the next-to-leading order in $1/N$ [4,9]. It is instructive to rewrite $F_{\rm bos}$ in Eq. (5) by converting the boson Matsubara sum into a contour integral distorted along the real axis,

$$F_{\rm bos} = -\frac{1}{2\pi}\sum_q \int_{-\infty}^{\infty} d\nu\, \Delta(q,\nu) n_b(\nu), \quad (9)$$

where n_b is the Bose distribution function and

$$\Delta(q,\nu) = -\arctan\left[\frac{{\rm Im\,Det}D^{-1}(q,\nu)}{{\rm Re\,Det}D^{-1}(q,\nu)}\right] \quad (10)$$

can be considered as a many-body phase shift due to scattering of the fermions by particle-hole excitations. We have numerically calculated the phase shift Δ at $T = 0$ from Eqs. (6) and (10). Its general behavior is shown in Fig. 1 for a fixed wave vector $q = (2\pi/3, 2\pi/3)$ as a function of frequency at different dopings. From intermediate to high frequencies, the scattering is in the unitary limit with $\Delta = \pi$, indicating the existence of a collective mode which is pulled out of the particle-hole continuum at low frequency where Δ drops from π to zero. Indeed, we find that ${\rm Det}D^{-1}$ has a branch cut along the real axis corresponding to the particle-hole continuum, and isolated poles corresponding to a collective mode which is well described by

$$\omega_q^2 \simeq c^2[\sin^2(q_x/2) + \sin^2(q_y/2)] + \epsilon_b^2(q), \quad (11)$$

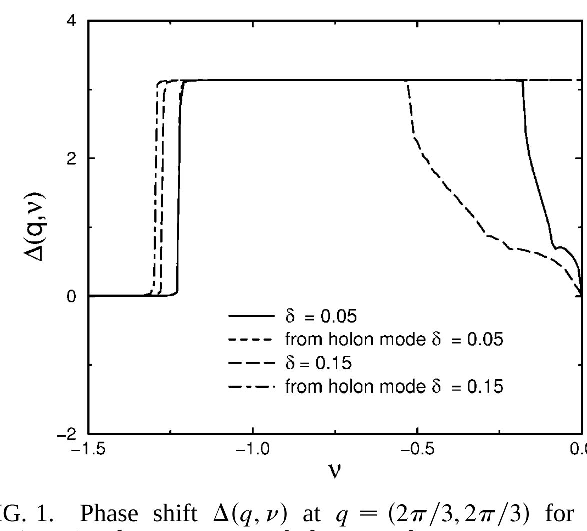

FIG. 1. Phase shift $\Delta(q,\nu)$ at $q = (2\pi/3, 2\pi/3)$ for $\delta = 0.05, 0.15$ and comparison to holon contributions.

where $c \propto \delta t$ is the zero sound velocity and $\epsilon_b(q)$ coincides with the original slave-boson dispersion. This mode has been identified as the "holon" in the t-J model [4,9]. At small doping, the holon contribution, with $\omega_q^* \simeq \pm\epsilon_b(q)$, dominates the particle-hole scattering as seen in Fig. 1. It disperses over the entire lower Hubbard band and carries the incoherent Mott-Hubbard spectral weight. Remarkably, the holon contribution leads to a density-density correlation function in excellent agreement with that obtained from exact diagonalization of the t-J model on small clusters [10].

Now we solve the self-consistent equations in (8) to next-to-leading order in $1/N$ including $F_{\rm bos}$. Writing $b = b_0 + b_1$, $\lambda = \lambda_0 + \lambda_1$, and $\mu = \mu_0 + \mu_1$, we find

$$b_1 = \frac{b_0}{2\beta} \sum_{q,\nu_n} D_{rr}(q, i\nu_n) e^{-i\nu_n 0^-}, \tag{12}$$

$$\mu_1 = \lambda_1 + \frac{1}{\rho} \sum_k \Sigma_n(k, \epsilon_k)\delta(\epsilon_k) + \frac{4tb_0 b_1 \epsilon_0}{N}, \tag{13}$$

$$\lambda_1 = -\frac{N}{2b_0^2\beta} \sum_{k,\omega_n} G_0(k, i\omega_n)\left[\Sigma_n(k, i\omega_n) - \frac{2tb_0^2}{N}\frac{1}{\beta}\sum_{q,\nu_n}\gamma_{k-q}D_{rr}(q, i\nu_n)e^{-i\nu_n 0^-}\right]$$
$$+ \frac{2t}{\beta}\sum_{k,\omega_n}\gamma_k G_0^2(k, i\omega_n)\Sigma_n(k, i\omega_n) + 2t|\epsilon_0|\sum_k \Sigma_n(k, \epsilon_k)\delta(\epsilon_k) + \frac{2}{\beta}\sum_{q,\nu_n}[D_{r\lambda}(q, i\nu_n) - D_{r\lambda}(q, \infty)]. \tag{14}$$

Here $G_0^{-1} = i\omega_n - \epsilon_k^0$ and $\Sigma_n(k, i\omega_n)$ is the usual self-energy to leading order in $1/N$ [4,9],

$$\Sigma_n(k, i\omega_n) = \frac{2tb_0^2}{N}\frac{1}{\beta}\sum_{q,i\nu_n}\gamma_{k-q}D_{rr}(q, i\nu_n)e^{-i\nu_n 0^-} - \frac{1}{\beta}\sum_{k,\nu_n}G_0(k+q, i\omega_n + i\nu_n)$$
$$\times [D_{\lambda\lambda}(q, i\nu_n)S_{\lambda\lambda} + 2D_{\lambda r}(q, i\nu_n)S_{r\lambda}(E_k + E_{k+q}) + D_{rr}(q, i\nu_n)(E_k + E_{k+q})^2], \tag{15}$$

where $E_k = -(2tb_0^2/N)\gamma_k$, $S_{r\lambda} = e^{-i\nu_n 0^-}$, and $S_{\lambda\lambda} = (e^{-i\nu_n 0^-} + e^{i\nu_n 0^-})/2$ are regularization factors for $D_{r\lambda}$ and $D_{\lambda\lambda}$, respectively. Without them, the theory in the radial gauge would be singular in the ultraviolet because $D_{r\lambda}$ and $D_{\lambda\lambda}$ approach constants at large frequencies [7].

Next, we present the results of our numerical evaluations of Eqs. (12)–(14), which were done on a 2D mesh of up to 60×60 points in the first quadrant of the Brillouin zone using the microzone method and a frequency grid size as small as $\Delta\omega/t = \delta/20$ to ensure convergence. The result for the slave-boson condensate to next-to-leading order in $1/N$ is shown in the inset of Fig. 2 for $N = 2$. Interestingly, b vanishes at a doping $\delta^* \simeq 0.12$. If we approximate the D_{rr} in Eq. (12) by the single holon mode in Eq. (11) at small doping, we find an analytical estimate $b/b_0 = 1 - 1/4N\delta$, which vanishes at a $\delta^* = 1/4N = 0.125$, in good agreement with the numerical result.

It is important to note that at this order the boson condensate is not simply related to the quasiparticle residue. To determine the Fermi liquid coherence factor Z, we follow Refs. [4,9] and write down the $1/N$-resummation of the single-electron Green's function,

$$G(k, i\omega_n) = \frac{b^2[1 + \Sigma_a(k, i\omega_n)]^2}{i\omega_n - \epsilon_k - \Sigma_n(k, i\omega_n)} + b^2\Sigma_i(k, i\omega_n), \tag{16}$$

where Σ_n is given in Eq. (15), Σ_a and Σ_i are the anomalous part due to the boson condensate, and the incoherent part of the self-energies, respectively. The latter are given by, to leading order in $1/N$,

$$\Sigma_i(k, i\omega) = -T\sum_{q,\nu_n}G_0(k+q, i\omega + i\nu_n)D_{rr}(q, i\nu_n), \tag{17}$$

$$\Sigma_a(k, i\omega) = -T\sum_{q,i\nu_n}G_0(k+q, i\omega + i\nu_n) \times [D_{\lambda r}(q, i\nu_n)S_{r\lambda} + (E_k + E_{k+q})D_{rr}(q, i\nu_n)]. \tag{18}$$

The quasiparticle residue on the interacting Fermi surface can be obtained from Eq. (16),

$$Z_{k_F} = \frac{b^2[1 + \mathrm{Re}\Sigma_a(k_F, 0)]^2}{1 - \partial\,\mathrm{Re}\Sigma_n(k_F, \omega)/\partial\omega|_{\omega=0}}. \tag{19}$$

Thus Z_{k_F} can be finite even if b^2 is vanishing, provided that the reduction of the condensate is compensated by the contributions from the self-energies. Remarkably, this turns out to be the route followed by the $1/N$ expansion. To next-to-leading order in $1/N$, one has

$$Z_{k_F}^{1/N} = b^2 + 2b_0^2\Sigma_a(k_F, 0) + b_0^2\partial\Sigma_n(k_F, \omega)/\partial\omega|_{\omega=0}. \tag{20}$$

In Fig. 2, $Z_{k_F}^{1/N}$ is plotted as a function of doping in the ΓM direction. The $1/N$ corrections are clearly small and Z_{k_F} stays close to the large-N limit value. Within the single holon mode [Eq. (11)] approximation, we found that the $1/\delta$ correction to b^2 in Eq. (20) is canceled out by those from the self-energy terms, leaving $Z_{k_F}^{1/N}$ weakly renormalized near δ^*. Thus we conclude that, while the boson condensate vanishes at δ^*, the Fermi liquid coherence remains finite.

We next turn to the compressibility of the model. In Fig. 3, the electron chemical potential $\mu = \mu_0 + \mu_1$ is

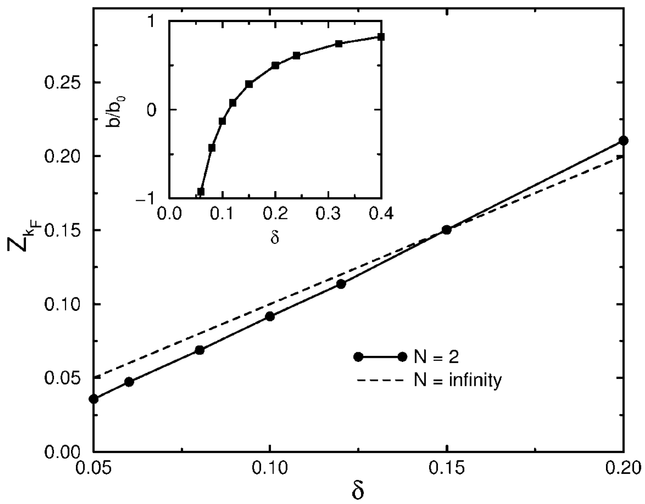

FIG. 2. Quasiparticle residue Z_{k_F} as a function of doping δ in the ΓM direction. Inset: Slave boson condensate amplitude b/b_0 as a function of doping.

shown as a function of doping, which is strongly modified from the $N = \infty$ result. The corresponding compressibility $\kappa = dn/d\mu$ is shown in the inset of Fig. 3. At moderate dopings, κ is approximately constant, but becomes strongly doping dependent as δ is reduced. Interestingly, there exists a critical doping $\delta_c = 0.07 \pm 0.01$, at which κ diverges. Thus, the Fermi liquid state becomes unstable below δ_c, while no singularity is present in Z_{k_F}. To further understand the nature of the instability, we have studied the quasiparticle mass renormalization defined by $m^*/m = N^*(0)/N(0)$, where $N(0) = \rho$ and $N^*(0)$ are the bare ($N = \infty$) and the renormalized (next-to-leading order in $1/N$) quasiparticle density of states, respectively. The numerical calculations of $N^*(0)$ show that while m^* is enhanced in the doping range $0.05 < \delta < 0.2$, it does not exhibit any singular behavior. A well-behaved $N^*(0)$, together with the general Fermi liquid result,

$$\kappa \equiv \frac{\partial n}{\partial \mu} = \frac{N^*(0)}{1 + F_s^0}, \tag{21}$$

suggests that the divergence of κ is a result of the Landau Fermi liquid parameter $F_s^0 \to -1$ at δ_c, indicative of phase separation and/or superconducting instability [11]. Note that the phase separation in the infinite-U case has a different origin than in models with strong antiferromagnetic correlations. For one hole, the ground state is known rigorously to be a Nagaoka state [12] of a saturated ferromagnet. For a finite density of holes, one expects ferromagnetic correlations to compete with the kinetic energy, and whether the Nagaoka state remains stable is a question of great interest. Both numerical [13] and analytical [14] results have shown that the *uniform* Nagaoka ferromagnetic state is unstable for any finite hole concentration. Our results naturally suggest a novel possibility that at low doping the system phase separates into hole-poor ferromagnetic and hole-rich paramagnetic regions. In the presence of long-range Coulomb repulsion, we expect the p-wave pairing instability [5] enhanced by the tendency towards phase separation to dominate [15,16]. We conclude that the breakdown of the Fermi liquid in our case is *not* due to a gradual reduction of the Fermi liquid coherence, but rather the enhanced interactions between the quasiparticles. This is the kind of Fermi liquid instability originally envisioned by Landau.

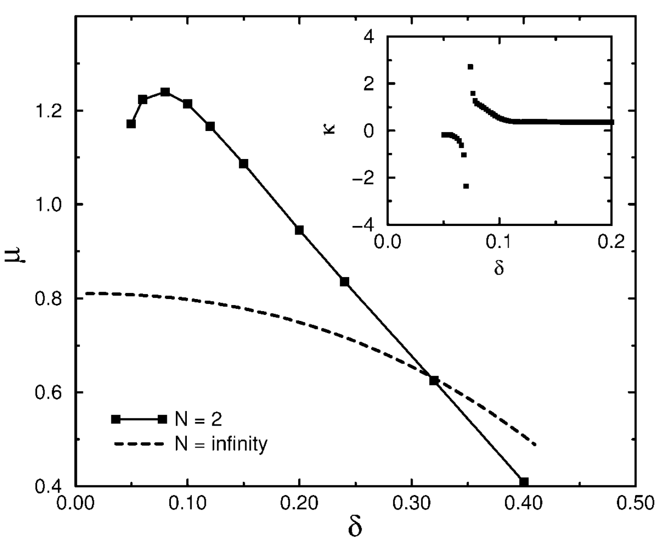

FIG. 3. Electron chemical potential and the compressibility (inset) as a function of doping.

We thank Jan Engelbrecht and Yong Baek Kim for useful discussions. This work was supported in part by DOE No. DE-FG02-99ER45747, the Research Corporation, and NSF No. DMR 95-29138.

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