Conserving Approximations for Strongly Correlated Electron Systems: Bethe-Salpeter Equation and Dynamics for the Two-Dimensional Hubbard Model

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In this Letter we describe a new technique for investigating phase transitions and dynamics in interacting electron systems. This technique is based on the derivation and self-consistent solution of infinite-order conserving approximations. It provides a new approach to the study of two-particle correlations with strong frequency and momentum dependence. We use this technique to derive a low-temperature phase diagram and dynamic correlation functions for the two-dimensional Hubbard model.

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Experimental studies of heavy-electron compounds,[1] the organic Bechgaard salts,[2] the recently reported bis-(ethylenedithiolo)-tetrathiafulvalene superconductors,[3] and the oxide superconductors[4] have emphasized the need for new approaches to strongly correlated electronic systems. While quantum Monte Carlo (QMC) techniques can, in principle, provide exact results for electronic correlation functions, such techniques are at present limited to relatively small systems and high temperatures. Furthermore, QMC furnishes direct information on imaginary-time, rather than real-time correlations; the treatment of real-time dynamics remains problematic. In this Letter, we describe a semianalytical approach to strongly correlated systems which satisfies microscopic conservation laws, treats strong frequency and momentum dependences, and provides information on both static and dynamic properties. This approach may be used to treat large systems and temperatures lower than those currently accessible to finite-temperature QMC. Furthermore, this approach naturally incorporates realistic features such as Fermi surface nonsphericity, which may explain property variations within a series of otherwise similar compounds.

In this Letter, we restrict attention to the two-dimensional Hubbard model. This lattice model is an interesting test for approximate many-body approaches since it involves a potential competition between antiferromagnetic and superconducting ground states. The simplest Hubbard Hamiltonian for electrons moving on a square lattice is characterized by a hopping integral t, which connects neighboring sites with separation a, an on-site Coulomb repulsion U, and a temperature-dependent chemical potential μ, which must be adjusted to fix the electronic filling n. A "conserving approximation" for this model, i.e., an approximation consistent with microscopic conservation laws for particle number, energy, and momentum, may be generated following an approach introduced by Baym[5] to treat the Coulomb gas: (a) First, write down a "free-energy" functional Φ of the dressed single-particle Green's function G and the interaction U. The diagrammatic representation of this functional formally resembles the expansion for the ground-state energy. (b) Generate an approximation for the single-particle self-energy Σ by functional differentiation of Φ with respect to G:

$$\Sigma(1,2)=\delta\Phi/\delta G(2,1)\,.$$

(Our notation is that of Ref. 5.) Compute G self-consistently using this self-energy. (c) Generate an approximation for particle-hole (or particle-particle) response functions L by computing G in the presence of an external potential $\mathcal{U}$, then performing a functional differentiation with respect to $\mathcal{U}$:

$$L(1,2;1',2')=\delta G(1,1')/\delta\mathcal{U}(2',2)\,|_{\mathcal{U}=0}\,.$$

The correlation functions generated in this way automatically obey microscopic conservation laws, are consistent with Luttinger's theorem,[6] and lead to Fermi-liquid behavior at low temperatures in the normal state. The Φ diagram describing the repulsion of opposite-spin electrons in the absence of fluctuations is shown in Fig. 1(a). The conserving approximation generated by this diagram is just Hartree-Fock, or mean-field, theory. The diagrams describing the interaction of electrons with spin, density, and two-particle fluctuations are shown in Figs. 1(b)–1(d). These diagrams lead to a "higher order" Hartree-Fock theory which consistently incorporates the effect of the simplest fluctuations. We shall hereafter refer to this approach as the "fluctuation-exchange approximation."[7,8] In the past, technical limitations have generally prevented the self-consistent solution of conserving approximations beyond mean-field level. We describe below a general approach for solving approximations which incorporate strong collective fluctuations, and use this technique to obtain a fully self-consistent solution of the fluctuation-exchange approximation for

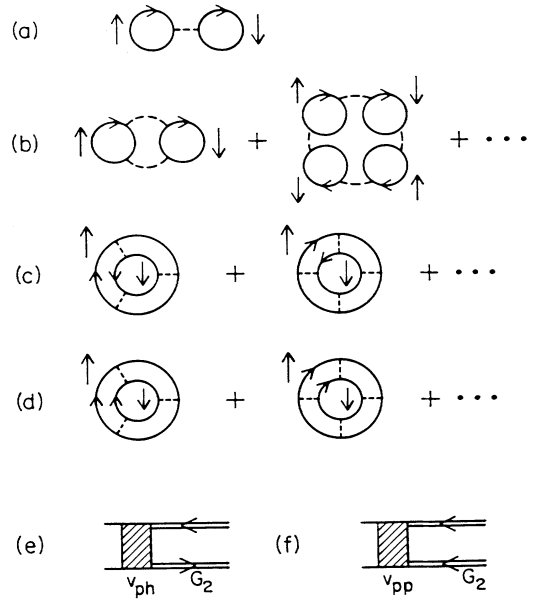

FIG. 1. Hubbard model diagrams for the fluctuation-exchange approximation. The interaction U is represented by a dashed line. (a) Lowest order Φ diagram (Hartree-Fock theory), (b) Φ ring diagrams representing the interaction of longitudinal spin and density fluctuations, (c) transverse spin fluctuations, (d) particle-particle fluctuations, (e) Bethe-Salpeter kernels for the particle-hole, and (f) particle-particle channels. The double lines represent self-consistent Green's functions based on the Φ approximation in (a)–(d).

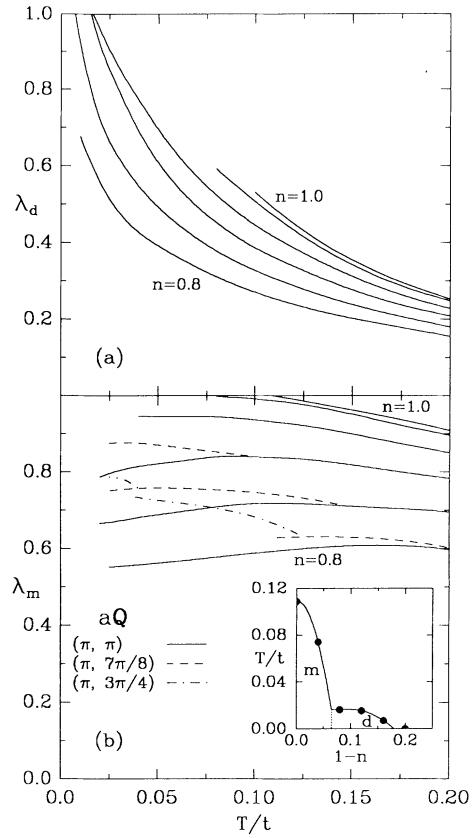

FIG. 2. (a) Leading d-wave singlet eigenvalues of the particle-particle kernel for $U/t=4$. These results are based on a 16×16 discretization of the Brillouin zone. Successive curves vary in n by increments of 0.04 from $n=1.0$ to 0.8. (b) Leading commensurate $[a\mathbf{Q}=(\pi,\pi)]$ and incommensurate magnetic eigenvalues of the particle-hole kernel. As in (a), values of the filling vary regularly by increments of 0.04. Incommensurate eigenvalues (for fillings $n=0.80$, 0.84, and 0.88) are shown only when they exceed the corresponding commensurate eigenvalues. Inset: Approximate phase diagram derived from the transitions (Ref. 10) in (a) and (b).

the Hubbard model.

In general, steps (b) and (c) above lead to singular integral equations in the Fourier transform variables $k=(\mathbf{k},\omega)$. These equations cannot be solved in closed form, but may be conveniently treated by (a) discretizing the Brillouin zone (or, equivalently, restricting the calculation to a finite lattice in real space), and (b) analytically continuing the energy variable ω to discrete Matsubara frequencies on the imaginary axis. Using the self-energy generated by Fig. 1, we have solved iteratively for the single-particle Green's function, taking into account its full momentum and frequency dependence. Use of symmetries in momentum and frequency space significantly reduces the computation time and storage requirements. Real-frequency correlation functions, including the one-electron density of states and the magnetic spectral density (or neutron-scattering function), may be recovered using N-point Padé approximants[9] to reverse the analytic continuation.

The competition between two or more ordering transitions[10] may be studied using the results of a conserving approximation and the Bethe-Salpeter equation. Singlet and triplet superconductivity correspond to the development of a scattering pole in the particle-particle channel, while spin and charge ordering correspond to a scattering pole in the particle-hole channel. In the nearly half-filled Hubbard model, an almost instantaneous attractive interaction occurs in the triplet particle-hole channel, corresponding to spin ordering with wave vector at or near the zone-boundary vector $a\mathbf{Q}=(\pi,\pi)$. On the other hand, it is believed from the random-phase-approximation[11,12] and from QMC[13] studies that a strongly retarded attractive interaction occurs in a particle-particle channel with singlet $d_{x^2-y^2}$ symmetry.[14] The Bethe-Salpeter equation, which treats time-dependent two-particle interactions, allows the study of both instabilities.

An instability occurs when an eigenvalue of the Bethe-Salpeter kernel K reaches unity. The imaginary-frequency kernel takes the form shown in Figs. 1(e) and 1(f). It is a product of two single-particle Green's functions and v, the effective particle-hole (or particle-

particle) interaction. We show in Figs. 2(a) and 2(b) the behavior of the leading magnetic and d-wave superconducting eigenvalues for calculations performed using the Φ approximation in Figs. 1(a)–1(d) with a 256-point discretization of the Brillouin zone and a frequency cutoff of $\pm 10t$. The Coulomb energy $U/t=4$ and results are shown for electronic fillings varying from 0.8 to 1.0. Leading eigenvalues and eigenvectors of K are computed by repeated projection on test vectors of the appropriate symmetry. The largest kernels we have treated with this technique have row dimension 256×322 in $(\mathbf{k},i\omega)$ space.[15] Finite-size studies with 16- and 64-point Brillouin zones suggest that discretization error in the calculated transition temperatures is on the order of 10% or less. For deviations of less than $\sim6\%$ from half filling, an antiferromagnetic state is favored, while for deviations between 6% and 18% a d-wave superconducting state is favored. A phase diagram is shown in the inset of Fig. 2(b). Note that the maximum predicted superconducting transition temperature is of order $0.01t$. This is an order of magnitude smaller than the random-phase-approximation estimate which would follow neglecting self-energies altogether. Combined with recent QMC results[13] which explore the effect of the two-particle vertex on pairing susceptibilities, these results strongly suggest that the Hubbard model has a d-wave superconducting ground state for a small range of fillings. The predicted transition temperature for a bare bandwidth $8t=1$ eV is $T_d\sim15$ K.

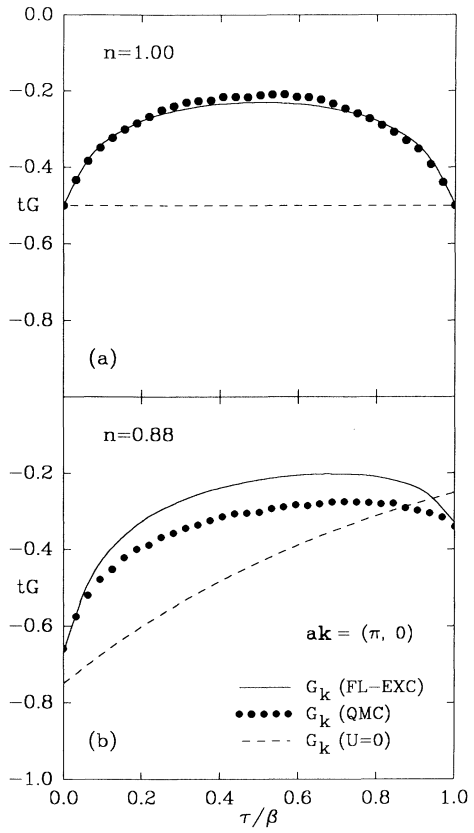

FIG. 3. Comparison of the imaginary-time Green's functions $G(\tau)$ derived from the fluctuation-exchange approximation and from QMC for $T/t=0.25$ with (a) $n=1.00$ and (b) $n=0.88$. Results are shown for the momentum-space Green's function $G_{\mathbf{k}}$ with $a\mathbf{k}=(\pi,0)$. The corresponding noninteracting functions are plotted as well to indicate the effect of interactions. All results shown are based on an 8×8 momentum-space discretization (or real-space lattice).

The accuracy of our conserving approximation for the Hubbard model may be gauged by direct comparison with QMC results.[16] We show in Fig. 3 results for the imaginary-time Green's function obtained from the fluctuation-exchange approximation and from QMC for fillings $n=0.88$ and 1.00. The approximate Green's function is particularly accurate at half filling; for smaller fillings, the two functions remain similar, though the fluctuation-exchange approximation underestimates G at intermediate values of τ. (This reduction is reflected in susceptibilities, which involve integrals of G.)

In order to illustrate the information on dynamics which may be obtained by this approach, we show in Fig. 4 a plot of the absorptive part of the magnetic susceptibility for $T/t=0.20$ at filling $n=0.96$. This plot shows the development of a sharp quasielastic peak at wave vector $a\mathbf{Q}^*=(\pi,\pi)$ and a softening of the paramagnon dispersion curve at the zone center, as well as the zone boundary. The velocity in the (1,1) direction is in this case approximately $0.35t/a^{-1}$, or $1.4t/\text{Å}^{-1}$ for a lattice constant of 4 Å. The one-electron density of states, scattering rate, and mass enhancement have also been obtained using the Padé technique[9] and will be discussed elsewhere.[17]

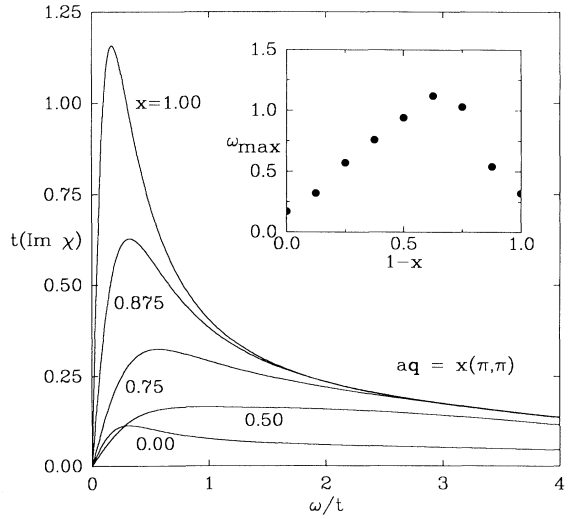

FIG. 4. Magnetic spectral density $\mathrm{Im}\chi(\mathbf{q},\omega)$ for $n=0.96$ and $T/t=0.20$. Inset: Peak locations $\omega_{\max}$, i.e., the paramagnon dispersion relation, for $a\mathbf{q}=(1-x)(\pi,\pi)$.

The calculation described above may be extended to more elaborate Hubbard or electron-phonon models and to more complex lattice structures. In the future, the self-consistent solution of conserving lattice approximations, which treat frequency and momentum dependence on an equal footing, may prove useful in developing a hybrid many-body band-theory approach to strongly interacting systems.

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[1]G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).

[2]D. Jerome, J. Phys. (Paris), Colloq. **44**, C3-755 (1983).

[3]K. Oshima, H. Urayama, H. Yamochi, and G. Saito, J. Phys. Soc. Jpn. **57**, 730 (1988).

[4]J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 18 (1986); M. K. Wu *et al.*, Phys. Rev. Lett. **58**, 908 (1987).

[5]G. Baym, Phys. Rev. **127**, 1391 (1962).

[6]J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).

[7]We have intentionally included spin, density, and two-particle fluctuations on the same footing. As expected from random-phase-approximation estimates, magnetic fluctuations are by far the most important contribution.

[8]This approximation satisfies approximate crossing symmetry and may be viewed as a first step toward a full summation of crossing-symmetric parquet diagrams.

[9]See, e.g., H. J. Vidberg and J. W. Serene, J. Low. Temp. Phys. **29**, 179 (1977).

[10]No true finite-temperature magnetic transition and only a possible Kosterlitz-Thouless superconducting transition are expected in the two-dimensional Hubbard model. For this reason, finite-temperature "transitions" should be interpreted as crossovers signaling the appearance of a large, but finite, correlation length. Weak three-dimensional coupling is sufficient to induce true long-range order in such phases.

[11]D. J. Scalapino, E. Loh, and J. E. Hirsch, Phys. Rev. B **35**, 6694 (1987).

[12]N. E. Bickers, D. J. Scalapino, and R. T. Scalettar, Int. J. Mod. Phys. B **1**, 687 (1987).

[13]S. R. White, D. J. Scalapino, N. E. Bickers, and R. T. Scalettar (to be published).

[14]A number of approximate approaches have been previously applied to investigate d-wave superconductivity: J. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **34**, 6554 (1986); C. Gros, R. Joynt, and T. M. Rice, Z. Phys. B **68**, 425 (1987); A. J. Millis, S. Sachdev, and C. M. Varma, Phys. Rev. B **37**, 4975 (1988); G. Kotliar, *ibid.* **37**, 3664 (1988); H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **57**, 1044 (1988).

[15]The only conserving diagrams omitted from the calculation of the vertex $v_{p\text{-}h}$ ($v_{p\text{-}p}$) describe the decay of a particle-hole (particle-particle) pair into two collective fluctuations. We have established, using studies with a sixteen-point Brillouin zone, that these contributions are small in comparison with the contributions retained.

[16]For a discussion of the QMC algorithm, see S. R. White, R. L. Sugar, and R. T. Scalettar (to be published).

[17]The one-electron self-energy is nontrivial and incorporates two opposing effects: The dressing of low-energy electrons by spin fluctuations tends to increase the electronic mass (in analogy with mass enhancement by phonons); on the other hand, the coupling of nearly degenerate electronic states in the presence of strong nesting repels electronic density from the Fermi level.