Spin-rotation-invariant slave-boson approach to the Hubbard model

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We present a slave-boson representation for the Hubbard model, introducing Bose fields for the empty, singly, and doubly occupied sites and show that the boson for the singly occupied site must transform as a tensor of rank two under spin rotations. This generalizes the formulation of Kotliar and Ruckenstein, which is not manifestly spin-rotation invariant. The paramagnetic saddle point of the corresponding functional integral is identical to Gutzwiller's solution. As an illustration of the method, we calculate the $T^3 \ln T$ spin-fluctuation contribution to the specific heat and find it to be fully consistent with Fermi-liquid theory. We discuss further applications of this approach.

The Hubbard model[1,2] has been a focal point in attempts to understand the recently discovered high-T_c superconductors.[3,4] It is known to embody many of the ingredients that appear to be essential for high-T_c materials: a metal-insulator transition, antiferromagnetic order, and possibly superconductivity. However, in spite of long and intense efforts to obtain solutions to this model in the regime of interest, i.e., near half filling and in the limit of strong on-site repulsion U, relatively few controlled results are available. The strong correlations present in the system in this regime appear to require techniques which go beyond the conventional treatments of many-body systems.

As far as the ground-state properties of the model are concerned, a powerful and well-known technique is the variational method. Indeed, one of the more promising approximate solutions to the Hubbard model was given early on by Gutzwiller.[2] The so-called Gutzwiller solution is based on an ansatz for the many-body wave functions consisting of a Slater determinant for free electrons acted on by a projection operator, which reduces the weight of configurations in position space containing doubly occupied sites by an amount determined variationally. In order to calculate the expectation value of the Hamiltonian with the projected state, Gutzwiller used a quasiclassical approximation. As a result, he found an instability at half filling at a finite value of U, which was later interpreted by Brinkman and Rice[5] and by Vollhardt[6] as a metal insulator, or localization transition. It has been shown recently by Vollhardt and collaborators that the Gutzwiller approximation (GA) used in evaluating the Gutzwiller wave function (GW) becomes exact in the limit of infinitie spatial dimensions $d=\infty$.[7] In one dimension $d=1$, however, the exact evaluation[8] of the GW leads to qualitative changes, the most important one being the absence of an instability (or transition) at finite U. There are reasons to suspect that there is no transition at finite U for any finite dimension,[9] in an exact evaluation of the GW.

Even so, the Gutzwiller solution remains an attractive starting point for a more systematic theory. It was in this spirit that Kotliar and Ruckenstein (KR) (Ref. 10) devised a functional integral method, which had the Gutzwiller solution (GW and GA) as a saddle point. The hope would then be that corrections to the saddle-point solution should improve the GA as well as account for new correlation effects not included in the GW.

However, the functional integral formulation of KR suffers from a serious problem: It is not manifestly spin-rotation invariant (SRI). This problem is generated by embedding the physical Hilbert space of fermion states, which possesses the full spin-rotation invariance, in a much larger Hilbert space of auxiliary bosons, which does not possess this symmetry. Any approximation to the functional integral should therefore project onto the SRI subspace, which is of course difficult to guarantee. It is much simpler to symmetrize the boson Hilbert space from the beginning. Any reasonable approximation will then preserve the symmetry automatically. In the following we present a generalization of KR's theory and give a simple illustration of the importance of maintaining SRI. We outline possible further applications of the theory.

Our starting point is the Hubbard model for interacting electrons on a lattice

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

Here $f^{\dagger}_{i\sigma}$ ($f_{i\sigma}$) creates (annihilates) an electron with spin projection $\sigma(=\pm 1)$ in an atomic state at site i, $t_{ij}(=t_{ji})$ is the hopping matrix element and U is the interaction matrix element for two electrons of opposite spin at the same site.

There are four atomic states per site i, $|0i\rangle, |\uparrow i\rangle, |\downarrow i\rangle, |\uparrow\downarrow i\rangle$, corresponding to the empty site, the singly occupied site with electron spin polarization $\uparrow$ or $\downarrow$, and the doubly occupied site. In the spirit of Gutzwiller's solution KR introduced four auxiliary bose fields to label these four states, e_i, $p_{i\uparrow}$, $p_{i\downarrow}$, d_i (here e_i and d_i stand for empty and doubly occupied sites). The squares of the classical values of these fields are supposed to give the occupation probabilities of the four states. Following KR we define an enlarged Hilbert space of fermion and boson states. The physical states are obtained by creating electrons and auxiliary bosons on the vacuum

state $|\text{vac}\rangle$

$$|0i\rangle = e_i^+ |\text{vac}\rangle \ , \tag{2a}$$

$$|\sigma i\rangle = f_{i\sigma}^\dagger p_{i\sigma}^+ |\text{vac}\rangle \ , \tag{2b}$$

$$|\uparrow\downarrow i\rangle = d_i^+ f_{i\downarrow}^\dagger f_{i\uparrow}^\dagger |\text{vac}\rangle \ . \tag{2c}$$

Introduction of the Bose fields allows one to linearize the interaction and to eliminate the fermion degrees of freedom. The resulting system of interacting bosons may then be shown to have a mean-field solution identical to Gutzwiller's solution. In addition, theories of this kind are attractive because the slave bosons correspond in a natural way to local charge and spin fluctuations present in the strong-coupling limit.

However, introduction of the boson operators $p_\uparrow, p_\downarrow$ poses problems with regard to the spin-rotation symmetry of the system. In KR's formulation the spin-rotation invariance in boson space is broken by the assumption of a spin quantization axis. This must be expected to lead to qualitatively wrong results in any approximate treatment, such as a gap in the excitation spectrum for spin waves in the antiferromagnetic ground state. Also, the fluctuation contributions from transverse spin fluctuations are found to be missing in a recent calculation[11] of the free energy, which yielded a $T^3 \ln T$ finite-temperature correction term to the specific heat. While the prefactor of the spin-fluctuation-induced term agreed in its detailed dependence on Fermi-liquid parameters with the exact result,[12] it was found to be smaller by a factor of 3, the spin multiplicity factor for spin fluctuations.

In order to understand the source of the difficulty and at the same time to develop a cure for it, we consider the transformation properties of the states (2) under rotations in spin space. We must require that the states $|0i\rangle$ and $|\uparrow\downarrow i\rangle$ transform as scalars, whereas the states $|\sigma i\rangle$ transform as spinor states under spin rotation

$$|\sigma i\rangle \rightarrow \sum_{\sigma'} U_{\sigma'\sigma}^+ |\sigma' i\rangle \ , \tag{3}$$

where

$$\underline{U} = \exp \frac{i}{2} \boldsymbol{\theta} \cdot \boldsymbol{\underline{\tau}} \tag{4}$$

and $\boldsymbol{\underline{\tau}}$ is the vector of Pauli matrices. Likewise, the fermion-field operators $f_{i\sigma}$ transform as spinors

$$f_{i\sigma} \rightarrow \sum_{\sigma'} U_{\sigma\sigma'} f_{i\sigma'} \ . \tag{5}$$

It follows that the boson-field operators $p_{i\sigma}^+$ transform as

$$p_{i\sigma} \rightarrow U p_i U^+ \tag{6}$$

and p_i is necessarily a 2×2 spin matrix operator $p_{i\sigma\sigma'}^+$ rather than a two-component spinor operator. The two operators $p_{i\uparrow}^+, p_{i\downarrow}^+$ introduced originally by KR are the eigenvalues of $p_{i\sigma\sigma'}$, i.e., the only nonzero components in a coordinate system where $p_{i\sigma\sigma'}^+$ is diagonal. The SRI form of (2b) is then given by

$$|\sigma i\rangle = \sum_{\sigma'} p_{i\sigma\sigma'}^+ f_{i\sigma'}^\dagger |\text{vac}\rangle \ . \tag{7}$$

It is useful to represent $p_{i\sigma\sigma'}^+$ in terms of its projections onto the Pauli matrices $\underline{\tau}_1, \underline{\tau}_2, \underline{\tau}_3$ and the unit matrix $\underline{\tau}_0$

$$p_{i\mu}^+ = \frac{1}{\sqrt{2}} \text{tr}(\underline{\tau}_\mu \underline{p}_i^+) \ . \tag{8a}$$

whence

$$p_{i\mu}^+ = \frac{1}{\sqrt{2}} \text{tr}(\underline{\tau}_\mu \underline{p}_i^+) \ . \tag{8b}$$

As might be expected, the boson fields $p_{i\sigma\sigma'}^+$ form a spin singlet p_{i0}^+ and a spin triplet $\mathbf{p}_i^+ = (p_{i1}^+, p_{i2}^+, p_{i3}^+)$. The set of triplet components $\mathbf{p}_i^+$ transforms a vector under spin rotations, while p_{i0}^+ transforms as a scalar. This should be interpreted as follows. The physical states according to (2) are constructed as combined objects of bosons and fermions. The singly occupied states specifically are represented by two particles, a boson p and a spin-$\frac{1}{2}$ fermion f, coupled to the total spin $\frac{1}{2}$. It follows that the boson can either have spin $S=0$ (singlet component p_{i0}) or spin $S=1$ (triplet components $\mathbf{p}_i$). The spin-zero bosons p_{i0} then represent the charge degrees of freedom of the spinor states (one unit of charge per site), whereas the spin-one boson describes the spin degrees of freedom. Note however, that these fields do not automatically represent the electron charge and spin operators, because the density operators involve the square of the matrix $\underline{p}$.

As each of the Bose fields is introduced to represent one particular atomic state, and since there is only one state per site, the boson fields are locally constrained by the following condition ("slave bosons"):

$$Q_i \equiv e_i^+ e_i + \text{tr}(\underline{p}_i^+ \underline{p}_i) + d_i^+ d_i = 1 \ , \tag{9}$$

or else

$$e_i^+ e_i + p_{i0}^+ p_{i0} + \mathbf{p}_i^+ \cdot \mathbf{p}_i + d_i^+ d_i = 1 \ .$$

Also, the number of electrons must match the number of p bosons and d bosons, i.e.,

$$\text{tr}(\underline{\tau}_\mu \underline{p}_i^+ \underline{p}_i) + 2\delta_{\mu,0} d_i^+ d_i = \sum_{\sigma\sigma'} f_{i\sigma}^\dagger (\tau_\mu)_{\sigma\sigma'} f_{i\sigma} \ ,$$

$$\mu = 0,1,2,3 \ . \tag{10}$$

There are thus two additional constraints involving the transverse spin components compared to KR's formulation. The particle-density and spin-density components of (10) may be expressed in terms of the singlet and triplet components of $\underline{p}_i$ as

$$L_{i0} \equiv p_{i0}^+ p_{i0} + \mathbf{p}_i^+ \cdot \mathbf{p}_i + 2 d_i^+ d_i - \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 0 \tag{11}$$

and

$$\mathbf{L}_i \equiv p_{i0}^+ \mathbf{p}_i + \mathbf{p}_i^+ p_{i0} + i(\mathbf{p}_i^+ \times \mathbf{p}_i) - \sum_{\sigma\sigma'} f_{i\sigma}^\dagger \tau_{\sigma\sigma'} f_{i\sigma'} = 0 \ . \tag{12}$$

The boson operators e_i, d_i, $p_{i\mu}$ ($\mu = 0,1,2,3$) obey the usual Bose commutation relations,

$$[p_{i\mu},p_{i\nu}^{+}]=\delta_{ij}\delta_{\mu\nu}\ ,$$
$$[e_i,e_j^{+}]=\delta_{ij}\ , \tag{13}$$
$$[d_i,d_j^{+}]=\delta_{ij}\ ,$$

all other commutators being equal to zero.

Following KR, the Hubbard Hamiltonian may now be written in terms of the original electron operators and the slave-boson operators as

$$H_{\rm SB}=\sum_{\substack{ij\\ \sigma\sigma'\sigma_1}} t_{ij}(f_{i\sigma}^{+}z_{i\sigma\sigma_1}^{+})(z_{j\sigma_1\sigma'}f_{j\sigma'})+U\sum_i d_i^{+}d_i\ . \tag{14}$$

In the interaction term the product of electron density operators $n_{i\sigma}n_{i-\sigma}$ has been replaced by $d_i^{+}d_i$, the occupation number operator for doubly occupied sites. Following KR we introduce additional projection operators z_i in the hopping term, whose eigenvalues would be unity if the constraints were satisfied exactly. The form of z_i is chosen such as to guarantee the correct weak-coupling limit ($U\to 0$) in mean-field theory. The projectors z_i describe the hopping process of slave bosons that must accompany any hopping process of electrons, i.e., if an electron hops from site i to j, the slave bosons must simultaneously change at j and i. Depending on whether site i is singly or doubly occupied, the bosonic state of i must change from $p_{i\sigma}^{+}$ to e_i^{+}, or from d_i^{+} to $p_{i-\sigma}^{+}$. Thus there are two transition channels, which add up, and the total transition probability must be equal to one. It is therefore useful to introduce a normalization factor, which guarantees the conservation of probability even in mean-field theory. Thus, we are led to define the spin matrix operator

$$\underline{z}_i=[(1-d_i^{+}d_i)\underline{\tau}_0-\underline{p}_i^{+}\underline{p}_i]^{-1/2}(e_i^{+}\underline{p}_i+\underline{\tilde{p}}_i^{+}d_i)\times[(1-e_i^{+}e_i)\underline{\tau}_0-\underline{\tilde{p}}_i^{+}\underline{\tilde{p}}_i]^{-1/2} \tag{15}$$

The operator $(e_i^{+}\underline{p}_i+\underline{\tilde{p}}_i^{+}d_i)$ in the center of the product on the rhs of (15) describes the sum of the processes (singly occupied site) $\to$ (empty site) and (doubly occupied site) $\to$ (singly occupied site with time-reversed spin). The operator $\underline{\tilde{p}}_i$ is defined by

$$\underline{\tilde{p}}_i\equiv\hat{T}\underline{p}\hat{T}^{-1}=\frac{1}{\sqrt{2}}(p_{i0}\underline{\tau}_0-\mathbf{p}_i\cdot\underline{\tau})\ , \tag{16}$$

where $\hat{T}$ is the time-reversal operator. Even though the eigenvalues of z_i are 0 and 1 if the local constraints are satisfied, and the eigenvalues of the square-root factors are exactly unity in this case, in any approximate treatment these normalization factors will make a difference.

The constraints (9), (11), and (12) may be incorporated by adding Lagrange multiplier terms to the Hamiltonian (14)

$$H_T=H_{SB}-\sum_i\lambda_i^{(1)}(Q_i-1)+\sum_i(\lambda_{i0}^{(2)}L_{i0}+\boldsymbol{\lambda}_i^{(2)}\cdot\mathbf{L}_i)\ , \tag{17}$$

where the Lagrange mutiplier fields $\lambda_i^{(1)}$ and $\lambda_{i\mu}^{(2)}$, $\mu=0,1,2,3$ may be chosen to be Bose fields. Note that the charge operators Q_i and $L_{i\mu}$ commute with H_T such that the λ fields are time independent.

The partition function of the model (17) may now be calculated from a functional integral over coherent fermion states $f_{i\sigma}(\tau)$ and boson states $e_i(\tau)$, $d_i(\tau)$, $p_{i\mu}(\tau)$, $\lambda_i^{(1)}$, $\lambda_{i\mu}^{(2)}$,

$$Z=\int[De][Dp_\mu][Dd][D\lambda^{(1)}][D\lambda_\mu^{(2)}]\times\exp\left[-\int_0^\beta d\tau\mathcal{L}_{\rm eff}(\tau)\right]\ , \tag{18}$$

where

$$\mathcal{L}_{\rm eff}(\tau)=\sum_i\left[e_i^{+}(\partial_\tau+\lambda_i^{(1)})e_i+\sum_{\mu=0}^{3}p_{i\mu}^{+}(\partial_\tau+\lambda_i^{(1)}-\lambda_{i0}^{(2)})p_{i\mu}-\boldsymbol{\lambda}_i^{(2)}\cdot[p_{i0}^{+}\mathbf{p}_i+\mathbf{p}_i^{+}p_{i0}+i(\mathbf{p}^{+}\times\mathbf{p})]+d_i^{+}(\partial_\tau+\lambda_i^{(1)}-2\lambda_{i0}^{(2)}+U)d_i\right]+\mathcal{L}_{\rm eff}^{F}(\tau)\ . \tag{19}$$

The fermion part of the effective action is defined by

$$\exp\left[-\int_0^\beta d\tau\mathcal{L}_{\rm eff}^{F}(\tau)\right]=\int[Df]\exp\left[-\int_0^\beta d\tau\mathcal{L}^{F}(\tau)\right]\ ,$$

where

$$\mathcal{L}^{F}(\tau)=\sum_{i\sigma\sigma'}f_{i\sigma}^{+}[(\partial_\tau-\mu_0+\lambda_{i0}^{(2)})\delta_{\sigma\sigma'}+(\boldsymbol{\lambda}_i^{(2)}-\mathbf{h})\cdot\boldsymbol{\tau}_{\sigma\sigma'}]f_{i\sigma'}+\sum_{ij\sigma\sigma_1\sigma'}t_{ij}f_{i\sigma}^{+}z_{i\sigma\sigma_1}^{+}z_{j\sigma_1\sigma'}f_{j\sigma'}\ . \tag{20}$$

Integration over the fermion fields yields

$$\mathcal{L}_{\rm eff}^{F}(\tau)=\mathrm{tr}\ln\{\delta_{ij}[(\partial_\tau-\mu_0+\lambda_0^{(2)})\underline{1}+(\boldsymbol{\lambda}^{(2)}-\mathbf{h})\cdot\underline{\tau}]+t_{ij}\underline{z}_1^{+}\underline{z}_j\}\ , \tag{21}$$

where the trace has to be taken over position and spin variables. In (20) μ_0 is the chemical potential ahd $\mathbf{h}$ is an external magnetic field.

The expressions (18), (19), and (21) for the partition function are manifestly spin-rotation invariant, and should form a better starting point for the calculation of spin-dependent quantities than the original formulation of KR. The price

one has to pay is the introduction of 4 additional Bose fields, increasing the total number of Bose fields from 7 to 11.

Let us now consider a simple mean-field solution, obtained as the saddle point of the functional integral under the assumption of spatial homogeneity, i.e., for $e_i=e_i^+=e$; $d_i=d_i^+=d$; $p_{i\mu}=p_{i\mu}^+=p_\mu$, etc. The free energy per lattice site then follows as

$$F=Ud^2-k_BT\int d\varepsilon\,\rho(\varepsilon)\mathrm{tr}_\sigma\ln[\underline{1}+\exp(-\beta\underline{E})]+\lambda^{(1)}\left[e^2+\sum_\mu p_\mu^2+d^2-1\right]-\lambda_0^{(2)}\left[\sum_\mu p_\mu^2+2d^2\right]-2\lambda^{(2)}\cdot\mathbf{p}p_0\ , \tag{22}$$

where

$$\underline{E}=\underline{z}^+\underline{z}\varepsilon+(\lambda_0^{(2)}-\mu_0)\underline{1}+(\boldsymbol{\lambda}^{(2)}-\mathbf{h})\cdot\underline{\tau} \tag{23}$$

and $\rho(\varepsilon)$ is the density of states of the tight-binding band defined by t_{ij}.

The equilibrium values of the classical field amplitudes e, d, p_μ, etc. are those for which the free energy is minimum and consequently $\partial F/\partial e=0$, etc. In order to find these values one performs a unitary transformation which diagonalizes $\underline{p}$, such that $p_\mu=(p_0,0,0,p_3)$. Then, the only remaining dependence on $\lambda_\mu^{(2)}$, $\mu=1,2$, comes from inside the logarithm, such that

$$\frac{\partial F}{\partial\lambda_{1,2}^{(2)}}=\int d\varepsilon\,\rho(\varepsilon)\mathrm{tr}_\sigma[\underline{\tau}_{1,2}f(\underline{E})]\ , \tag{24}$$

where $f(E)$ is the Fermi function. The derivatives $\partial F/\partial\lambda_{1,2}^{(2)}$ are zero for diagonal spin matrix $\underline{E}$, i.e., for $\lambda_{1,2}^{(2)}=0$ and $\mathbf{h}=(0,0,h)$. A possible solution is then given by a diagonal matrix $\underline{p}$ with elements $p_\uparrow$ and $p_\downarrow$ in the frame where the magnetic field is parallel to the z axis, i.e.,

$$F=ud^2-k_BT\int d\varepsilon\,\rho(\varepsilon)\sum_\sigma\ln(1+\exp-\beta E_\sigma)\ , \tag{25}$$

with

$$E_\sigma=q_\sigma\varepsilon+\lambda_0^{(2)}-\mu_0+(\lambda_3^{(2)}-h)\sigma\ , \tag{26}$$

$$q_\sigma=\frac{e^2p_\sigma^2+d^2p_{-\sigma}^2+2e\,dp_\sigma p_{-\sigma}}{(1-d^2-p_\sigma^2)(1-e^2-p_{-\sigma}^2)} \tag{27}$$

and the constraints

$$e^2+p_\uparrow^2+p_\downarrow^2+d^2=1\ , \tag{28a}$$

$$p_\uparrow^2+p_\downarrow^2+2d^2=\int d\varepsilon\,\rho(\varepsilon)\sum_\sigma f(E_\sigma)\ , \tag{28b}$$

$$p_\uparrow^2-p_\downarrow^2=\int d\varepsilon\,\rho(\varepsilon)\sum_\sigma\sigma f(E_\sigma)\ . \tag{28c}$$

This is the result obtained by KR for a spin-polarized state with magnetization given by (28c), which agrees with the results obtained from the Gutzwiller solution,[6] if e^2, p_σ^2, and d^2 are identified as the probabilities for a lattice site to be empty, singly or doubly occupied, respectively.

We now proceed to calculate the effect of fluctuations about the mean-field solution for the half-filled band case in the paramagnetic state $p_\uparrow=p_\downarrow$. As a first step, following Rasul and Li,[11] we separate out the phase fluctuations. This is most easily done in the representation where the matrix operator $\underline{p}_i$ is diagonal. In a representation of the Bose fields by modulus and phase (radial gauge),

$$\begin{aligned}e_i&=x_ie^{i\theta_i}\ ,\\ d_i&=\eta_ie^{i\phi_i}\ ,\\ p_{i\sigma}&=q_{i\sigma}e^{i\chi_{i\sigma}}\ ,\end{aligned} \tag{29}$$

the phase factors may be gauged away and absorbed into the Fermi fields at the cost of adding time-dependent gauge terms to the previously time-independent Lagrange multiplier fields as

$$\begin{aligned}\alpha_i(\tau)&=\lambda_i^{(1)}+i\dot\theta_i(\tau)\ ,\\ \beta_{i\sigma}(\tau)&=\lambda_{i\sigma}^{(2)}+i\dot\theta_i(\tau)-i\dot\chi_{i\sigma}(\tau)\ .\end{aligned} \tag{30}$$

Note that the integration over the fields ϕ_i is removed by a gauge fixing term due to the local invariance with respect to simultaneous gauge transformations of e, d, and p_σ. In (30) the spin-dependent fields $\beta_{i\sigma}$ again have to be interpreted as the two eigenvalues of a 2×2 matrix field generated by rotations in spin space, $\beta_{i\alpha\beta}=(1/\sqrt{2})\sum_{\mu=0}^3\beta_{i\mu}(\tau_\mu)_{\alpha\beta}$. The effective action is then given by (18)–(21), with (i) $\lambda_i^{(1)}$, $\lambda_{i\mu}^{(2)}$ replaced by $\alpha_i(\tau)$ and $\beta_{i\mu}(\tau)$, respectively, (ii) the time derivative terms involving e_i, d_i, $p_{i\mu}$ deleted, and (iii) real valued fields e_i, d_i, $p_{i\mu}$.

We now expand the effective action thus defined in lowest order in the fluctuations about the (paramagnetic) mean-field solution. At $T=0$ such an expansion can be shown to converge[10] for an N-orbital generalization of the Hubbard model in the limit $N\to\infty$. On the other hand, the contribution of the thermal fluctuations at low temperatures $T\ll T_F$ is given simply by the leading order term since further terms are of higher order in T/T_F. Spin-rotation invariance requires that the fluctuations of the spin-singlet type $\delta x,\delta y,\delta q_0,\delta\alpha,\delta\beta_0$ and those of the spin-triplet type $\delta\mathbf{q},\delta\boldsymbol{\beta}$ are decoupled (one can not form a vector quantity in spin space out of the paramagnetic mean-field solution). Spin fluctuations as described by the spin-triplet contributions are dominant at low energy for strong repulsive interaction near half-filling. We therefore concentrate on their contribution here. From the corresponding part in the (Fourier-transformed) effective action

$$S_{\mathrm{sf}}=\sum_k\{(S_+-S_-)[\mathbf{q}(k)\cdot\mathbf{q}(-k)]+\chi^0(k)[\boldsymbol{\beta}(k)\cdot\boldsymbol{\beta}(-k)]+q[\mathbf{q}(k)\cdot\boldsymbol{\beta}(-k)]\}\ , \tag{31}$$

where

$$\begin{aligned}S_+-S_-&=-\tfrac{1}{4}U(1-u)(2+u)\ ,\\ \chi^0(k)&=\sum_p G(p+k)G(p)\ ,\end{aligned}$$

with $G(p)\equiv G(\mathbf{p},\omega)=(\omega-E_p)^{-1}$, one finds a contribution to the free energy

$$F_{\rm sf}=kT\sum_k \ln[q^2+(S_+-S_-)\chi^0(k)]^3 \ . \tag{32}$$

In the long-wavelength approximation, evaluation of (32) yields a specific-heat contribution at low temperatures

$$C_v=\delta_{\rm SF}T^3\ln(T/T_0) \ , \tag{33}$$

with

$$\delta_{\rm SF}=(9\pi^4/40)(n/T_F^3)(A_0^a)^2[1-(\pi^2/12)A_0^a] \ ,$$

where $A_0^a=F_0^a/(1+F_0^a)$ and $F_0^a=-au(2+u)/(1+u)^2$. Here A_0^a and F_0^a are the spin-antisymmetric isotropic components of the quasiparticle scattering amplitude and the Fermi-liquid interaction, respectively, and the expression for F_0^a is the Gutzwiller result[6] [$u=U/U_c$, where U_c is the critical value of U and $a=\rho(0)\int d\varepsilon|\varepsilon|\rho(\varepsilon)\simeq 1$]. The result (33) agrees with the one derived within Fermi-liquid theory itself[12] and, in the weak-coupling limit, with the result of paramagnon theory.[13] We note that the above calculation can be extended to include high momentum processes ($k\simeq 2k_F$) not accessible in Fermi-liquid theory. In particular, we recover the spin multiplicity factor of 3 missing in the work of Rasul and Li.[11]

In summary, we have discussed a slave-boson representation of the Hubbard model, which has a paramagnetic saddle point identical with the Gutzwiller solution. In contrast to an earlier formulation by Kotliar and Ruckenstein[10] our theory is manifestly spin-rotation invariant. We have calculated the contribution of thermal fluctuations in the spin-type variables to the free energy in one-loop order and found a $T^3\ln T$ term in the specific heat. The prefactor of this term agrees with the result obtained from a finite temperature extension of Fermi-liquid theory in the sense that the phenomenlogical Landau parameters there are now expressed in terms of the microscopic interaction parameter U. This implies that the Fermi-liquid behavior at finite frequencies and wave numbers for a strongly interacting system has been derived here on a microscopic basis.

From the preceding discussion it should be clear that the present theory will give results different from KR (a) in the mean-field theory whenever the spin quantization axis is spatially nonuniform, (b) in any approximate calculation of the spin dynamics, and (c) whenever fluctuations are included. This gives rise to a number of interesting applications of the SRI formalism. For example, a proper treatment of spin-rotated singly occupied states is clearly necessary to study incommensurate spiral states thought to play a role in the destruction of Néel order with doping in the strong-coupling regime,[14] or general antiferromagnetic order in nonbipartite lattices. Furthermore, approximate calculations of spin dynamics, especially in the antiferromagnetic state, depend sensitively on the preservation of spin-rotation invariance. It should be interesting to calculate the spin-wave spectrum, as well as the incoherent excitation part, as a function of U and filling. Finally, one expects quantum fluctuations to strongly modify the mean-field ground state, rendering a straightforward expansion in fluctuations impossible for the spin-$\frac{1}{2}$ case. It is possible that a self-consistent one-loop theory of interacting fluctuations may provide a controlled approach to the problem. Interacting fluctuations should also be important at higher temperatures, where the mean-field theory is known to give unphysical results.[10] Work along these lines is in progress.

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