Stability of Nagaoka phase, spin effective action and delocalized free holes

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Abstract

The Hubbard model in the limit of infinite $U$ is investigated within a projected slave fermion representation and following a previous work of the author and collaborators [1]. The stability of the Nagaoka’s phase with respect to a non vanishing concentration of holes ($\delta_h$) is analyzed by envisaging the existence of a spin effective action for itinerant magnetism of the Hubbard model. It is considered that, as the hole doping increases away from the half filled insulating limit, free holes are expected to be more delocalized. Depending on treatment for the hopping: a ferromagnetic or anti-ferromagnetic ordering might arise and the Nagaoka phase might have some stability with respect to $\delta_h \neq 0$.

Key words: Strong correlations, Nagaoka phase, concentration of holes, Hubbard model, hopping, spin effective action

1. Introduction

One of the few exact results for the Hubbard model (HM) is the ferromagnetic Nagaoka limit for $U = \infty$ [1]. This phase appears when one hole hops in the half filled band. Although this limit is not found in any material, it can be reached in optical traps [4]. The investigation of the Nagaoka mechanism provides relevant information about the phase diagram of the model and one starting point for understanding further the role of strong electronic correlations [1,5,6,7] and of realistic mechanism for itinerant ferromagnetism [5,3]. In the limit of infinite Coulomb repulsion the HM is written as:

$$H = -\sum_{ij,\sigma} t_{ij} \tilde{c}^\dagger_{i\sigma} \tilde{c}^\sigma_{j\sigma} + \mu \sum_{i\sigma} (1 - \tilde{c}^\dagger_{i\sigma} \tilde{c}^\sigma_{i\sigma}),$$

where $t_{ij}$ is a symmetric matrix with elements representing the hopping amplitude $t$ only non-zero between the nearest-neighbor sites; $\tilde{c}^\dagger_{i\sigma}$ is the projected electronic operator [5]. In this expression the chemical potential $\mu$ is to control the number of vacancies (away from half filling), and the projected electronic operator carries the effect of the strong correlations, i.e. it excludes the doubly occupied states.

It is difficult to handle the strong electronic correlations and thus to provide exact results, in particular concerning the stability of the Nagaoka phase. However, a common trend is that this FM phase is unstable with respect to a finite concentration of holes in particular in the thermodynamic limit $S^{\delta_h = \infty}$. In the present work we investigate the role of the delocalization of (free) holes for the appearance and for the stability of the Nagaoka’s phase following the long-wavelength approach with slave fermion representation worked out in Ref. [1]. By envisaging the derivation of a spin-effective action ($S_{eff}$) for the HM with very large $U$, a previous analysis was performed in Ref. [1]. On the other hand, in the present work, the role of delocalization of free holes close to half filling is investigated. It is considered that the increase of the number or concentration of holes should increase the mobility of holes departing from the half filled limit. An itinerant magnetic phase (ferromagnetic or anti-ferromagnetic) emerges depending on the structure and treatment of the hopping of spinless holes.

2. Slave fermion for the $U = \infty$ Hubbard model

To account for the strong correlations that forbid doubly occupied states, consider the slave-fermion decomposition for projected electronic operators [16] given by: $\tilde{c}^\dagger_{i\sigma} = b^\dagger_{i\sigma} f_i$, where two operators have been used: $b_{i\sigma}$ stands for a spinon boson and $f_i^\dagger$ creates a charged spinless fermion. The functional generator for the $U = \infty$ Hubbard model is given by:

$$Z^{U=\infty} = \int D[b, b^\dagger; f, f^\dagger] \exp \left( S^{SF}_{U=\infty} [b_i, b_i^\dagger; f_i, f_i^\dagger] \right).$$

The action can be written, with the time-dependent phase, as [11]:

$$S^{SF}_{U=\infty} = -\int d\tau \sum_{i,j} f_i \left( \delta_{ij} + \sum_\sigma t_{ij} b^\dagger_{i\sigma} b_{j\sigma} \right) f_j^\dagger.$$
\[-\int d\tau \sum_i \left( \sum_\sigma b^\dagger_{i\sigma} \partial_\tau b_{i\sigma} - H_{\text{const}} \right) \]  

The local non doubly occupancy (NDO) constraint is imposed by a (local) Lagrange multiplier, \(\lambda_i\), by adding the term: \(H_{\text{const}} = \lambda_i (f_i^\dagger f_i + \sum_{\sigma=\uparrow,\downarrow} b^\dagger_{i\sigma} b_{i\sigma} - 1)\).

The slave-fermion decomposition is equivalent to a particular (lowest weight) representation of the \(su(2|1)\) supersymmetric projected electronic operators \([6,17]\): spinless holes are super-partners of spinons. A mapping for the variables, incorporating implicitly the non-doubly-occupancy (NDO) constraint, is given by \([1]\):

\[(b_{i\uparrow}, b_{i\downarrow}, f_i) = \left( \frac{e^{i\phi_i} z_i e^{-i\phi_i}, \xi_i e^{i\phi_i}}{\sqrt{1 - z_i^* z_i + \xi_i^* \xi_i}} \right), \tag{2}\]

and the corresponding variables for \(b_{i\sigma}^\dagger\) and \(f_i^\dagger\). With these new variables \((z_i, \xi_i, \phi_i)\) respectively for bosonic spinons, spinless fermions and a local phase) the Lagrange multiplier \(\lambda_i\) is naturally eliminated, being the NDO constraint incorporated. With the spinon variables \(z_i\), the images of the spin \(su(2)\) algebra - \(\hat{S}\) - can be rewritten \([11,17]\), for example: \(S_{ij} = \frac{1}{2} \frac{z_i z_j}{1 - z_i^* z_j} \). There is a local gauge invariance as consequence of the redundancy in parameterization of the electron operator in terms of the auxiliary boson/fermion fields. After some manipulation, decomposing the measure of the path integral into the new variables \(D[b, b^\dagger; f, f^\dagger] \to D\mu_{\text{spin}}(z, \xi) \times D\mu_{\text{fermion}}(\xi, \tilde{\xi})\), with the corresponding Jacobian \([17]\), the action reads \([17,1]\):

\[S = \sum_i \int_0^\beta \! i a_i(\tau) d\tau - \sum_i \int_0^\beta \! \xi_i (\partial_\tau + \mu + i a_i) \xi_i d\tau \]

\[-\int_0^\beta \! \sum_j (\xi_j z_i < z_i z_j > + hc) d\tau \tag{3}\]

The first term of this action is a kinematical term and the second is the classical image of the Hamiltonian. The spin “kinetic” term (Berry phase): \(ia = -<z|\partial_\tau z|z> = \frac{1}{2} \frac{z_i^* z_i}{1 + z_i^* z_i}\), with \(z\) being the \(su(2)\) coherent state \([17,1]\). The inner product of the \(su(2)\) coherent states is written as: \((z_i|z_j) = \frac{1 - z_i^* z_j}{\sqrt{(1 + z_i^* z_i)(1 + z_j^* z_j)}} = \frac{1}{\tilde{t}_{ij}} \Sigma_{ij}\).

3. Factorization of the hopping

By introducing more holes in the half filled HM, it can be expected they become progressively more delocalized. Consider that the band structure is such that the hopping term can be decomposed into two parts. One of them endows the holes with a dispersion relation (labeled by \(\gamma_1\)) and the other is treated as a perturbation (labeled by \(\gamma_2\)), eventually from a different band. It will be considered schematically that:

\[\xi_i \Sigma_{ij} \xi_j \rightarrow \gamma_1 \xi_j^{(1)} \Sigma_{ij}^{(1)} + \gamma_2 \xi_j^{(2)} \Sigma_{ij}^{(2)} + \hbar c. \tag{4}\]

Where \(\gamma_1\) and \(\gamma_2\) keep track of each of the different parts of the hopping. The procedure and idea will be clearer and useful when working in the momentum space. We will consider that these terms are characterized by different ranges of momenta of holes \(\xi_1^{(1)}(k_1)\) and \(\xi_2^{(2)}(k_2)\), associated respectively to the terms \(\Sigma^{(1)}\) and \(\Sigma^{(2)}\), such that \(k_1\) and \(k_2\) can belong to different parts of the band. With this decomposition, the following ansatz for the free hole Green’s functions can be envisaged:

\[(G_0^{-1})_{ij} = (\partial_\tau - \mu) \delta_{ij} \delta(\tau) + \gamma_1 \Sigma^{(1)}_{ij}, \tag{5}\]

and \(\gamma_2 \Sigma^{(2)}_{ij} = \gamma_2 \xi_j^{(2)} < z_i z_j >\) is a perturbation. The upper indices \((2)\) stand for the perturbation due to the corresponding part of the hopping term, separated according to expression \([4]\). Since this separation is generic and not calculated microscopically, for the sake of generality we can have \(\xi^{(2)} \neq \xi^{(1)}\) depending on the hopping (and band) structure. This procedure can be considered such as to provide a measure of the (de)localization of the free holes. For instance, in a normal conducting phase, we should recover \(\gamma_2 \rightarrow 0\), that is used in the usual mean field approximation \([15,1]\). On the other hand, at the half filling limit (and very close to it) the hopping parameter would be such that \(\gamma_1 = 0\), suitable for the hopping (loop) expansion as discussed in details in Ref. \([4]\).

3.1. Delocalization of free holes and spin effective action

We take a continuum limit of the full action, given by \([3]\), to derive a spin-effective action, \(S_{eff}\), by integrating out the fermion variables with the prescription \([5]\) in the same lines as it was done in Ref. \([1]\). Using a finite difference method for the term labeled by \(\gamma_1\), we take: \(\xi_j = i a + \xi(i) + \nabla \xi(i)\) and perform a Fourier transformation. Therefore we consider free holes are endowed with a dispersion relation \(\epsilon(k_{(1)})\), being that \(k_{(1)} \rightarrow \xi(i)\) refers to the momenta of modes labeled by \(\gamma_1\). This yields the momentum dependent Green’s function: \(G_0[i; \epsilon(k_{(1)})]\). The particular dispersion relation \(\epsilon(k_{(1)})\) is completely defined by the lattice (geometry and dimensionality). For the sake of the main argument, we consider a two dimensional square lattice, for which it follows:

\[\epsilon(k_{(1)}) \simeq 2 \gamma_1 t \sum_{k,\sigma} \phi_{k,\sigma}^2 (\cos(k_x) + \cos(k_y))\]

from what the continuum limit is extracted. Prescription \([4]\) might also be associated to a superposition of (nearly) localized and (fully) delocalized states. In order simplify the notation \(k_{(1)}\) momenta will be denoted simply by \(k\) from here on.

The corresponding effective action, with the integration of fermions variables, can be written as \([4]\):

\[S_{eff} = TrLogG^{-1} = TrLog\left(G_0^{-1} - ia + \Sigma^{(2)}\right) = TrLogG_0^{-1} + TrLog(1 - G_0ia + G_0\Sigma^{(2)}). \tag{6}\]

The different modes of the fermions are decoupled such that the corresponding \(\Sigma^{(i)}\) are treated (nearly) independently. The free hole Green’s function can be calculated,
for the sake of generality, for a given (sub)lattice $A$, instead of an unique lattice, being written as: $\langle G_{\alpha}^{-1}\rangle^{A}(\mu^{A},k) = \left(\partial_{\tau} - \mu^{A} + \epsilon_{\alpha}(k)\right)^{-1}\delta(\tau)$. This case of (at least) two sublattices will not be worked out here, and this might be considered when there are different hoppings in the sublattices or between each of them. This can yield the terms labeled by $\gamma_{1}$ and $\gamma_{2}$ contributing in each of the different sublattice. The long-wavelength expansion is done by considering $G_{\alpha}^{-1} >> \Sigma^{(2)}$. The reliability of this expansion depends on several parameters, seen in expressions (1) and (3). Basically it is required that $\mu + \epsilon(k) >> \Sigma^{(2)}$ where $\Sigma^{(2)}$ is only part of the full hopping term. We remind further that $\Sigma^{(2)}$ is basically proportional to $t$ and the long-wavelength limit corresponds to a gradient expansion of $t < z_{i}z_{j} >$. Therefore we expect to provide a complementary investigation to the loop expansion analyzed in Ref. [1].

Keeping track of the time ordering in the effective action, is obtained in the very same way as shown in Ref. [1].

The particular dispersion relation for the holes was not explicitly written so far. For the sake of generality, two cases are considered of the following usual forms:

\[ \epsilon_{i}(k) = \gamma_{1}a_{i}k \equiv a_{i}k \text{ and } \epsilon_{f}(k) = \gamma_{2}b_{i}k^{2} \equiv b_{i}k^{2}. \]

Changing variables for each of the cases, we write:

\[ j_{\text{eff}}^{(I)} = \gamma_{2}^{2} \frac{2\Omega_{D}\beta}{4(2\pi)^{D}a_{1}\beta} \int_{X_{0}^{(I)}}^{X_{1}^{(I)}} dx \left[ \frac{1}{\cosh^{2}(x)} \right]^{D-1} \]

\[ j_{\text{eff}}^{(II)} = \gamma_{2}^{2} \frac{2\Omega_{D}\beta}{4(2\pi)^{D}b_{1}\beta} \int_{X_{0}^{(II)}}^{X_{1}^{(II)}} dx \left[ \frac{1}{\cosh^{2}(x)} \right]^{D-2} \]

where $\Omega_{D}$ is the integral of the $D$ dimensional solid angle; and the cutoffs are: $X_{0}^{(I)} = \frac{(\mu - a_{1}k_{0})^{2}}{2}$, $X_{1}^{(I)} = \frac{(\mu - a_{1}k_{0})^{2}}{2}$, $X_{0}^{(II)} = \frac{(\mu - b_{1}K_{0}^{2})^{2}}{2}$, $X_{1}^{(II)} = \frac{(\mu - b_{1}K_{0}^{2})^{2}}{2}$, with the eventual formation of a Fermi surface for the (spinless) vacancies in a normal metallic phase, we could identify the chemical potential to: $\mu = \epsilon(k_{F})$, where $k_{F}$ is the momentum at the Fermi surface. The result for the quadratic $\epsilon_{f}(k)$ in 2-dim is the same as for $\epsilon_{f}(k)$ in 1-dim, apart from a normalization.

The integrations, in 2-dim, yield respectively:

\[ j_{\text{eff}}^{(I),D=2} = -\gamma_{2}^{2} \frac{t^{2}}{4\pi a_{1}\beta} \left[ X_{1}^{(I)} \tanh(X_{1}^{(I)}) - X_{0}^{(I)} \tanh(X_{0}^{(I)}) \right] \]

\[ j_{\text{eff}}^{(II),D=2} = \frac{2}{\beta} \log \left( \frac{\cosh X_{1}^{(II)}}{\cosh X_{0}^{(II)}} \right) \]
A short example can be taken, for $T = 0$, by choosing $K_1 > K_0 \simeq k_F \simeq \mu/a_1$ for the first of these expressions, in which case $K_0$ might be the momentum at a Fermi surface for the holes. The resulting spin-effective coupling at zero temperature is given by:

\[ J_{\text{eff}}^{(i)} \sim \frac{2}{a_1^2 \pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{\sqrt{2k+1}} \frac{2}{\pi a_1^2 \beta} \left(\ln 2\right) \]

\[ J_{\text{eff}}^{(I)} = -\mu \frac{2}{a_1^2 \pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{\sqrt{2k+1}}. \]

We notice that these couplings might depend on $\mu$. They provide anti-ferromagnetic spin Heisenberg couplings.

4. Final remarks

We have shown that the delocalization of free holes might be a relevant issue for the understanding of the stability of the Nagaoka's phase with respect to a finite concentration of holes. More generally we proposed a framework for investigating different magnetic orderings in the limit of very large Coulomb repulsion and low concentration of holes for the Hubbard model. A spin effective action was found to have a form of localized Heisenberg coupling in the long wavelength limit along with the work presented in Ref. [1]. It can be ferromagnetic (Nagaoka-type phase) or anti-ferromagnetic depending on the relation among the chemical potential and the eventual values of the limitation on the summation/integration of momenta carried by the holes. For that, the hopping term was separated in two parts, corresponding to high and low momentum modes or to hopping among different bands.\(^1\) A microscopic derivation of the prescriptions adopted was not yet presented and for the sake of the main argument it was considered that the holes are reasonably decoupled from the spinons. In particular, by endowing holes with a dispersion relation such that a kind of Fermi surface can be formed, it was found that the Nagaoka’s phase at finite concentration of holes can have some stability in a long-wavelength limit. A more complete analysis will be presented elsewhere.

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\[^{1}\] Eventually the parameters $\gamma_i$ introduced to label $\Sigma^{(i)}$ might be expected to depend on the temperature, $U$ and concentration of holes $\delta_h$. Eventually,变得 phenomenological. For example, one might want to account the variation of $\gamma_i$ due to a finite value for the Coulomb repulsion by means of prescriptions. They might be given by:

\[ \gamma_1 = \frac{\alpha_0}{\alpha_0 + \alpha_0 U}, \quad \gamma_2 = \frac{\alpha_U}{\alpha_0 + \alpha_0 U}, \]

\[ \gamma_1 = \frac{2\alpha_1 + \alpha_2 U}{2(\alpha_1 + \alpha_2 U)}, \quad \gamma_2 = \frac{\alpha_3 U}{2(\alpha_1 + \alpha_2 U)}. \]
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