RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 42, NUMBER 10 1 OCTOBER 1990

Dynamics of quasiparticles in the two-dimensional Hubbard model

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(Received 9 July 1990)

The Hubbard model at half-filling is a collective, antiferromagnetic insulator. We study added electrons or holes. The insulating energy gap and the dispersion of the added carriers are calculated variationally in two dimensions with use of a Monte Carlo evaluation of the electronic correlation functions in the insulating phase. Both E_g and m^* are found to be temperature dependent.

INTRODUCTION

For a variety of reasons, attention has recently focused on two-dimensional (2D) interacting electrons. At $N_{\rm el}=N$, the number of sites, the Hubbard model is a collective, antiferromagnetic insulator with energy gap E_g. Away from half-filling there are a number of hypotheses but no consensus as to the nature, number, and dispersion of the carriers in the many-body system,[1] although it is widely conceded that solving this problem is prerequisite to any theory of high-T_c superconductivity. The evidence on the normal phase of CuO_2-based layered metals has been construed to favor a modified Fermi liquid[2] over ordinary band-structure theory.[3] Varma *et al.*[4] have characterized them as "marginal" Fermi liquids. Numerical analysis[5] of the strong-coupling-limit t-J model reveals quasiparticle peaks in the spectrum of added electrons or holes.

This paper analyzes the charge carriers in the Hubbard model by means of correlation functions that are accurately calculable *only* for the insulating half-filled band. When doping introduces a fraction x of charge carriers, we determine that they constitute a spin-$\frac{1}{2}$ Fermi liquid of xN, *not* $(1\pm x)N$, particles, with anisotropic dispersion and an effective mass m^* at the gap edge functionally related to E_g.

THE MODEL

The Hamiltonian for the Hubbard model $\mathcal{H}$ is

$$\mathcal{H}=-t\sum_{ij}(c_{i\sigma}^{*}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i,+}n_{i,-}-(U/2)N_{\rm el}\,, \quad (1)$$

with electrons hopping from sites i to nearest-neighbor sites j. With the chemical potential μ here set at $U/2$, on a bipartite lattice $\mathcal{H}$ is invariant under charge conjugation (followed by a phase transformation on the odd-numbered sublattice): $c_{r\sigma},c_{r\sigma}^{*}\rightarrow(-)^{r}c_{r,-\sigma}^{*},(-)^{r}c_{r,-\sigma}$. This invariance creates extra symmetries.[6]

The exact ground state at half-filling is $|\Psi_0\rangle$,[7] its energy E_0. For a particle deleted or added, the energy is $E(\mathbf{k};t,U)\equiv E_0+e(\mathbf{k};t,U)\pm U/2$, its minimum lying on the star of a wave vector $\mathbf{k}_0$, independent of σ. It is known[1,2] that $\mathbf{k}_0$ is $(\pi/2,\pi/2)$ at all $t/U>0$,[5,8] both for deleted and for added particles. It follows that $E_g=U+2e_{\rm del}(\mathbf{k}_0;t,U)$. The stability of the insulating phase is guaranteed by $E_g\geq 0$. However, if E_0 and $E(\mathbf{k};t,U)$, both $O(N)$, are obtained numerically, their differences, including E_g, which are $O(1)$, become difficult—if not impossible—to calculate reliably and other means must be sought.[9,10]

STATES OF ONE PARTICLE ADDED OR DELETED

We define

$$a^{*}(\mathbf{k},\sigma)\equiv N^{-1/2}\sum_{i}e^{i\mathbf{k}\cdot\mathbf{R}_i}\sum_{j}\Gamma_{ij}c_{i\sigma}^{*}\,,$$

with Γ_{ij} an operator incorporating the reaction of the medium at j to the extra carrier at i. For $N+1$ particles there are $2N$ orthogonal states $a^{*}(\mathbf{k},\sigma)|\Psi_0\rangle$ with which to estimate the $e(\mathbf{k};t,U)$ directly:

$$e\leq\frac{(\Psi_0|a(\mathbf{k},\sigma)[\mathcal{H},a^{*}(\mathbf{k},\sigma)]|\Psi_0)}{(\Psi_0|a(\mathbf{k},\sigma)a^{*}(\mathbf{k},\sigma)|\Psi_0)}+U/2\,. \quad (2)$$

The better the choice of Γ, the tighter is this variational bound. By successive applications of $(\mathcal{H}-E_0)$ to $c_{\mathbf{k}\sigma}^{*}|\Psi_0\rangle$, one determines the form of Γ at any given $\mathbf{k},\sigma$:

$$\sum_{j}\Gamma_{ij}(\mathbf{k},\sigma)=1+g_{0\mathbf{k}}n_{i,-\sigma}+\sum_{j\neq i}g_{1\mathbf{k}}(\mathbf{R}_{ij})(n_{j\uparrow}+n_{j\downarrow})+\cdots\,. \quad (3)$$

Because many-body perturbation theory in U fails about the singular point $U=0$, the g's have to be obtained variationally. But already the leading approximation $\Gamma=1$ yields sensible results, such as locating the minimum at $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$.[5,11] The next term ($\propto g_{0\mathbf{k}}$) considerably improves the calculated energies without substantial complication. Higher-order terms which parametrize charge and spin polarization[12] of the environment assume increasing importance at large $U\geq 8t$. But they also greatly complicate the programs, and we are forced to defer them for future investigations. In the present work, we opt for a simple operator designed for accuracy in the little-studied weak-coupling regime, $U<8t$; for *added*

particles we choose

$$\Gamma_{ij}(\mathbf{k},\sigma)=[U_{\mathbf{k}}n_{r,-\sigma}+v_{\mathbf{k}}(1-n_{r,-\sigma})]\delta_{ij}\,.$$

By the aforementioned symmetry[6] ($\mathbf{k}\rightarrow-\mathbf{k}+\pi$, $\sigma\rightarrow-\sigma$, and $c^*\leftrightarrow c$), this also yields the operator for *deleted* particles.

At each $\mathbf{k}$ we determine $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ by optimizing $e(\mathbf{k})$. Using these, we also construct the Wannier operators of the composite particle. Their effective radius is found to be quite small.[13]

The numerator and denominator in (2) are each sums of correlation functions in the half-filled ground state of $\mathcal{H}$, and are calculated by quantum Monte Carlo.[14] Identities which keep our calculations to a manageable minimum include[7]

$$(\Psi_0|n_{i,-\sigma}c_{i\sigma}^*c_{j\sigma}|\Psi_0)\equiv\tfrac{1}{2}(\Psi_0|c_{i\sigma}^*c_{j\sigma}|\Psi_0)\neq 0$$

for i,j on different sublattices, and $(\Psi_0|c_{i\sigma}^*c_{j\sigma}|\Psi_0)\equiv\frac{1}{2}\delta_{ij}$ if i,j are on the same sublattice. Our studies centered on the range of parameters $0<U/t\leq 8$, where neither the t-J model nor perturbation theory (the energies are not analytic in U at $U=0$) are applicable. To keep the systematic error as small as possible, we used different imaginary-time discretizations $\Delta\tau$, extrapolating the results to $\Delta\tau=0$. Simulations are on 8×8 lattices at $\beta=6/t$. At small U we verified that the β dependence was negligible by simulating also at $\beta=9/t$. Figure 1 (bottom curve) shows $e_{0,\mathrm{del}}(t,1)$, i.e., $e_{\mathrm{del}}(\mathbf{k}_0;t,U)$ at $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$ and $U=1$, calculated at $t/U=0$ (where $e_{0,\mathrm{del}}\rightarrow 0$), $\frac{1}{6}$, $\frac{1}{5}$, $\frac{1}{4}$, $\frac{1}{2}$, 1, and ∞ (where $e_{0,\mathrm{del}}/U\rightarrow-0.5$), and fitted to a smooth polynomial curve; accuracy is indicated by error bars. At $t/U<\frac{1}{8}$ our curve joins smoothly with the strong-coupling results of Dagotto *et al.*:[5] $e_{0,t\text{-}J}=-3.17t+2.83t(J/t)^{0.73}$ (dashed curve), with $J=4t^2/U$. While the $t-J$ model is closely related to the Hubbard model in strong coupling, it is not identical, and the upturn at $t/U>\frac{1}{8}$ in the dashed curve makes it clear that the two models differ substantially in weak coupling.

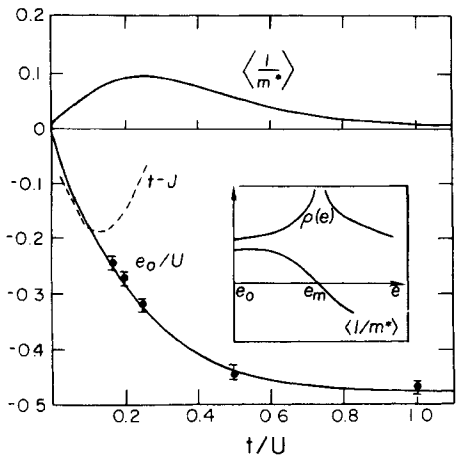

FIG. 1. Lower curve: $e_0(t,U)/U$ (e_0 plotted here is minimum energy to *delete* particle from half-filled band) vs t/U. Calculated points are indicated by error bars, curve is best polynomial fit. Dashed line marked t-J is from Dagotto *et al.* (Ref. 5). Upper curve: $\langle 1/m^*\rangle$ at $\mathbf{k}_0$, in units of $(1/m_0)(U/4\times 13.6\text{ eV})(a/a_0)^2$ vs t/U as calculated from $e_0(t,U)$ using Eq. (5). (m_0 is the free-electron mass, U is in eV, and a/a_0 is the lattice parameter in units of the Bohr radius, 0.529 Å.) Inset: Schematic plots of $\langle 1/m^*\rangle$ and the density of states $\rho(e)$ (at fixed t,U) as functions of energy measured from e_0, demonstrating that $\langle 1/m^*\rangle$ changes sign at e_m where ρ has its maximum (Ref. 15).

MANY-PARTICLE STATES

Consider at first the *scattering states* of two added particles,

$$|\mathbf{k},\sigma;\mathbf{k}',\sigma')=a^*(\mathbf{k},\sigma)a^*(\mathbf{k}',\sigma')|\Psi_0)+N^{-1}\sum_{\mathbf{q}\sigma''\sigma'''}\mathcal{L}_{\sigma''\sigma'''}(\mathbf{q})a^*(\mathbf{k}+\mathbf{q},\sigma'')a^*(\mathbf{k}'-\mathbf{q},\sigma''')|\Psi_0)\,. \tag{4}$$

As usual in scattering theory, the energy of the pair is additive: $e(\mathbf{k})+e(\mathbf{k}')+2(U/2)+O(1/N)$. But what is their statistics? If the Γ's were in the form of long strings, these could become entangled in 2D and lead to parastatistics (exotic representations of the braid group) under interchange of the two members of this pair. But in the present context, our variationally determined Γ's have a small radius.[13] Therefore, one readily forms wave packets such that the two particles are well separated in space and devoid of interaction with each other. From this it follows that the a^*'s anticommute. If the medium were spin polarized about each carrier, i.e., if the Γ's created a "Nagaoka bubble" of spin S about each carrier, the a^*'s would be creation operators for exotic fermions of spin $S\pm\frac{1}{2}$. Again, as our choice of Γ's carries only $S=0$ (as is appropriate in the weak-coupling regime), our fermions have the usual spin $\frac{1}{2}$.

Extending the arguments to a dilute fraction x of added or deleted particles, one concludes that they behave as an ordinary spin-$\frac{1}{2}$ Fermi liquid of xN charge carriers superposed onto a background of N non-current-carrying electrons. Their unusual dispersion is detailed below. Even if the residual interparticle forces were to favor bound states over the scattering states (4), as is claimed in some small-cluster calculations,[10] and this resulted in the many-body ground state of the presumed Fermi liquid becoming unstable against some condensed phase, the statistics of the particles under interchange and their dispersion would be required ingredients in constructing the new ground state.

DISPERSION OF QUASIPARTICLES

Figure 2 shows the calculated dispersion in $e(\mathbf{k};1,U)$ along two orthogonal axes centered at $\mathbf{k}_0$. The extreme anisotropy diminishes somewhat with increasing U. With increasing carrier concentration, the Fermi surface follows disjoint contours surrounding each $\mathbf{k}_0$, portions of which are show in Fig. 2 (inset). Such a topology was earlier conjectured by Lee.[2] The density of states $\rho(e)$ starts at a finite value ρ_0 ($\rho_0\propto m^*$) at e_0, and increases with in-

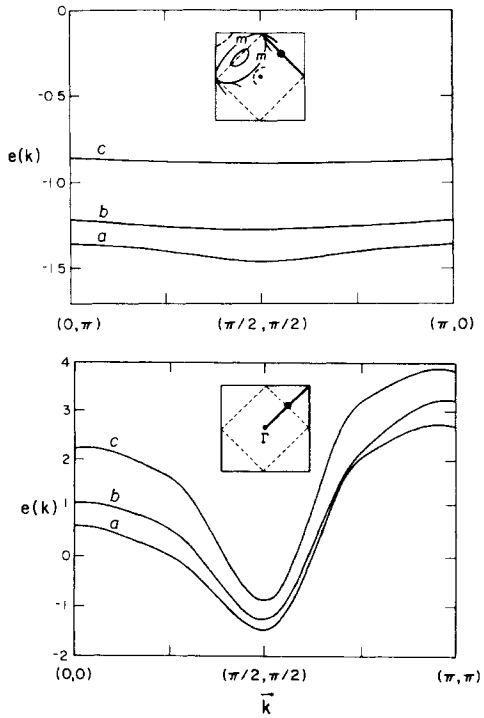

FIG. 2. Curves labeled a are for $U/t=6$, b are for $U/t=43$, and c are for $U/t=2$, respectively. Top: $e_{\rm del}(\mathbf{k})/t$ (energy to delete particle at $\mathbf{k}$ from half-filled band) plotted along perimeter of inscribed diamond. Inset: $\mathbf{k}_0=(\pi/2,\pi/2)$ shown as big dot. Portions of constant energy contours are shown; curves labeled m are the locus of e_m (cf. inset of Fig. 1) (Ref. 15). Bottom: $e_{\rm del}(\mathbf{k})/t$ along (1,1) direction. Note the anisotropy: m^* in this direction is smaller than along the perimeter by 1 order of magnitude.

creasing energy until, at e_m, the four contours merge. Their perimeter is then at a maximum, as is ρ.[15] For $e>e_m$, both $d\rho/de$ and $\langle 1/m^*\rangle$ become negative—shown schematically in Fig. 1 (inset). (By way of comparison, both in Hartree-Fock and in band-structure theory, where the many-body correlations are treated in an average way, e_m merges with e_0 and the low-energy dynamics are given incorrectly.[3])

THE EFFECTIVE MASS

We estimate the average inverse mass $\langle 1/m^*\rangle$ directly as a function of $\mathbf{k}$, t, U, and T by combining Galilean invariance with Feynman's theorem:[16]

$$\langle 1/m^*\rangle(\mathbf{k}) = -(t/2)\partial e(\mathbf{k};t,U)/\partial t\,. \tag{5}$$

$\langle 1/m^*\rangle(\mathbf{k}_0)$ as a function of t/U, plotted in the upper curve of Fig. 1, is found by differentiating the lower curve. Our results demonstrate that a correlated system can produce truly "heavy,"[17] yet delocalized, fermions at all U.

The addition or deletion of each particle affects not just the total energy of the medium, but its entropy as well. With $f(\mathbf{k})$ the excess free energy of an excess particle at $\mathbf{k}$, the $T\neq 0$ generalization of (5) is[16]

$$\langle 1/m^*\rangle(\mathbf{k}) = -(t/2)\partial f(\mathbf{k})/\partial t - (\beta/2)[\langle(\mathbf{v}-\langle\mathbf{v}\rangle)^2\rangle - \langle(\mathbf{v}-\langle\mathbf{v}\rangle_0)^2\rangle_0]\,, \tag{6}$$

where $\beta=1/kT$, $\mathbf{v}=(v_x,v_y)$ with $v_x=2t\sum_{k,\sigma}\sin k_x \times c^*(\mathbf{k},\sigma)c(\mathbf{k},\sigma)$, and $\langle\cdots\rangle$ indicates thermal average in the presence of the extra particle, while $\langle\cdots\rangle_0$ refers to such an average in the half-filled state.

CONCLUSION

By combining a variational ansatz with quantum Monte Carlo techniques, we have estimated the properties of low-lying eigenstates of a small number of extra holes or electrons introduced into the Mott insulating phase of the two-dimensional Hubbard model. In weak coupling, we conclude that they constitute a dilute fluid of spin-$\frac{1}{2}$ fermions with heavy, anisotropic, temperature- and energy-dependent masses.

ACKNOWLEDGMENTS

The authors thank the ISI (Torino) and Professor Mario Rasetti for his hospitality during the early stages of this work. Support was provided by U.S. Army Electronics Technology and Devices Laboratory, SLECT-E, Ft. Monmouth, New Jersey (D.C.M.), and by the Bundesministerium für Forschung und Technologie and Esprit Program No. 3041 (M.D. and X.Z.). Publication of this work was supported by ONR Grant No. N00014-86K-0710.

[1]For a perspective, see *High-Temperature Superconductivity*, Proceedings of the Los Alamos Symposium, 1989, edited by K. S. Bedell *et al.* (Addison-Wesley, Redwood, CA, 1990).

[2]G. A. Sawatzky, Nature (London) **342**, 480 (1989); P. E. Sulewski *et al.*, Phys. Rev. B **36**, 2357 (1987); also see review by P. A. Lee, in *High-Temperature Superconductivity* (Ref. 1), p. 96.

[3]In addition to some other inadequacies, band-structure theory yields the incorrect sign of the Hall constant; see review by N. P. Ong, in *Physical Properties of High-Temperature Superconductors II*, edited by D. M. Ginsberg (World Scientific, Singapore, 1990).

[4]C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 1996 (1989).

[5]S. A. Trugman, Phys. Rev. B **41**, 892 (1990); E. Dagotto *et al.*, *ibid.* **41**, 2585 (1990); with $J\approx 4t^2/U$, the t-J model is believed to mimic the strong-coupling limit ($t\ll U$) of the Hubbard model.

[6]E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[7]$|\Psi_0\rangle$ is invariant under the point group of the lattice, translations, and charge conjugation. Its total momentum, angular momentum, and spin is zero for $N=$even. For details, see

Ref. 6.

[8]Although at $U=0$ the locus of $\mathbf{k}_0$ in the Brillouin zone is the inscribed diamond given by $(\cos k_x+\cos k_y)=0$, this degeneracy is lifted at all $U\neq 0$. See, for example, P. A. Lee, in *High-Temperature Superconductivity* (Ref. 1).

[9]The calculational error in each E is $O(1)$ for exact diagonalization but $O(\sqrt{N})$ if Monte Carlo is used. In the former case, the uncertainty in the energy differences $e(\mathbf{k})$ is serious and in the latter, fatal. Our procedure avoids this pitfall, as do some other recent schemes (see Ref. 10).

[10]E. Dagotto *et al.*, Phys. Rev. B **41**, 811 (1990), find a two-hole bound state with small binding energy on 4×4 clusters. (Note that such binding might not be sturdy against longer-range Coulomb forces.)

[11]According to Trugman (Ref. 5) at $t=U/8$ the fractional spectral intensity of the quasiparticle peak is only 0.358 (in the state which corresponds to $\Gamma=1$ in our notation.) Thus, quasiparticle eigenstates must include local-density and antiferromagnetic (Ref. 12) correlations, i.e., have $\Gamma\neq 1$.

[12]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. Lett. **60**, 944 (1988); Z. Y. Weng, C. S. Ting, and T. K. Lee, Phys. Rev. B **41**, 1990 (1990).

[13]The Wannier operators are lattice Fourier transforms of the $a^*(\mathbf{k},\sigma)$. The Fourier transform $u(\mathbf{R}_{ij})$ of $u_{\mathbf{k}}/(\Psi_0|a(\mathbf{k},\sigma)\times a^*(\mathbf{k},\sigma)|\Psi_0)^{1/2}$, and the Fourier transform $v(\mathbf{R}_{ij})$ of $v_{\mathbf{k}}/(\Psi_0|a(\mathbf{k},\sigma)a^*(\mathbf{k},\sigma)|\Psi_0)^{1/2}$ have been computed by us. At $U=0$, the Wannier functions are trivially pointlike: $u(\mathbf{R})=v(\mathbf{R})=\delta(\mathbf{R})$. But even at $U/t=6$, where the correlations are consequential and $v(\mathbf{0})\approx 2u(\mathbf{0})$, the functions $v(\mathbf{R})$ and $u(\mathbf{R})$ decrease rapidly with distance with alternating signs, the effective radius being no more than a few interatomic spacings.

[14]Following R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981), as extended to 2D by J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985), and later by S. R. White *et al.*, *ibid.* **40**, 506 (1989).

[15]We compute $(e_m-e_0)/t$ to be 0 (at $U=0$), 0.03 (at $U=2t$, curves c in Figs. 2) 0.06 (at $U=4t$, curves b), and 0.12 (at $U=6t$, curves a).

[16]D. C. Mattis (unpublished).

[17]Z. Fisk *et al.*, Science **239**, 33 (1988).