Effective Action for Strongly Correlated Fermions from Functional Integrals

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The Hubbard model is investigated using functional integrals and a Hubbard-Stratonovich decomposition of the interaction term. Using a spin-space reference frame that fluctuates in time and space, the effective action both is spin-rotation invariant and exhibits the correct Hartree-Fock saddle point. For strong correlation the effective action for free carriers and spins coupled via a gauge field is obtained as a systematic expansion in t/U. The spiral state existing for small doping is discussed. The formalism allows straightforward generalization to intermediate and weak coupling.

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It hardly needs to be emphasized anymore that a theoretical understanding of strongly correlated fermion systems is of crucial importance for the interpretation of the physical properties of high-temperature superconducting materials.[1] Strong electron-electron correlations also play an important role in heavy-fermion systems, itinerant ferromagnets, and a large variety of other systems. The theoretical description of correlated fermion systems is frequently based on the Hubbard model and its generalizations. A standard method to treat interacting many-body Hamiltonians is a Hubbard-Stratonovich decomposition of the interaction combined with some approximate treatment of the resulting functional integral. For the Hubbard model, however, this kind of approach has not been very successful, in large part due to the apparent impossibility to take into account properly spin-rotation invariance,[2] as briefly discussed below.

In the present paper I will show that the difficulties with the functional-integral formulation can be overcome using a spin-space reference frame that varies in time and space. The fluctuations of the orientation of the reference frame then allow for a rather natural inclusion of spin-rotation invariance. As will be seen below, in the strong correlation limit it then becomes possible to derive microscopically the effective action for carriers doped into a Mott-type insulator. Mainly based on phenomenological and symmetry arguments, effective actions have been proposed previously,[3-7] and the present approach then establishes the connection between these and microscopic models.

To be concrete, in the following I will consider the Hubbard model, but generalization to other models should be rather straightforward. The partition function can be represented as a functional integral over Grassmann variables,

$$Z=\int \mathcal{D}\Psi^{\dagger}(\tau)\mathcal{D}\Psi(\tau)\exp(-S)\,, \tag{1}$$

where Ψ is a Grassmann spinor defined at all lattice sites at imaginary time τ: $\Psi_{\mathbf{r}}=(\psi_{\mathbf{r}\uparrow},\psi_{\mathbf{r}\downarrow})^{T}$. The action is

$$S=\int_0^{\beta} d\tau\left[\sum_{\mathbf{r}}\Psi_{\mathbf{r}}^{\dagger}(\tau)(\partial_{\tau}-\mu)\Psi_{\mathbf{r}}(\tau)+H(\Psi^{\dagger},\Psi)\right] \tag{2}$$

($\beta=1/T$), with the Hamiltonian given by

$$H(\Psi^{\dagger},\Psi)=-t\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}(\Psi_{\mathbf{r}}^{\dagger}\Psi_{\mathbf{r}'}+\Psi_{\mathbf{r}'}^{\dagger}\Psi_{\mathbf{r}})+\frac{U}{4}\sum_{\mathbf{r}}(n_{\mathbf{r}}^{2}-s_{z\mathbf{r}}^{2})\,. \tag{3}$$

Most of what follows is independent of spatial dimension, but to be specific I consider the two-dimensional case: $\langle\mathbf{r}\mathbf{r}'\rangle$ indicates summation over nearest-neighbor bonds on a square lattice, each bond being counted once, and $n_{\mathbf{r}}=\Psi_{\mathbf{r}}^{\dagger}\Psi_{\mathbf{r}}$ and $s_{z\mathbf{r}}=\Psi_{\mathbf{r}}^{\dagger}\sigma_{z}\Psi_{\mathbf{r}}$ are the local particle and spin (along z) densities, respectively.

A standard way to handle the interaction term in Eq. (3) is the Hubbard-Stratonovich transformation, introduced at each point in space and time:

$$\exp\left[-\frac{U}{4}(n_{\mathbf{r}}^{2}-s_{z\mathbf{r}}^{2})\right]=\frac{1}{\pi U}\int d\Delta_{c}\,d\Delta_{s}\exp\left[-\frac{1}{U}(\Delta_{c}^{2}+\Delta_{s}^{2})+i\Delta_{c}n_{\mathbf{r}}+\Delta_{s}s_{z\mathbf{r}}\right]. \tag{4}$$

Formally, it is then possible to integrate out the fermions and to obtain an effective action for the fields Δ_s,Δ_c. In the saddle-point approximation one recovers the Hartree-Fock approximation. However, the fluctuations of Δ_s,Δ_c around the saddle points are massive; i.e., the low-frequency spin-wave modes which are crucial for the physics of the model are not easily recovered. Alternatively, one might write the interaction as $(U/6)\mathbf{s}_{\mathbf{r}}^{2}$ ($\mathbf{s}_{\mathbf{r}}$ is the local spin-density *vector),* and then use a decomposition with a *vector* field $\boldsymbol{\Delta}$. The angular fluctuations of $\boldsymbol{\Delta}$ then certainly are massless; however, due to the factor $U/6$ the saddle point does not even reproduce the Hartree-Fock results, certainly a very unsatisfactory situation.

As will be seen, a theory that in the saddle-point approximation reproduces Hartree-Fock *and* explicitly exhibits the correct low-energy excitations can be constructed using a spin reference frame that varies in space and time. For this purpose I introduce identities $1=R_{\mathbf{r}}R_{\mathbf{r}}^{\dagger}$ into (2), where $R_{\mathbf{r}}$ is a SU(2) matrix,

parametrized by a unit vector $\mathbf{\Omega}$ which varies in time and space: $R_r\sigma_z R_r^\dagger = \mathbf{\Omega}_r(\tau)\cdot\sigma$ [more precisely $R_r \in \mathrm{SU}(2)/\mathrm{U}(1) = S^2$]. Then

$$S = \int_0^\beta d\tau \left[\sum_r \Psi_r^\dagger R_r R_r^\dagger (\partial_\tau - \mu) R_r R_r^\dagger \Psi_r + H(\Psi^\dagger, \Psi) \right]. \tag{5}$$

Now, introducing at each point in space and time an integration over $\mathbf{\Omega}_r(\tau)$ with invariant integration measure normalized to unity, and performing the unitary transformation $\Phi_r = R_r^\dagger \Psi_r$, the action becomes

$$S(\Phi^\dagger, \Phi, \mathbf{\Omega}) = \int_0^\beta d\tau \left\{ \sum_r \Phi_r^\dagger (\partial_\tau - \mu + R_r^\dagger \dot{R}_r) \Phi_r + H(\Phi^\dagger, \Phi, \mathbf{\Omega}) \right\}, \tag{6}$$

$$H(\Phi^\dagger, \Phi, \mathbf{\Omega}) = -t \sum_{\langle rr' \rangle} \left(\Phi_r^\dagger R_r^\dagger R_{r'} \Phi_{r'} + \text{c.c.} \right) + \frac{U}{4} \sum_r [(\Phi_r^\dagger \Phi_r)^2 - (\Phi_r^\dagger \sigma_z \Phi_r)^2]. \tag{7}$$

Because of spin-rotation invariance $\psi_{r\uparrow}^* \psi_{r\downarrow}^* \psi_{r\downarrow} \psi_{r\uparrow} = \phi_{r\uparrow}^* \phi_{r\downarrow}^* \phi_{r\downarrow} \phi_{r\uparrow}$, and therefore the spin-rotation matrices do not appear in the interaction term in (7). Note that an $\uparrow$ spin in the Φ variables points along $\mathbf{\Omega}$ in the original (laboratory) reference frame; i.e., in going from the Ψ's to the Φ's there is a change from a fixed reference frame in spin space to a reference frame (or quantization axis) varying in space and time.

I now apply the scalar Hubbard-Stratonovich decomposition (4) to the Hamiltonian (7). In the saddle-point approximation, this reduces to the Hartree-Fock results. On the other hand, the angular variables $\mathbf{\Omega}$ explicitly appear in the functional integral, and consequently the fluctuation spectrum around the saddle point does contain the low-energy spin-wave modes.

As will be briefly discussed below, the fluctuating-reference-frame approach can be used for arbitrary U, e.g., to obtain the effective nonlinear σ model for the antiferromagnetic state at half filling. Here I will concentrate on the strongly correlated case. Then arbitrary variations of $\mathbf{\Omega}_r(\tau)$ around the saddle point can be taken into account. For reasons of simplicity it is convenient to choose the ferromagnetic saddle point $\Delta_{s0} = i\Delta_{c0} = -U/2$. One can then decompose the total action as $S = S_0 + S_\Omega + S_\delta$, where S_0 is the action at the saddle point, S_Ω contains the contributions from the fluctuations of $\mathbf{\Omega}$, and S_δ describes the fluctuations of $\Delta_{s,c}$ ($\delta_{s,c} = \Delta_{s,c} - \Delta_{s,c0}$):

$$\begin{aligned} S_0 &= \int_0^\beta d\tau \left[\sum_r \Phi_r^\dagger [\partial_\tau - \mu + \tfrac{1}{2} U(1+\sigma_z)] \Phi_r - t \sum_{\langle rr' \rangle} (\Phi_r^\dagger \Phi_{r'} + \Phi_{r'}^\dagger \Phi_r) \right], \\ S_\Omega &= \int_0^\beta d\tau \left[\sum_r \Phi_r^\dagger R_r^\dagger \dot{R}_r \Phi_r - t \sum_{\langle rr' \rangle} \{ \Phi_r^\dagger (R_r^\dagger R_{r'} - 1) \Phi_{r'} + \text{c.c.} \} \right], \\ S_\delta &= \int_0^\beta d\tau \sum_r [-i\delta_{cr}(n_r - 1) - \delta_{sr}(s_r + 1) + U^{-1}(\delta_{cr}^2 + \delta_{cr}^2)]. \end{aligned} \tag{8}$$

I consider the case of more than one electron per site, so that S_0 represents a completely filled band of $\downarrow$ electrons ("lower Hubbard band") and a partially filled band of $\uparrow$ electrons ("upper Hubbard band"), but by electron-hole symmetry, the case of less than one electron can be treated completely analogously.

I now want to derive the effective action for the physical degrees of freedom: fermions in the upper Hubbard band, and spins represented by $\mathbf{\Omega}$. This can be achieved by doing the trace over $\phi_\downarrow$ and $\delta_{s,c}$ explicitly. The effective action then is obtained as a cumulant expansion in diagrams connected by $s_z = \downarrow$ (lower Hubbard band) Green's functions. This function is

$$G_{0\downarrow}(\mathbf{r}, \tau) = -\theta(-\tau) e^{U\tau} \delta(\mathbf{r}) \approx -\delta(\tau^-)\delta(\mathbf{r})/U.$$

Consequently, to obtain the effective action to order $(t/U)^n$, the cumulant expansion has to be carried to order $n+1$. To zeroth order in t/U I find

$$S_{\text{eff}}^0 = \int_0^\beta d\tau \left\{ \sum_r [\phi_r^* (\partial_\tau - \mu + U) \phi_r - \tfrac{1}{2} i\varphi_r (1 - \cos\vartheta_r)(1 - \phi_r^* \phi_r)] - t \sum_{\langle rr' \rangle} [\alpha(\mathbf{\Omega}_r, \mathbf{\Omega}_{r'}) \phi_r^* \phi_{r'} + \text{c.c.}] \right\}, \tag{9}$$

$$\alpha(\mathbf{\Omega}_r, \mathbf{\Omega}_{r'}) = |\alpha| e^{i\chi_{rr'}} = [(1 + \mathbf{\Omega}_r \cdot \mathbf{\Omega}_{r'})/2]^{1/2} \exp[i\hat{A}(\mathbf{\Omega}_r, \mathbf{\Omega}_{r'}, \hat{\mathbf{z}})/2]. \tag{10}$$

Here ϕ refers to fermions in the upper Hubbard band, the spin index being omitted, φ_r, ϑ_r are the polar angles of $\mathbf{\Omega}_r$, $\hat{A}(\mathbf{\Omega}_1, \mathbf{\Omega}_2, \mathbf{\Omega}_3)$ is the signed solid angle spanned by the vectors $\mathbf{\Omega}_1, \mathbf{\Omega}_2, \mathbf{\Omega}_3$,[8] and $\hat{\mathbf{z}}$ is the unit vector along z.

In the absence of particles in the upper Hubbard band, in S_{eff}^0 only the purely imaginary term remains, which is the Berry phase of an isolated spin $\frac{1}{2}$; i.e., as expected, the half-filled Hubbard model becomes a collection of independent spins for $U = \infty$. Introducing more fermions, two effects occur. (i) The factors $1 - \phi_r^* \phi_r$, previously introduced by

Shankar from semiphenomenological arguments,[4] cancel the Berry-phase term whenever there is an extra particle on site $\mathbf{r}$; i.e., one is in a spin singlet whenever two particles occupy the same site. Here this effect is seen directly from a microscopic calculation. (ii) The kinetic-energy term plays a role: In particular, going around an elementary plaquette (1234) the lattice curl of the phases $\chi_{\mathbf{r}\mathbf{r}'}$ equals

$$\Phi_{1234}=[\hat{A}(\mathbf{\Omega}_1,\mathbf{\Omega}_2,\mathbf{\Omega}_3)+\hat{A}(\mathbf{\Omega}_3,\mathbf{\Omega}_4,\mathbf{\Omega}_1)]/2\,,$$

i.e., there is an effective magnetic field proportional to the solid angle spanned by $\mathbf{\Omega}_1,\ldots,\mathbf{\Omega}_4$. Φ_{1234} is the lattice analog of the familiar winding-number density of the continuum nonlinear σ model.[8] Note that, while the gauge potential in (10) depends explicitly on $\hat{\mathbf{z}}$ and therefore is not rotational invariant, the physical fluxes are. For coplanar configurations, $\Phi_{1234}=0$; i.e., the phases can be removed by a gauge transformation of the ϕ's. One then sees straightforwardly that the kinetic term is optimized by a ferromagnetic arrangement of the spins. This is the familiar Nagaoka phenomenon.[9] Whether noncoplanar configurations of $\mathbf{\Omega}_\mathbf{r}$ with a nonzero winding-number density can lead to an energy lower than the Nagaoka state is not currently clear.[10]

The first-order contribution to the action is

$$S^1_{\rm eff}=\frac{t^2}{U}\int_0^\beta d\tau\left\{\frac{1}{2}\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}(2-\phi^*_\mathbf{r}\phi_\mathbf{r}-\phi^*_{\mathbf{r}'}\phi_{\mathbf{r}'})(\mathbf{\Omega}_\mathbf{r}\cdot\mathbf{\Omega}_{\mathbf{r}'}-1)\right.$$
$$\left.+\sum_{\langle\mathbf{r}\mathbf{r}'\mathbf{r}''\rangle}[\alpha(\mathbf{\Omega}_\mathbf{r},-\mathbf{\Omega}_{\mathbf{r}'})\alpha(-\mathbf{\Omega}_{\mathbf{r}'},\mathbf{\Omega}_{\mathbf{r}''})\phi^*_\mathbf{r}\phi_{\mathbf{r}''}+\text{c.c.}]+\frac{1}{4t^2}\sum_\mathbf{r}(1-\phi^*_\mathbf{r}\phi_\mathbf{r})\dot{\mathbf{\Omega}}^2_\mathbf{r}\right\}. \tag{11}$$

Here $\mathbf{r}$ and $\mathbf{r}''$ are second- or third-nearest neighbors, and the sum over $\mathbf{r}'$ is over all sites that are nearest neighbors of both $\mathbf{r}$ and $\mathbf{r}''$.

In the absence of fermions in the upper Hubbard band, only the ϕ-independent part of the first term in $S^1_{\rm eff}$ contributes and represents the antiferromagnetic exchange interaction between nearest-neighbor sites; e.g., in this case $S^0_{\rm eff}+S^1_{\rm eff}$ is the action of the antiferromagnetic Heisenberg model. This model has long-range antiferromagnetic order at zero temperature. Neglecting quantum fluctuations completely, one then has $\mathbf{\Omega}_\mathbf{r}\cdot\mathbf{\Omega}_{\mathbf{r}'}=-1$, and consequently one finds for the energy of one extra electron $\varepsilon_\mathbf{k}=(4t^2/U)(\cos k_x+\cos k_y)^2$. This expression has a degenerate minimum along $|k_y|=\pi-|k_x|$, as is well known from Hartree-Fock theory. One should, however, notice that the inclusion of zero-point spin fluctuations will immediately lift this degeneracy: The kinetic term in $S^1_{\rm eff}$ contains contributions like $(\mathbf{\Omega}_\mathbf{r}\cdot\mathbf{\Omega}_{\mathbf{r}'})(\mathbf{\Omega}_{\mathbf{r}'}\cdot\mathbf{\Omega}_{\mathbf{r}''})$, and these averages will be different according to whether $\mathbf{r}$, $\mathbf{r}'$, and $\mathbf{r}''$ lie along a straight line or not. This then may explain the minimum of $\varepsilon_\mathbf{k}$ at $(\pi/2,\pi/2)$ found in numerical calculations.

In the presence of a finite concentration n of extra electrons, one immediately sees the instability of the Néel state: In the Néel state the term proportional to t in $S^0_{\rm eff}$ does not contribute. If, however, $\mathbf{\Omega}_\mathbf{r}\cdot\mathbf{\Omega}_{\mathbf{r}'}=-1+\varepsilon^2$, there is an effective nearest-neighbor hopping of order $t|\varepsilon|$, and a corresponding gain of kinetic energy of order $-t|\varepsilon|n$. The loss of exchange energy is of order ε^2; e.g., $\varepsilon\neq0$ is energetically favored for any nonzero n. For an $\mathbf{r}$-independent ε one then finds a spiral, as proposed by Shraiman and Siggia.[3] Neglecting the quantum fluctuations of $\mathbf{\Omega}_\mathbf{r}$ completely (i.e., in the Hartree-Fock approximation) the magnetic structure can be determined by numerical minimization of the total energy. With the spin lying in the x-y plane I find the optimal structure to be characterized by the azimuthal angle $\varphi_\mathbf{r}=\pi(1-\delta)(x+y)$, with δ varying continuously as a function of n and t/U (Fig. 1). As can be seen from Fig. 1, at fixed t/U there is a *continuous* transition from the antiferromagnetic ($\delta=0$) to the ferromagnetic ($\delta=1$) state, via an intermediate spiral phase. As expected, this "unwinding" of the antiferromagnet into the ferromagnet occurs more rapidly for strong correlation. A number of comments are however in place: (i) In the present theory the minimum of the single-particle dispersion in the antiferromagnetic state is along the *lines* $|k_y|=\pi-|k_x|$, not at isolated points. Consequently, the direction of the spiral pitch is along the lattice diagonal, not along a lattice direction as found in Ref. 3. The direction found here is in agreement with a Schwinger-boson mean-field calculation.[11] (ii) Over the whole spiral region in Fig. 1 one has $\partial^2E_0/\partial n^2<0$; i.e., the calculation really shows phase separation into ferromagnetic and antiferromagnetic domains, in agreement with

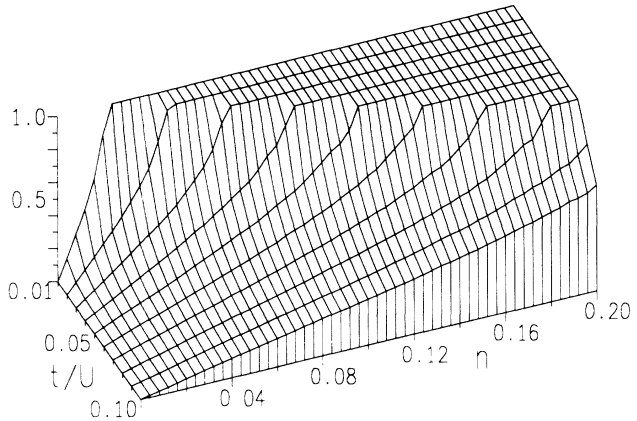

FIG. 1. Variation of the spiral pitch parameter δ with band filling n and strength of the correlations. $\delta=0$ is the antiferromagnet, and $\delta=1$ is the ferromagnet.

other theories.[12] This instability will, however, be suppressed if one includes long-range Coulomb interactions. (iii) The energy gain *per particle* due to the formation of the spiral is of order tn, much smaller than the energy gain due to domain-wall formation, which is of order t.[13] One should, however, notice that the carriers in the spiral state are free to move and can gain additional kinetic energy of order t by distorting their local spin environment, whereas in the domain-wall case the carriers are bound to the domain walls. It is therefore plausible that for strong correlation the spiral state is stable compared to domain walls.

Also note that the factors $1-\phi_{\mathbf{r}}^{*}\phi_{\mathbf{r}}$ in Eqs. (9) and (11) increase the coupling constant in the effective nonlinear σ model and therefore bring the Néel state closer towards its instability against quantum fluctuations.[14] It would be interesting to obtain a theory for the analogous "quantum melting" of the spiral phase, which possibly will lead to a Fermi-liquid-like state.

The spiral instability of the Néel state is due to the coupling between fermions and spins in S_{eff}^{0}. As pointed out in Ref. 3, for a nearly antiferromagnetic structure ($\mathbf{\Omega}_{\mathbf{r}}\cdot\mathbf{\Omega}_{\mathbf{r}'}\approx -1$) this interaction couples fermion and spin currents. The U(1) gauge field appearing in S_{eff}^{0} is identical to the one considered previously by Baskaran and Anderson.[15] In S_{eff}^{1} another term appears, coupling fermion motion to the winding number of the *antiferromagnetic* order parameter $(-1)^{\mathbf{r}}\mathbf{\Omega}_{\mathbf{r}}$. The continuum version of this term has been investigated by Shankar[4] and by Lee.[6] In the present case, the coupling constant is t^{2}/U, much smaller than the coupling in S_{eff}^{0}, which is of order t. It thus seems likely that the spin-fermion coupling in S_{eff}^{0} is predominant in the Hubbard model. The situation is quite different in the model considered by Shankar and by Lee: There is no nearest-neighbor hopping, and consequently the coupling between fermions and antiferromagnetic winding number dominates.

In conclusion, I have shown here that starting from a Hartree-Fock saddle point and using a Hubbard-Stratonovich decomposition in a fluctuating spin-space reference frame, the effective action for carriers in a quantum antiferromagnet can be obtained via a systematic procedure. In fact, generalizing the functional integration over $\mathbf{\Omega}_{\mathbf{r}}$ to the full SU(2) manifold, the effective action is closely related to the Schwinger-boson formulation of the problem. One should, however, notice that the present approach can be straightforwardly extended to intermediate and weak coupling: In the vicinity of half filling one can expand around the antiferromagnetic saddle point. The t/U expansion then becomes impractical; however, a long-wavelength expansion is possible for arbitrary U, and one finds terms of the same structure as in (9) and (11), with an additional coupling to a scalar field representing the amplitude of the spin modulation. Further away from half filling one can expand around the paramagnetic solution, and one obtains an explicit description of amplitude and orientational fluctuations of the local spin density. The present formulation thus provides a convenient starting point for a discussion of the similarities and differences between weak and strong correlation.

The present approach allows an interesting generalization: Using the matrix representation[16]

$$\Psi_{\mathbf{r}}=\begin{pmatrix}\psi_{\mathbf{r}\uparrow} & \psi_{\mathbf{r}\downarrow}\\ (-1)^{\mathbf{r}}\psi_{\mathbf{r}\downarrow}^{*} & -(-1)^{\mathbf{r}}\psi_{\mathbf{r}\uparrow}^{*}\end{pmatrix}, \tag{12}$$

the Hamiltonian can be written in a SU(2) × SU(2)-invariant way: Multiplying $\Psi_{\mathbf{r}}$ by a SU(2) matrix from the right, one generates the spin rotations discussed above, but multiplication from the left generates electron-hole transformations [in the Heisenberg model this becomes a SU(2) gauge symmetry[16]]. The above formalism then can be rather straightforwardly generalized to include variable reference frames in both SU(2) spaces. In the large-U limit, that formulation becomes equivalent to a slave-boson description.[17] It thus seems possible to relate slave-boson mean-field theories to approximate functional-integral theories of, e.g., the Hubbard model. Given that functional-integral methods are applicable for arbitrary interaction strength, this may prove helpful in understanding similarities and differences between weakly and strongly correlated systems.

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