New Functional Integral Approach to Strongly Correlated Fermi Systems: The Gutzwiller Approximation as a Saddle Point

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We propose a new functional integral representation of the Hubbard and Anderson models of lattice fermions. The simplest saddle-point approximation leads, at zero temperature, to the results derived from the Gutzwiller variational wave function. This approach uncovers the limitations of the Gutzwiller approximation and clarifies its connection to the "auxiliary-boson" mean-field theory of the Anderson model. This formulation leads to a novel strong-coupling mean-field theory which allows for a unified treatment of antiferromagnetism and ferromagnetism, metal-to-insulator transition, and Kondo compensation effects.

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Recently there has been an upsurge of interest in strongly correlated Fermi systems, mainly triggered by the remarkable properties of the newly discovered "heavy-electron" materials.[1] Interest in the problem was also stimulated by speculations concerning the interplay between disorder and correlation effects near the metal-to-insulator transition in doped semiconductors.[2] A theoretical understanding of these systems is still lacking and further progress appears to require new techniques, outside the scope of conventional weak-coupling approximations.

Apart from Monte Carlo simulations,[3] two analytical approaches to strongly correlated fermions have received a great deal of attention: the Gutzwiller variational approach, which originated in the context of the Hubbard model,[4] and the so-called "slave-boson" or auxiliary-boson formulation first proposed by Barnes[5] and rediscovered and extended by Coleman[6] and Read and Newns[7] in their work on the mixed-valence problem. The first is an appealing but uncontrolled approximation scheme for calculating the ground-state energy of a variational trial wave function. The second has so far been mainly used to treat the infinite-U Anderson model and consists of replacing the infinite correlations by a local constraint which is then handled by standard field-theoretical methods (see, however, Ref. 5). In this Letter we present a new functional integral formulation which (i) extends the collective boson approach to any value of the correlation[8]; (ii) reproduces for the first time the results of the Gutzwiller approach in a saddle-point approximation, and thus uncovers the limitations of the Gutzwiller approximation and suggests, at least in principle, systematic ways of improving it; and (iii) allows for a unified treatment of ferromagnetism, antiferromagnetism, and metal-insulator transitions in a mean-field theory which in the weak-coupling case agrees with Hartree-Fock theory while for strong coupling incorporates the qualitative physics expected from the few available exact results. (iv) In the Anderson model the resulting saddle point builds in the collective quenching of the local moments (Kondo effect) and will ultimately allow us to study the competition between the Kondo effect and magnetic order. To our knowledge this is the first method by which such a large number of phenomena become easily accessible within the same framework.

Qualitatively our approach is based on the idea that, in a strongly correlated system, in the process of hopping the electron is accompanied by a "backflow" of spin and density excitations of the medium. (In a quasiparticle picture this shows up as a renormalization of the hopping amplitude and simply leads to a change of the effective mass.) Formally, this qualitative idea can be realized by rewriting the original Hamiltonian in terms of the original fermions and a set of four projection operators which keep track of the environment by measuring the occupation numbers in each of the four possible states available for hopping.

To be explicit, we first concentrate on the Hubbard model[9] which is expected to capture the main features of the physics of lattice fermions in a narrow energy band. The corresponding Hamiltonian includes a nearest-neighbor hopping, t_{ij}, and an on-site repulsion between electrons of different spins, U:

$$H=\sum_{ij,\sigma} t_{ij} f_{i\sigma}^{\dagger} f_{j\sigma}+U \sum_{i} f_{i\sigma}^{\dagger} f_{i\sigma} f_{i-\sigma}^{\dagger} f_{i-\sigma}, \tag{1}$$

where $f_{i\sigma}^{\dagger}$ ($f_{i\sigma}$) are creation (annihilation) operators for an electron of spin σ ($=\pm 1$) at site i. In analogy with the "slave boson" approach we enlarge the Fock space at each site, to contain in addition to the original fermions a set of four bosons represented by the creation (annihilation) operators $e_i^{\dagger}$ (e_i), $p_{i\sigma}^{\dagger}$ ($p_{i\sigma}$), $d_i^{\dagger}$ (d_i). This enlarged space contains unphysical states which can be eliminated by imposing the set of constraints

$$\sum_{\sigma} p_{i\sigma}^{\dagger} p_{i\sigma}+e_i^{\dagger} e_i+d_i^{\dagger} d_i=1, \tag{2a}$$

$$f_{i\sigma}^{\dagger} f_{i\sigma}=p_{i\sigma}^{\dagger} p_{i\sigma}+d_i^{\dagger} d_i, \quad \sigma \pm 1. \tag{2b}$$

When restricted by (2) the Bose fields e_i, $p_{i\sigma}$

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$(\sigma=-1)$, and d_i act respectively as projection operators onto the empty, singly occupied (with spin up and down), and doubly occupied electronic states at each site. Equation (2a) can then be interpreted as a completeness relation and reflects the fact that no more and no less than one of the four possible states must be occupied at each site; the second constraint equates the two ways of counting the fermion occupancy of a given spin. It is easy to check that in the physical subspace defined by Eqs. (2) the Hamiltonian

$$\tilde{H}=\sum_{ij,\sigma} t_{ij} f_{i\sigma}^\dagger f_{j\sigma} z_{i\sigma}^\dagger z_{j\sigma} + U\sum_i d_i^\dagger d_i, \tag{3a}$$

$$z_{i\sigma}=e_i^\dagger p_{i\sigma}+p_{i-\sigma}^\dagger d_i, \tag{3b}$$

has the same matrix elements as those calculated for (1) in the original Hilbert space.

To calculate observable quantities we write down the partition function Z of model (3) as a functional integral over coherent states of Fermi and Bose fields.[6,7] We note that the constraints (2) commute with the Hamiltonian (3) and thus the physical Hilbert space is preserved under time evolution. The constraints (2a) and (2b) are thus enforced at each site by time-independent Lagrange multipliers, which we symbolize below by $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$ $(\sigma=\pm 1)$, respectively. We integrate out the Fermi fields (by using standard rules for integration over Grassmann variables) to reexpress Z in terms of the effective action for the bosons, $\tilde{S}$, as

$$Z=\int [De][Dp_{\pm\sigma}][Dd]\prod_{i\sigma}[d\lambda_i^{(1)}][d\lambda_{i\sigma}^{(2)}]\exp\left[-\int_0^\beta d\tau\, \tilde{S}(\tau)\right], \tag{4a}$$

$$\tilde{S}(\tau)=\sum_i \Big[e_i^\dagger(\partial_\tau+\lambda_i^{(1)})e_i+\sum_\sigma p_{i\sigma}^\dagger(\partial_\tau+\lambda_i^{(1)}-\lambda_{i\sigma}^{(2)})p_{i\sigma}+d_i^\dagger(\partial_\tau+U+\lambda_i^{(1)}-\lambda_{i\sigma}^{(2)})d_i\Big]$$
$$-\lambda_i^{(1)}+\operatorname{tr}\ln[\delta_{ij}(\partial_\tau-\mu-\sigma h+\lambda_{i\sigma}^{(2)})+t_{ij}z_{i\sigma}^\dagger z_{j\sigma}], \tag{4b}$$

where μ is the chemical potential which is adjusted to fix the average occupation of the site, $n=1-\delta$, and h is an external magnetic field. (Since the physics is symmetric about $n=1$ [10] we restrict ourselves to the case $\delta\geqslant 0$.)

We note that in the atomic limit $(t_{ij}=0)$ the functional integral (4) can be calculated exactly and leads to the known results.[9] For $t_{ij}\neq 0$ the simplest approach to (4) is the saddle-point approximation in which all Bose fields and Lagrange multipliers are taken to be independent of space and time. Unfortunately, the resulting saddle-point equations lead to the incorrect result in the noninteracting limit (which occurs either for $U=0$ or in the case of fully polarized spins). This is because in this approximation the constraints are only satisfied on the average, and not explicitly at each site of the lattice. For example, when $U=0$ and $\delta=0$, $e^2=d^2=p_\sigma^2=\frac{1}{4}$ and thus

$$\langle z_{i\sigma}^\dagger z_{j\sigma}\rangle = e^2p_\sigma^2+d^2p_{-\sigma}^2+2edp_\sigma p_{-\sigma}=\tfrac{1}{4},$$

rather than unity as it should be for the noninteracting system.

In order to resolve this problem we make use of the fact that the procedure described above is not unique; there are many different Hamiltonians, $\tilde{H}$, with different properties in the enlarged Hilbert space which lead to the same spectrum as (1) when restricted to the physical subspace defined by (2). Clearly this arbitrariness presents no difficulty as long as the constraints are handled exactly. However, any approximation which relaxes the constraints is sensitive to the precise choice of $\tilde{H}$. In any practical calculation this ambiguity can be used to our advantage, and the form of $\tilde{H}$ can be determined by requiring that the approximation scheme leads to physically sensible results in known limiting cases. In particular, in this case we replace $z_{i\sigma}$ in (3b) by another operator, $\tilde{z}_{i\sigma}$:

$$\tilde{z}_{i\sigma}=(1-d_i^\dagger d_i-p_{i\sigma}^\dagger p_{i\sigma})^{-1/2}z_{i\sigma}(1-e_i^\dagger e_i-p_{i-\sigma}^\dagger p_{i-\sigma})^{-1/2}, \tag{5}$$

which has the same eigenvalues and eigenvectors as z_i in the physical subspace but also leads to the correct $U=0$ limit in the saddle-point approximation.[11] The resulting saddle-point free-energy functional $f=-k_BT\ln Z/N$ can then be written as

$$f=Ud^2-k_BT\sum_\sigma\int_{-\infty}^{+\infty}d\xi\,\rho(\xi)\ln[1+e^{-\beta(q_\sigma\xi-\mu-\sigma h+\lambda_\sigma^{(2)})}]+\lambda^{(1)}\Big(\sum_\sigma p_\sigma^2+e^2+d^2-1\Big)-\sum_\sigma\lambda_\sigma^{(2)}(p_\sigma^2+d^2) \tag{6}$$

where $q_\sigma\equiv\langle\tilde{z}_{i\sigma}^\dagger\tilde{z}_{j\sigma}\rangle$, and T is the temperature.

As the simplest illustration of our approach we consider (6) in the paramagnetic phase of the half-filled-band Hubbard model (i.e., $n=1$, $\delta=0$). From general arguments as well as by a direct inspection of the saddle-point equations, $\mu=U/2$; also we set $h=0$, and we assume a symmetric density of states, $\rho(\xi)$. The Lagrange multipliers can then be easily eliminated to arrive at a (free energy) functional of d alone, $f=\bar{\epsilon}-Ts$. Here, $\bar{\epsilon}=2\int_{-\infty}^{+\infty}d\xi\,\rho(\xi)q\xi f(q\xi)+Ud^2$, and $q=8d^2(1-2d^2)$; s is the entropy per particle calculated for a lattice gas of free fermions with an effective hopping amplitude $\tilde{t}_{ij}=qt_{ij}$, and f is the Fermi function $f(\xi)=(e^{\beta\xi}+1)^{-1}$. At $T=0$, $\bar{\epsilon}$ is minimized by $d^2=1/4(1-U/U_c)$ with $U_c=16\int_0^\infty d\xi\,\rho(\xi)\xi$. Within our approximation this corresponds to the vanishing of the number of doubly occupied sites and indicates that the system is undergoing a metal-insulator transition at a finite critical value of U. The same result was derived by Brinkman and Rice[12] by using the variational wave function and the approximation scheme proposed by Gutzwiller.[4] The Gutzwiller approach to the half-filled Hubbard model has recently received a great deal of attention as a model for liquid ^{3}He close to the solidification curve.[13]

At sufficiently high temperatures we expect on physical grounds that the correlation effects become unimportant and q should approach unity. However, in the rigid-band picture the entropy favors $q=0$ and the system undergoes a first-order transition at a temperature of order W^2/U. We stress that none of the "slave boson" mean-field or Gutzwiller-type theories proposed to date[14] give a sensible crossover between low and high temperatures and we expect that new techniques treating fluctuations in fermion and boson degrees of freedom on an equal footing will be required in order to remedy this problem. Even so, it is likely that the behavior predicted from the finite-temperature saddle point to (4) is qualitatively correct at the lowest temperatures. In particular, it is appealing to interpret the initial decrease of q with temperature in terms of an increase of the coherent low-frequency fluctuations accompanying the hopping particle.

Our approach also provides a natural framework for studying magnetic properties of the Hubbard model. We have investigated the stability of the paramagnetic ground state with respect to both ferromagnetism and antiferromagnetism. At the ferromagnetic saddle point $p_\uparrow^2 - p_\downarrow^2 = m$ (m is the magnetization), while antiferromagnetism can be parametrized as usual by dividing the system into two sublattices, A and B, with the sublattice Bose fields satisfying the relations $e_A = e_B$, $d_A = d_B$, $p_{A\uparrow} = p_{B\downarrow}$, $p_{A\downarrow} = p_{B\uparrow}$, and $p_{A\uparrow}^2 - p_{A\downarrow}^2 = m_s$, the staggered magnetization. The ferromagnetic and antiferromagnetic phase boundaries (as determined by the vanishing of the inverse magnetic and staggered susceptibilities) are shown in Fig. 1.[15] It is intriguing that in this mean-field theory the possibility for ferromagnetism is restricted to very large values of U in contrast to the predictions of Stoner-type weak-coupling theories.[16] The tendency towards ferromagnetism for infinite U is in accordance with Nagaoka's theorem[10] which asserts that the ground state of a system with $d^2=0$ and $\delta = 1/N$ is ferromagnetic (N is the number of sites), while the disappearance of ferromagnetism at large U for $\delta \approx 0.38$ agrees qualitatively with the corresponding result of Kanamori.[17] Also, we stress that, as expected in lattices with perfect nesting, and in contrast with a previous calculation based on the Gutzwiller wave function due to Ogawa *et al.*,[18] the ground state of the half-filled Hubbard model is antiferromagnetic for an infinitesimal interaction U; for values of U up to $U \approx 40\,W$ the corresponding energy is lower than that given by Hartree-Fock theory.[16] The competition between ferromagnetism and antiferromagnetism, and the full phase diagram of the Hubbard model will be discussed elsewhere.[19]

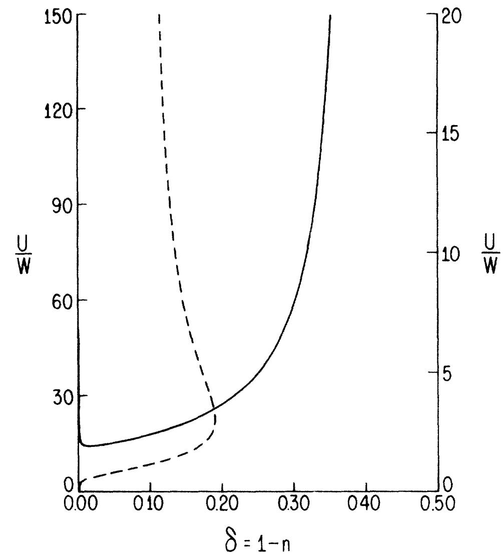

FIG. 1. The boundaries of stability of the paramagnetic phase of the Hubbard model with respect to ferromagnetism (solid line, left axis) and antiferromagnetism (dashed line, right axis) as determined from the vanishing of the inverse magnetic and staggered susceptibilities, respectively.

Finally, the approach outlined above can also be used to study the Anderson-lattice Hamiltonian[6,7,20] for all values of U. Here we make two comments about our results[19]: (i) In the paramagnetic phase and for infinite U ($d=0$) our calculation exactly agrees with that of Rice and Ueda,[20] who applied the Gutzwiller variational approach to the Anderson lattice. Their intriguing result that, for infinite U and in the Kondo regime, the spin-$\frac{1}{2}$ Anderson lattice has an instability with respect to ferromagnetism appears in our formulation as a consequence of the delocalization of "holes" in the f band, in analogy with the Nagaoka limit of the Hubbard model. (ii) We note that the boson introduced by Coleman[6] for the infinite-U case corresponds, strictly speaking, to the e_i ($e_i^\dagger$) of our treatment. It can then be easily seen that the resulting mean-field theories can only agree in the paramagnetic regime and in the limit of infinite spin degeneracy.

In this Letter we presented a new approach to strongly correlated Fermi systems, in the context of which we derive a new strong-coupling mean-field theory. While in the simplest physical situations the mean-field results are equivalent to those of the Gutzwiller variational approach, our formulation is systematic and is applicable with equal ease to both magnetic and nonmagnetic phases of these systems. In the case of the Anderson model this mean-field theory incorporates the competition between magnetism and the Kondo effect. This work can be extended in several directions: One can study the effect of Gaussian fluctuations about the saddle point, and one can apply this mean-field approach to richer physical situations (disorder, several bands, deformable lattice). Work in these directions is currently in progress.

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