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Quasiparticle properties of the two-dimensional Hubbard model in a propagator-renormalized fluctuation-exchange approximation

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We calculate the self-energy and thermodynamic potential of the two-dimenisonal Hubbard model in a propagator-renormalized conserving approximation, for lattices as large as 128 × 128 and temperatures as low as 0.002 times the bandwidth. For densities near quarter filling we see no evidence of deviations from the predictions of Fermi-liquid theory, such as those expected in a Luttinger liquid or a marginal Fermi liquid.

In spite of intense theoretical effort sparked by the normal-state properties of the high-T_c superconductors, controversy continues over the ground-state and low-lying excitations of the two-dimensional Hubbard model, with Hamiltonian

$$H = -t \sum_{<i,j>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Anderson has recently argued that the two-dimensional (2D) Hubbard model describes a Luttinger liquid (LL), in which the renormalization factor $a(\varepsilon)$ of a quasiparticle with energy ε approaches zero as ε^α $(0 < \alpha \ll 1)$ for all $U > 0$ and all densities.[1] Similarly, in the marginal-Fermi-liquid (MFL) theory abstracted from the experimental phenomenology of the high-T_c materials, the quasiparticle weight vanishes as an inverse logarithm at low energy.[2] A microscopic basis for these models is still lacking, and the weak nature of the proposed anomalies means that they would not be apparent in numerical calculations on small lattices or at relatively high temperatures. An alternative is to carry out approximate calculations for large enough lattices and low enough temperatures that the proposed anomalies might be seen. In this paper we report numerical calculations using self-consistent Green's-function approximations, which indicate that if a LL or MFL really occurs for all $U > 0$ and all densities, then within this framework the anomalous behavior must have a more subtle origin than anything studied in the past.

The quasiparticle excitations of a Fermi liquid are described by the retarded self energy, $\Sigma^R(\mathbf{k},\varepsilon)$. The quasiparticle energy $\xi_{\mathbf{k}}$ and the crystal momentum are related by

$$\xi_{\mathbf{k}} - \xi^0_{\mathbf{k}} - \mathrm{Re}\,\Sigma^R(\mathbf{k},\xi_{\mathbf{k}}) = 0, \quad (2)$$

where both $\xi_{\mathbf{k}}$ and the noninteracting single-particle energy $\xi^0_{\mathbf{k}}$ are measured from the chemical potential. The renormalization factor for a quasiparticle with energy ε and crystal momentum $\mathbf{k}$ can be expressed as

$$a(\mathbf{k},\varepsilon) = \left(1 - \frac{\partial \mathrm{Re}\,\Sigma^R(\mathbf{k},\varepsilon)}{\partial\varepsilon}\right)^{-1}. \quad (3)$$

We have studied the quasiparticle properties of the Hubbard model within a propagator-renormalized theory for the temperature Green's function $G(\mathbf{k},\varepsilon_n)$, in which the self-energy is given as a nonlinear functional of the interacting Green's function, which is, in turn, related to the self-energy by Dyson's equation,

$$\Sigma(\mathbf{k},\varepsilon_n) = \frac{1}{2}\frac{\delta\Phi[G]}{\delta G(\mathbf{k},\varepsilon_n)}, \quad (4)$$

$$G(\mathbf{k},\varepsilon_n) = [G_0^{-1}(\mathbf{k},\varepsilon_n) - \Sigma(\mathbf{k},\varepsilon_n)]^{-1}. \quad (5)$$

The thermodynamic potential density $\Omega(T,\mu)$ can also be expressed in terms of the Green's function, self-energy, and the functional $\Phi[G]$,

$$\Omega(T,\mu) = -2\,\mathrm{Tr}[\Sigma G + \ln(-G_0^{-1} + \Sigma)] + \Phi[G], \quad (6)$$

where $\mathrm{Tr}[A] = (T/N)\sum_{\mathbf{k}}\sum_n A(\mathbf{k},\varepsilon_n)$ and N is the number of lattice sites.[3] Viewed as a functional of Σ and G, this expression is stationary whenever Eqs. (4) and (5) are satisfied. Although originally derived by resummation of perturbation theory, this framework is formally exact,[4] and should be capable of describing a LL or MFL as well as a Fermi liquid. The complexities are, of course, hidden in the functional $\Phi[G]$, which is usually approximated by some infinite subset of the one-particle irreducible closed Feynman diagrams.

Following Bickers, Scalapino, and White[5] we take for $\Phi[G]$ the sum of all particle-hole and particle-particle bubble chains,

$$\Phi = \Phi_2 + \Phi^{df}_{\mathrm{ph}} + \Phi^{sf}_{\mathrm{ph}} + \Phi_{\mathrm{pp}}, \quad (7)$$

$$\Phi_2 = -\tfrac{1}{2}\mathrm{Tr}\left[\chi^2_{\mathrm{ph}}\right], \quad (8)$$

$$\Phi^{df}_{\mathrm{ph}} = \tfrac{1}{2}\mathrm{Tr}\left[\ln(1+\chi_{\mathrm{ph}}) - \chi_{\mathrm{ph}} + \tfrac{1}{2}\chi^2_{\mathrm{ph}}\right], \quad (9)$$

$$\Phi^{sf}_{\mathrm{ph}} = \tfrac{3}{2}\mathrm{Tr}\left[\ln(1-\chi_{\mathrm{ph}}) + \chi_{\mathrm{ph}} + \tfrac{1}{2}\chi^2_{\mathrm{ph}}\right], \quad (10)$$

$$\Phi_{\mathrm{pp}} = \mathrm{Tr}\left[\ln(1+\chi_{\mathrm{pp}}) - \chi_{\mathrm{pp}} + \tfrac{1}{2}\chi^2_{\mathrm{pp}}\right], \quad (11)$$

where the particle-hole and particle-particle susceptibility bubbles are

$$\chi_{\mathrm{pp}}(\mathbf{q},\omega_m) = U(T/N)\sum_{\mathbf{k}}\sum_n G(\mathbf{k}+\mathbf{q},\varepsilon_n+\omega_m)G(-\mathbf{k},-\varepsilon_n) \quad (12)$$

$$\chi_{\mathrm{ph}}(\mathbf{q},\omega_m) = -U(T/N)\sum_{\mathbf{k}}\sum_n G(\mathbf{k}+\mathbf{q},\varepsilon_n+\omega_m)G(\mathbf{k},\varepsilon_n). \quad (13)$$

The corresponding approximation for the self-energy consists of the single second-order diagram plus exchanged density fluctuations, spin-density fluctuations, and (singlet) pair fluctuations. Although this approximation is not expected to give an accurate description of the Hubbard model in the large-U limit, it does have two notable virtues: (1) the infinite-order resummation of perturbation theory can be carried out analytically, in terms of the susceptibility bubbles; (2) in the absence of an external magnetic field, every instability or anomaly of which we are aware manifests itself at this level of approximation. The repeated particle-particle scattering described by Φ_{pp} has recently been discussed as a possible mechanism for the breakdown of Fermi-liquid theory in two dimensions.[1,6] We have not explicitly included the Hartree self-energy, which for the Hubbard model has the simple form $nU/2$ and hence can always be eliminated by a redefinition of the chemical potential.

For this $\Phi[G]$ we have generated self-consistent solutions of Eqs. (4) and (5) on a 128 × 128 lattice with periodic boundary conditions, for temperatures between $T/t = 0.015$ and $T/t = 0.12$. Since the noninteracting bandwidth is $W = 8t$, at our lowest temperature we have $T/W \approx 0.0019$. The large lattice used in these calculations is required in order to avoid finite-size effects at low temperature; with a 64x64 lattice, deviations from the correct T^2 dependence of the noninteracting thermodynamic potential are significant at $T/t = 0.015$. We have been able to obtain the temperature dependence of thermodynamic properties and of the self-energy over a range of temperature where differences between a Fermi liquid and a LL or MFL should be apparent.

We have looked for evidence of deviations from Fermi-liquid behavior in the temperature dependence of the thermodynamic potential and of a quantity closely related to the quasiparticle renormalization factor. The calculations reported here were carried out for an approximately quarter-filled band ($n \approx 0.53$) with $U/t = 8$. Consequently these calculations are not relevant to models such as that of Virosztek and Ruvalds in which marginal-Fermi-liquid behavior is predicated on Fermi-surface nesting.[7] (We have verified that our approach does generate a MFL-like self-energy near half filling and hence that we can identify such an anomaly; details will be reported elsewhere.[8])

Numerical solution of Eqs. (4) and (5) requires the introduction of a high-energy cutoff in the discrete frequency sums. While implementing this cutoff is relatively straightforward in simple sums such as those in the thermodynamic potential, it is less clear how to handle the frequency convolutions that appear in the susceptibilities and self-energies. We have evaluated these frequency convolutions by imposing periodic boundary conditions on the frequency dependence of the Green's function, susceptibilities, and self-energy. Although this procedure may at first appear unnatural, it is exactly the form of cutoff in frequency implied by a discretization of the corresponding (and in some respects more fundamental) equations in imaginary time, where all functions are periodic with period 2β. An important practical advantage to this cutoff scheme is that it allows both frequency and momentum convolutions to be evaluated very efficiently using fast Fourier transforms (FFT's).[9] At the cost of doubling the number of Matsubara frequencies, one can also impose a sharp frequency cutoff on the formally periodic Green's function by padding the Green's function with zeros between the cutoff and twice the cutoff. We have found no significant difference between the quasiparticle properties obtained with these two cutoff schemes, and hence we have generally used the former on account of its computational economy.

The resulting FFT-based algorithm is well suited to highly parallel computer architectures; our calculations were carried out on the Naval Research Laboratory (NRL) Connection Machine. A minor disadvantage of doing convolutions with FFT's is that the lattice size and the number of frequency points are restricted to powers of two. This is particularly significant for the frequency dimension, because in order to avoid spurious temperature dependences the calculations must be carried out at a constant cutoff energy. The cutoff energy is proportional to the product of the temperature and the number of Matsubara frequencies, and hence we can only extract meaningful temperature dependences from calculations at temperatures that differ by powers of two.

We have minimized the effect of the high-frequency cutoff by calculating differences between expressions evaluated with the interacting and noninteracting Green's functions in cases when the latter frequency sums can also be evaluated analytically without cutoffs. In particular, we have used this trick for the number density, the thermodynamic potential, and the susceptibilities. In order to ensure that our results for the quasiparticle properties and thermodynamic potential are cutoff independent, we have used cutoffs up to 12 times the bandwidth.

Numerical calculations of temperature Green's functions all suffer from a well-known problem of interpretation, because they yield the self-energy at the discrete Matsubara frequencies $\varepsilon_n = (2n+1)\pi T$ along the imaginary frequency axis, while the quasiparticle properties are defined most directly in terms of the self-energy for real frequencies. To circumvent this problem we recall that the frequency-dependent part of the retarded self-energy has the following spectral representation:

$$\Sigma^R(\mathbf{k}, z) = \int \frac{d\varepsilon}{\pi} \frac{\mathrm{Im}\,\Sigma^R(\mathbf{k}, \varepsilon)}{\varepsilon - z}. \tag{14}$$

We use this representation to evaluate the self-energy $\Sigma(\mathbf{k}, \varepsilon_n) = \Sigma^R(\mathbf{k}, i\varepsilon_n)$ at the smallest Matsubara frequency, and define an imaginary-frequency approximation to the quasiparticle renormalization factor,

$$a_M(\mathbf{k}, T)^{-1} = 1 - \frac{\mathrm{Im}\,\Sigma(\mathbf{k}, \varepsilon_0)}{\varepsilon_0}, \tag{15}$$

$$= 1 - \int \frac{d\varepsilon}{\pi} \frac{\mathrm{Im}\,\Sigma^R(\mathbf{k}, \varepsilon)}{\varepsilon^2 + (\pi T)^2}. \tag{16}$$

For a Fermi liquid, $a_M(\mathbf{k}, T)^{-1}$ is well behaved for $T \to 0$ and approaches $a(\mathbf{k}, 0)^{-1}$, while for the LL or MFL $a_M(\mathbf{k}, T)^{-1}$ diverges in this limit. For example, the MFL theory of Varma *et al.* has

$$\mathrm{Im}\,\Sigma^R(\mathbf{k},\varepsilon) = -\alpha \max(|\varepsilon|, T)\,\Theta(\omega_c - |\varepsilon|), \qquad (17)$$

with ω_c a high-energy cutoff of order the bandwidth and α a dimensionless coupling constant of order unity. The integral in Eq. (16) yields

$$\frac{\mathrm{Im}\,\Sigma_{\mathrm{MFL}}(\mathbf{k},\varepsilon_0)}{\varepsilon_0} = -\frac{\alpha}{\pi}\left[\frac{2\arctan(1/\pi)}{\pi} + \ln\left(\frac{\omega_c^2 + (\pi T)^2}{(\pi^2+1)T^2}\right)\right]. \qquad (18)$$

In Fig. 1 we show $\Sigma(\mathbf{k},\varepsilon_0)/\varepsilon_0$ with $\mathbf{k}$ on the Fermi surface in the (10) direction, from calculations with a cutoff of six times the bandwidth, together with the MFL result for three different values of the cutoff ($\omega_c = 8t, 4t, 2t$), with the coupling strength α adjusted to agree with the fluctuation exchange approximation at one temperature ($\alpha = 0.42, 0.49, 0.60$). The temperature dependence in the (11) direction is similar.[8] It is apparent that over this temperature range the results from the fluctuation exchange approximation are inconsistent with the MFL theory (and presumably also with a LL theory) for any reasonable choice of parameters.

As a further check on the Fermi-liquid character of the fluctuation-exchange approximation, we have examined the temperature dependence of the thermodynamic potential obtained from Eq. (6). Figure 2 shows $\Omega(T,\mu)$ from the three lowest-temperature runs in Fig. 1, plotted versus T^2 for comparison with the expected leading temperature dependence for a Fermi liquid,

$$\Omega_{\mathrm{FL}}(T,\mu) = \Omega(0,\mu) + \tfrac{1}{2}\gamma(\mu)T^2 + \cdots . \qquad (19)$$

Although these points do show some small curvature,

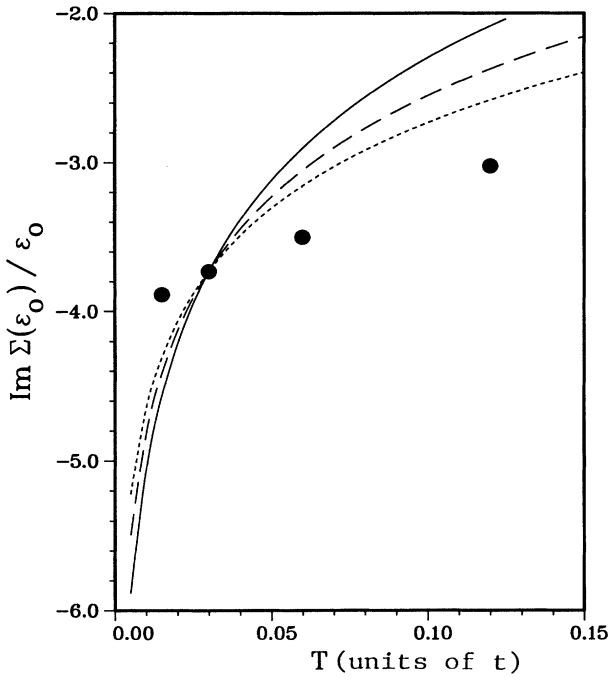

FIG. 1. $\mathrm{Im}\,\Sigma(\varepsilon_o)/\varepsilon_o$ vs T for the fluctuation-exchange approximation (•) with $U/t = 8$, $n \approx 0.53$, and a cutoff energy of $48t$. The points shown are for a (10) point on the Fermi surface. The MFL prediction [Eq. (18)] for cutoff energies $\omega_c = 8t$ (short dashed), $4t$ (dashed), and $2t$ (solid) is shown for comparison. At each cutoff the coupling strength was adjusted to fit the fluctuation-exchange approximation at $T/t = 0.03$.

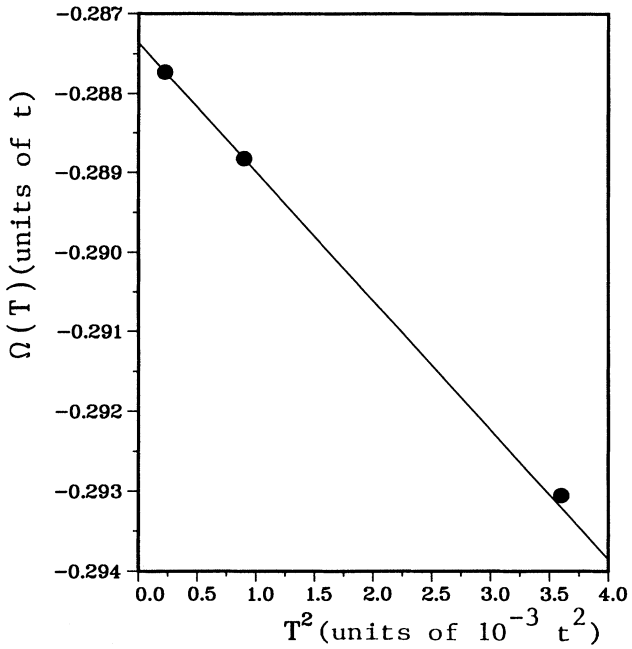

FIG. 2. The thermodynamic potential $\Omega(T)$ plotted vs T^2 for the fluctuation-exchange approximation with $U/t = 8$ and a cutoff energy of $48t$. The solid line is a fit to the lowest temperature points.

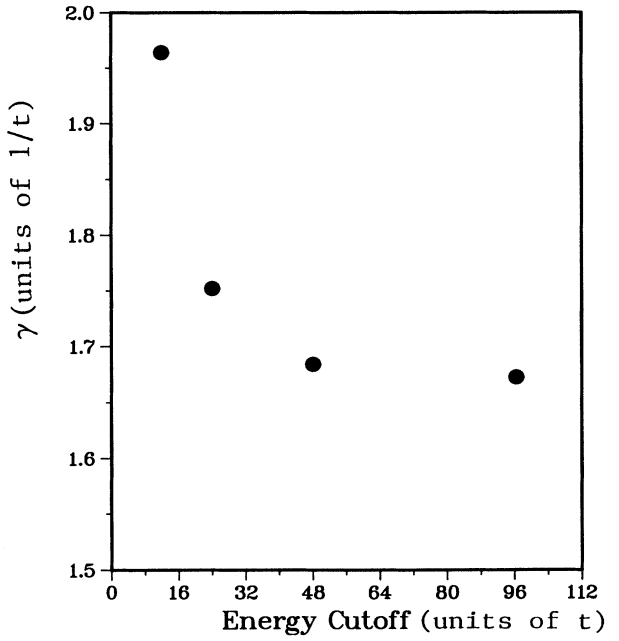

FIG. 3. The coefficient of the T^2 term in the thermodynamic potential as calculated from the Fermi-surface integral in Eq. (20) at $T/t = 0.03$, as a function of cutoff energy.

deviations from a pure T^2 dependence of this magnitude are not unexpected for a Fermi liquid; ^{3}He has a comparable mass enhancement and exhibits significant finite-temperature corrections at corresponding temperatures.[10]

For a Fermi liquid, the coefficient $\gamma(\mu)$ is given by the same expression as for a noninteracting Fermi gas, but with the noninteracting single-particle energy $\xi^0_{\mathbf{k}}$ replaced by the $(T = 0)$ quasiparticle energy $\xi_{\mathbf{k}}$ defined in Eq. (2).[11] In terms of the self-energy, this is equivalent to the following Fermi-surface integral:

$$\gamma(\mu) = (1/6) \int_{\mathrm{FS}} ds \frac{a(\mathbf{k},0)^{-1}}{|\nabla[\xi^0_{\mathbf{k}} + \mathrm{Re}\,\Sigma^R(\mathbf{k},0)]|}. \quad (20)$$

We have evaluated this expression using a discrete-lattice approximation to the Fermi-surface integral and approximating $a(\mathbf{k},0)$ by $a_M(\mathbf{k},T)$ and $\mathrm{Re}\,\Sigma^R(\mathbf{k},0)$ by $\mathrm{Re}\,\Sigma(\mathbf{k},\varepsilon_0)$. In Fig. 3 we show this approximation to $\gamma(\mu)$, evaluated at $T/t = 0.03$, as a function of cutoff energy. The cutoff dependence appears to have saturated at a cutoff of six times the bandwidth. The approximate $\gamma(\mu)$ has a residual temperature dependence similar to that of $\Sigma(\mathbf{k},\varepsilon_0)/\varepsilon_0$ in Fig. 1. Although for a Fermi liquid the slope of $\Omega(T,\mu)$ versus T^2 and the coefficient $\gamma(\mu)$ evaluated from Eq. (20) should agree as $T \to 0$, we do not feel confident about extrapolating our numerical results for either of these to $T = 0$; the finite-temperature corrections to these quantities are presumably different (the difference corresponds roughly to that between statistical and dynamical quasiparticle energies[10]), and their functional forms are not known. As a crude consistency check, we note that the value obtained from the two lowest-temperature points in Fig. 2 is $1.62/t$, while the limiting value of the Fermi-surface integral at $T/t = 0.03$ is $1.67/t$. The agreement seems satisfactory in light of the uncertainties noted above.

Another quantity of both theoretical and experimental interest is the crystal-momentum distribution function,

$$n(\mathbf{k}) = 2T \sum_n G(\mathbf{k},\varepsilon_n) + 1. \quad (21)$$

In Fig. 4 we show our result for $n(\mathbf{k})$ at $T/t = 0.015$ with $\mathbf{k}$ along the (10) direction. In a Fermi liquid $n(\mathbf{k})$ is the sum of a continuous incoherent background and a quasiparticle part described by a Fermi distribution with weight $a(\mathbf{k},0)$,

$$n(\mathbf{k}) = n_{inc}(\mathbf{k}) + a(\mathbf{k},0) f(\xi_{\mathbf{k}}). \quad (22)$$

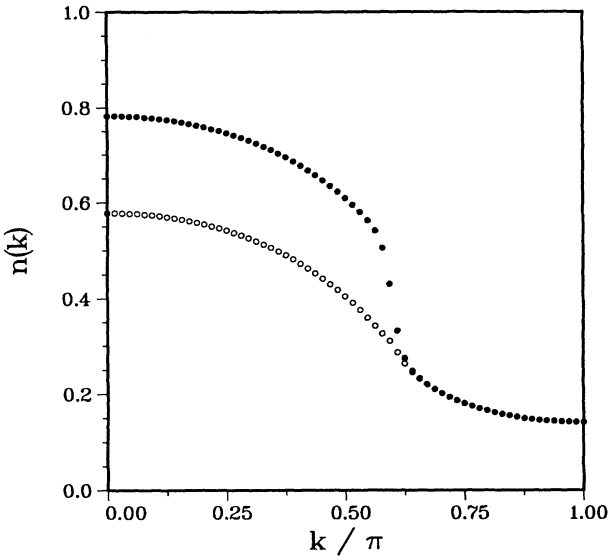

FIG. 4. The momentum distribution function $n(\mathbf{k})$ plotted for $\mathbf{k}$ along the (10) direction and $T/t = 0.015$. The open circles are the incoherent part from Eq. (22).

If we evaluate the quasiparticle contribution using the same approximations as we used in Eq. (20), the corresponding approximation for the incoherent contribution (open symbols in Fig. 4) appears to be continuous at k_F. This figure provides further evidence for the quasiparticle interpretation of our results and also warns against a naive interpretation of experimentally determined momentum distributions, such as those extracted from positron-annihilation experiments.

In conclusion, we emphasize that the results reported here should not necessarily be interpreted as evidence against the occurrence of a Luttinger liquid or a marginal Fermi liquid in the 2D positive-U Hubbard model. We have simply presented evidence that the self-consistent propagator-renormalized fluctuation exchange approximation leads to conventional Fermi-liquid behavior (at least well away from half filling), and hence that the origin of a Luttinger liquid or marginal Fermi liquid must be sought in more sophisticated approximations.

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