Functional Integrals for Correlated Fermions

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Functional integral methods provide a way to define mean-field theories and to systematically improve them. For the Hubbard model and similar strong-correlation problems, methods based in particular on the Hubbard–Stratonovich transformation have however been plagued by difficulties to formulate the problem in a spin-rotation invariant way. Here a formalism circumventing this problem by using a space- and time-dependent spin reference axis is discussed. This formulation is then used to suggest a possible alternative to Nagaoka ferromagnetism in the strongly correlated Hubbard model in the vicinity of half-filling. Finally, some aspects of single-particle spectra in a simplified model for a short-range ordered antiferromagnet are discussed.

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1. INTRODUCTION

It has been pointed out soon after the discovery of high-temperature superconductivity in the cuprates that electron-electron correlations are likely to play the crucial role in determining the physics of these compounds. This observation is based on the fact that compounds with a nominally half-filled band like La$_2$CuO$_4$ are antiferromagnetic insulators rather than metals (as would be expected from band theory). This of course is explained by the well-known Mott–Hubbard effect, implying important correlation effects. Rather small amounts of doping away from half-filling than lead to an unusual metallic state which becomes superconducting at high temperatures.

As pointed out by Anderson, the (strongly correlated) Hubbard model can be expected to reproduce many of the essential features: at half-filling the model can be mapped onto the antiferromagnetic Heisenberg model and therefore gives rise to the antiferromagnetic insulating state, and it is equally clear that doping will eventually lead to a conducting state. How exactly this happens is however not clear at present: for weak correlation doping initially gives rise to an incommensurate antiferromagnetic (or spin density wave) insulator, and only upon further doping is a conducting state reached. For stronger correlation, the situation may well be different. In particular, the spiral state proposed by Shraiman and Siggia is conducting already at the smallest doping level, even though long-range magnetic
H.J. Schulz

order may persist. Moreover, neither the anomalous properties of the normal state in the conducting regime nor the origin of superconductivity are currently well-understood in the framework of the Hubbard model or of its possible generalizations.

Whatever the critical value of doping $\delta_c$ at which magnetic order disappears, one can expect that for $\delta \gtrsim \delta_c$ short-range antiferromagnetic order with a more or less important correlation length $\xi$ still exists. It is then important to understand the electronic properties in this regime, in particular in view of understanding the unusual properties of the metallic state of the cuprates. Moreover, the ordered state at half-filling can be understood in quite some detail (even for strong correlation) from Hartree–Fock theory supplemented by spin–wave corrections. At least for large (but finite) $\xi$ it therefore seems reasonable to start from a description of the ordered state and then, in a second step, to add the effects of the fact that the order is only short ranged. Ideally, this might even help to understand the situation of very short $\xi$. In fact for large $U$ (and hole doping) a site is either empty and thus non-magnetic or singly occupied and thus represents, on some short time scale, a magnetic moment. The physics of strong correlation thus is closely related to that of more or less short ranged magnetic order. In fact, the dynamics of the strongly correlated fermions can be seen as that of fermions moving in a space– and time–dependent spin “background” which however is generated by the fermions themselves and therefore has to be determined self-consistently.

In the following section a generalization of the standard Hubbard–Stratonovich functional integral formalism will be described that explicitly exhibits the local spin dynamics and therefore can be expected to make a formally satisfying treatment of the situation discussed above possible. Some simple applications will then be discussed in the subsequent sections.

2. FORMALISM

The standard Hubbard Hamiltonian has the form

$$H = -t \sum_{\langle \mathbf{r} \mathbf{r}' \rangle} (a_{\mathbf{r} \sigma}^\dagger a_{\mathbf{r}' \sigma} + h.c.) + U \sum_{\mathbf{r}} n_{\mathbf{r} \uparrow} n_{\mathbf{r} \downarrow},$$

where $a_{\mathbf{r} \sigma}^\dagger$ creates a fermion at site $\mathbf{r}$ with spin projection $\sigma$, $t$ is the nearest-neighbor hopping integral, $U$ is the onsite interaction, and $\langle \mathbf{r} \mathbf{r}' \rangle$ indicates summation over nearest-neighbor bonds, each bond being counted once. Introducing a spinor notation via

$$\Psi_{\mathbf{r}} = \begin{pmatrix} \psi_{\mathbf{r} \uparrow} \\ \psi_{\mathbf{r} \downarrow} \end{pmatrix}$$

the partition function can be written as a functional integral over Grassmann variables:

$$Z = \int \mathcal{D} \Psi e^{-S_0 - S_{int}}.$$ 

The free and interaction parts of the action are respectively

$$S_0 = \int_0^\beta d\tau \left\{ \sum_{\mathbf{r}} \Psi_{\mathbf{r}}^* (\partial_\tau - \mu) \Psi_{\mathbf{r}} - t \sum_{\langle \mathbf{r} \mathbf{r}' \rangle} (\Psi_{\mathbf{r}}^* \Psi_{\mathbf{r}'} + c.c.) \right\},$$

$$S_{int} = \int_0^\beta d\tau \left\{ \sum_{\mathbf{r}} \Psi_{\mathbf{r}}^* \Psi_{\mathbf{r}} \right\}.$$
Functional Integrals for Correlated Fermions

\[ S_{\text{int}} = U \int_0^\beta d\tau \sum_r \psi_{r\uparrow}^\dagger \psi_{r\uparrow} \psi_{r\downarrow}^\dagger \psi_{r\downarrow} . \]  

(5)

In the following, the interaction term will be treated using a Hubbard–Stratonovich decomposition.

For repulsive interactions \((U > 0)\) the appropriate decomposition is

\[ e^{-\varepsilon U \psi_\uparrow^\dagger \psi_\uparrow \psi_\downarrow^\dagger \psi_\downarrow} = \frac{\varepsilon}{\pi U} \int d\Delta_c d\Delta_s \exp \left[ -\frac{\varepsilon}{U} (\Delta_c^2 + \Delta_s^2) + i\varepsilon \Delta_c n + \varepsilon \Delta_s \sigma_z \right] . \]  

(6)

Here \(\Delta_c, \Delta_s\) are real variables, and \(n = \psi_\uparrow^\dagger \psi_\uparrow + \psi_\downarrow^\dagger \psi_\downarrow\), \(\sigma_z = \psi_\uparrow^\dagger \psi_\uparrow - \psi_\downarrow^\dagger \psi_\downarrow\). One inserts this at each point in space and time and thus obtains a functional integral over charge and spin fields \(\Delta_{c,s}(r, \tau)\), coupled bilinearly to the fermions. A saddle point approximation reproduces the Hartree–Fock results, and in particular at half–filling one finds an antiferromagnetic (or spin–density wave in another terminology) ground state. The unpleasant feature of this way of proceeding is that both \(\Delta_c\) and \(\Delta_s\) are scalar fields, and one therefore cannot construct easily the effective action for the low–energy excitations of the antiferromagnetic state which are spin–waves, the existence of which is of course closely related to the vectorial character of the order parameter.

Alternatively, one might use a Hubbard–Stratonovich decomposition using a vector auxiliary field. One then however does not even obtain the Hartree–Fock solution as a saddle point. A number of other, equally unsatisfactory decompositions have been discussed in the literature. In order to obtain a spin–rotation invariant effective action for fluctuations around the Hartree–Fock solution, I noticed that in writing down the Hamiltonian the choice of the spin quantization axis is a priori arbitrary at each lattice site, and in a functional integral formulation can also vary in time. I then leave the quantization axis \(\Omega_r(\tau)\) arbitrary and integrate over all possible \(\Omega_r(\tau)\), with the appropriate invariant and normalized integration measure at each point in space and time. In practice, this is achieved by introducing \(SU(2)\) rotation matrices \(R_r(\tau)\) at each point of space and time which satisfy \(R_r(\tau) \sigma_z R_r^+ (\tau) = \Omega_r(\tau) \cdot \sigma\). A convenient choice is

\[ R(\Omega) = \left( \begin{array}{cc} \cos(\frac{1}{2} \theta) & -e^{i\varphi} \sin(\frac{1}{2} \theta) \\ e^{i\varphi} \sin(\frac{1}{2} \theta) & \cos(\frac{1}{2} \theta) \end{array} \right) , \]  

(7)

where \(\theta\) and \(\varphi\) are the usual polar angles. I then introduce identities \(R_r(\tau) R_r^+ (\tau) = 1\) at the appropriate places in the functional integral and integrate over all configurations \(\Omega_r(\tau)\). Finally, new spinor variables are introduced via

\[ \Phi = R^+ \Psi . \]  

(8)

This means that the \(\phi\)–particles now have their spin along \(\pm \Omega_r(\tau)\). The Hubbard interaction term is invariant under this transformation, and now the Hubbard–Stratonovich transformation can be used in its form without loosing the spin excitations which are contained in the functional integral over \(\Omega_r(\tau)\). This also means that a nonzero saddle point value of the spin field \(\Delta_s\) does not necessarily imply the existence of magnetic long–range order. For this to occur, the angular degrees of freedom have also to be ordered.
H.J. Schulz

Given that at least at half–filling Hartree–Fock theory handles \textit{local} correlations rather well even for large $U$, one can now start by using a saddle point approximation for the scalar fields $\Delta_{c,s}$. The partition function then becomes

$$Z = \int \mathcal{D}\Omega \, \mathcal{D}\Phi \, \mathcal{D}\delta \, e^{-S_{HF} - S_{\Omega} - S_{\delta}}.$$  

(9)

Here $S_{HF}$ is the action corresponding to the saddle point, and $S_{\Omega}$ represents the coupling between the angular fluctuations and the fermions. Finally $S_{\delta}$ represents the massive fluctuations of $\Delta_c$ and $\Delta_s$ around their respective saddle point values, and will be neglected in the following.

For large $U$ an effective action for the spin degrees of freedom and the doped carriers can be derived, because in fact arbitrary space–time variations of $\Omega(r,\tau)$ can be treated. For simplicity, one can then start from a ferromagnetic saddle point which is characterized by lower and upper Hubbard band separated by a gap $U$.

One then has

$$S_{HF} = \int_0^\beta d\tau \left\{ \sum_r \Phi^*_r (\partial_\tau - \mu + \frac{1}{2} U \sigma_z) \Phi_r - t \sum_{\langle rr' \rangle} (\Phi^*_r \Phi_{r'} + \text{c.c.}) \right\}, \quad (10)$$

and

$$S_{\Omega} = \int_0^\beta d\tau \left\{ \sum_r \Phi^*_r R^+_r \hat{R}_r \Phi_r - t \sum_{\langle rr' \rangle} [\Phi^*_r (R^+_r R_{r'} - 1) \Phi_{r'} + \text{c.c.}] \right\}. \quad (11)$$

For the case of electron doping, the chemical potential is somewhere in the upper Hubbard bands, and the lower Hubbard band then can be integrated out. In this way one obtains the effective action for the local spin orientation and particles in the upper Hubbard band order by order in $t/U$. To zeroth order in $t/U$ I find

$$S_{\text{eff}}^0 = \int_0^\beta d\tau \left\{ \sum_r [\phi^*_r (\partial_\tau - \mu + U) \phi_r - \frac{i}{2} \hat{\phi}_r (1 - \cos \partial_\tau)(1 - \phi^*_r \phi_r)] \right\} - t \sum_{\langle rr' \rangle} [\alpha(\Omega_r, \Omega_{r'}) \phi^*_r \phi_{r'} + \text{c.c.}]. \quad (12)$$

Here $\phi$ refers to fermions in the upper Hubbard band, the spin index being omitted, and $\phi_r, \partial_r$ are the polar angles of $\Omega_r$. The coefficients $\alpha(\Omega_r, \Omega_{r'})$ come from the expression for the product of two $R$ matrices and are given by

$$\alpha(\Omega_r, \Omega_{r'}) = |\alpha| e^{i \theta_{rr'}} = [(1 + \Omega_r \cdot \Omega_{r'})/2]^{1/2} \exp [i \hat{A}(\Omega_r, \Omega_{r'}, \hat{z})/2], \quad (13)$$

where $\hat{A}(\Omega_1, \Omega_2, \Omega_3)$ is the signed solid angle spanned by the vectors $\Omega_1, \Omega_2, \Omega_3$, and $\hat{z}$ is the unit vector along $z$. To next order in $t/U$ one recovers the usual $t^2/U$ antiferromagnetic exchange term.

3. A POSSIBLE INSTABILITY OF THE NAGAOKA STATE

In the absence of particles in the upper Hubbard band, in $S_{\text{eff}}^0$ only the purely imaginary term remains, which is the Berry phase of an isolated spin $1/2$, 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 semi-phenomenological arguments, cancel the Berry phase term whenever there is an extra particle on site $r$, i.e. one is in a spin singlet whenever two particles occupy the same site. (ii) the kinetic energy term plays a role: in particular, going around an elementary plaquette (1234) the lattice curl of the phases $\chi_{rr'}$ equals $\Phi_{1234} = [\hat{A}(\Omega_1, \Omega_2, \Omega_3) + \hat{A}(\Omega_3, \Omega_4, \Omega_1)]/2$, i.e. there is an effective magnetic field proportional to the solid angle spanned by $\Omega_1, ..., \Omega_4$. $\Phi_{1234}$ is the lattice analogue of the familiar winding number density of the continuum nonlinear $\sigma$ model. Note that, while the gauge potential in (13) depends explicitly on $\hat{z}$ 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 $\phi$'s. One then straightforwardly sees that the kinetic term is optimized by a ferromagnetic arrangement of the spins. This is the familiar Nagaoka phenomenon.

One can now ask the question whether non-coplanar configurations of $\Omega_r$ with a nonzero winding number density can lead to an energy lower than the Nagaoka state. A configuration giving rise to a spatially constant effective field (i.e. a constant lattice curl of $\chi_{rr'}$) seen by the fermions is shown in fig. 1. At the mean-field level, one assumes the $\Omega_r$ to be static, and only the first and third terms in eq. (12) contribute. It is then easy to convince oneself that if this field is such that the lowest Landau level is completely filled and all the other Landau level are empty the energies of the ferromagnetic and the textured states are nearly identical. More precisely, the energy of the textured state is higher than that of the ferromagnetic state only due to the fact that now $\Omega_r \cdot \Omega_{r'} < 1$, i.e. the global scale of the kinetic

Fig. 1. A spin arrangement (“texture”) giving rise to a constant effective magnetic field acting on the fermions.
energy term is reduced. This leads to an energy difference

$$\Delta E \approx tn^2,$$

\(14\)
in favor of the ferromagnet. Here \(n\) is the dopant density, i.e. \(n = 1\) corresponds to half-filling. However, one should notice that the fully polarized ferromagnet \((\Omega_r \equiv \hat{z})\) is an exact eigenstate of the Hamiltonian, whereas the textured state is a mean-field trial state, i.e. its mean-field energy is an upper limit to its exact energy. In particular, one can calculate the first order quantum fluctuation corrections:\[\text{14}\] the collective modes have a spectrum \(\omega(q) = v|q|\), with a velocity given by

$$v = 2t\sqrt{2\pi n}.$$

This then gives rise to a fluctuation correction to the ground state energy of order

$$\Delta E_{\text{fluc}} \approx -tn^2,$$

\(16\)
i.e. of the same order of magnitude but with opposite sign as the correction due to the band narrowing, eq.\(14\). To determine which of the two corrections is more important, a detailed calculation taking into account short-distance cutoffs would be necessary. In the absence of such a calculation one can only point out that a textured state is a possible candidate for the destabilization of Nagaoka ferromagnetism.

The existence of a textured state might in fact have interesting consequences: (i) there is a large class of spin textures that all give rise to a constant effective magnetic field. It is conceivable that this large degeneracy gives rise to sufficiently strong quantum fluctuations to destroy long-range magnetic order. The effective magnetic field seen by the fermions would however still persist, i.e. the PT symmetry breaking inherent in a textured state would survive. This then could lead to a state similar to those proposed in the context of anyon superconductivity.\[\text{15, 16}\] (ii) even if long-range order exists the true ground state would be a spin singlet, due to the absence of any spontaneous magnetization. This might explain the strong variation of the total ground state spin observed in finite-size studies.\[\text{17}\] Moreover, with twisted boundary conditions, the small-doping ground state is in fact found to be fully polarized in finite-size calculations.\[\text{18}\] The twist necessary to lead to the polarized ground state may well be a remnant of the spin texture which (hypothetically) is present in the thermodynamic limit.

4. SINGLE PARTICLE STATES

It is clearly of importance to understand the single-particle properties in a doped and short-range ordered antiferromagnet. Fully understanding this problem, even based on the simplified action, eq.\(12\), and possibly the correction of order \(t/U\), is still a formidable unsolved problem. Nevertheless, some insight can be gained transforming eqs.\(10\) and \(11\) back to the original \(\Psi\) variables, via eq.\(8\). One obtains

$$S_{HF} + S_\Omega = \int_0^\beta d\tau \left\{ \sum_r \Psi_r^\dagger (\partial_\tau - \mu + \frac{1}{2} U \Omega_r \cdot \sigma) \Psi_r \right\}.$$
Functional Integrals for Correlated Fermions

\[-t \sum_{\langle rr' \rangle} (\Psi^*_r \Psi_{r'} + c.c.) \]  

\[ (17) \]

i.e. effectively a problem of electrons moving in a space and time–dependent field of constant magnitude but varying orientation. A priori all possible time and space dependent configurations \( \Omega_r(\tau) \) should be summed over. However, it seems likely that the dominant configurations will have some degree of short–range antiferromagnetic order. At least in one dimension such a state can be considered as an antiferromagnet disordered by defects, and I therefore consider configuration where there is antiferromagnetic order and just one defect changing the sign of the order parameter. To obtain a calculationally tractable problem, I further consider static configurations. In a truly disordered antiferromagnet with some finite correlation length, one of course has a finite density of defects (provided these can still be defined), but the present highly simplified calculation may still give some helpful ideas. In figs. 2 and 3 I show some defect configurations together with their electronic spectrum. In particular, in fig. 2 local antiferromagnetic order is preserved nearly everywhere. One observes that the separation of states into upper and lower Hubbard bands remains unless the width of the defect becomes very small (the lowest panel in the figure). If one the other hand in the vicinity of the defect there is some form of local ferromagnetic order (fig. 3), one always has states in the middle of the band. One can expect that the two rather different types of spectra for local antiferromagnetic or ferromagnetic alignment persist in higher dimensions. The two alternative types of spectra (or spectral densities) thus might be observed in photoemission spectroscopy. Moreover, configurations like those of fig. 3 because of their local ferromagnetic order should give rise to an enhanced spin susceptibility.

In the present calculations the spin structure \( \Omega_r \) was assumed to be static. This is probably a reasonable approximation if the electronic excitation energy (as measured from the Fermi level) is high compared to a typical frequency of the spin dynamics. If on the other hand one is at low excitation energy, i.e. in somewhere in the middle of the spectra of figures 2 and 3 if the band is approximately half–filled, the spin dynamics will be effectively fast compared to the electronic dynamics. One can then speculate that some form of “motional narrowing” will transform the states close to the center of the spectra into plane–wave like states, giving rise to Fermi–liquid or possibly non–Fermi–liquid like properties. It should also be noted that the spectra shown here are symmetric about the horizontal axis, in particular there is no “spectral weight transfer” from the upper to the lower Hubbard band. This is due to the neglect of the charge interaction contained in the \( S^\delta \) term in eq.(4).

5. CONCLUSION

I have discussed here a way to give a spin–rotation invariant functional integral formulation of the strong correlation problem. This formulation makes the role of local (in space and time) magnetic order particularly apparent. For half–filling, this formulation allows one to recover the mapping to the antiferromagnetic Heisenberg model for large \( U \), and more generally to obtain the effective spin dynamics for arbitrary \( U \). As discussed here alternatives to Nagaoka ferromagnetism arise at strong coupling, and properties of single–particle spectra for different types of local
Fig. 2. Single particle states for electrons moving in a magnetic field of constant magnitude but varying orientation (see eq. (17)). The spin configurations are shown together with the corresponding spectrum and represent a defect in an otherwise antiferromagnetically ordered state. Here in all cases approximate antiferromagnetic order is preserved even within the defect. The width of the defect decreases from top to bottom.
Fig. 3. The same as fig. 2 but here there is a strong ferromagnetic component of the magnetization at the defects.
H.J. Schulz

magnetic order can be discussed.

It should be pointed out that the method can be generalized so as to include the electron–hole symmetry of the Hubbard model. One then obtains a formulation with a fluctuating reference frame in an $SU(2) \times SU(2)$ space. This can in particular be used to treat particle–particle and particle–hole type instabilities on an equal footing in a Ginzburg–Landau like formulation. For example, one can include Kanamori–type $T$–matrix renormalizations into a microscopic formulation of a Ginzburg–Landau theory of magnetic ordering. Also, the large $U$ limit of the present formulation can be related to the slave–fermion Schwinger boson approach.

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