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Insulator-to-metal crossover induced by local spin fluctuations in strongly correlated systems

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Abstract

We study the simplified Hubbard (SH) model in the presence of a transverse field in the infinite-dimension limit. The relevant one-particle Green's functions of the model are obtained by means of a perturbative treatment of the hopping and of the transverse field around the atomic limit. We consider an analytical solution for the impurity problem. It is shown that this solution is very accurate in describing the spectral properties of the heavy particles of the SH model for intermediate and strong values of the on-site Coulomb interaction U. We find that for large values of U an insulator–metal transition takes place as a function of the transverse field. We analyse the metallic phase through the behaviour of the density of states and those of the optical conductivity and static resistivity. Our results for the latter quantity agree with what is observed in experiments on Bi₂Sr₂CuO_y.

1. Introduction

In the last few years, several experimental works have considered the problem of the magnetic response in strongly correlated electronic systems. For example, the spin blockade problem in quantum dots in magnetic fields has been considered by different groups [1, 2]. The farinfrared transmission in thin films of YBaCu₃O₇ has been measured by Drew *et al* [3] and Lihn *et al* [4], and a magneto-optical study of the magnetization for this compound was performed by Uspenskaya *et al* [5]. The study of the magnetic properties of quantum dots [2] as well as high- T_c thin films [6–8] in the presence of *transverse* magnetic fields has also been of great interest.

An important problem related to high- T_c compounds is that of understanding the normalstate properties of the in-plane (ρ_{ab}) and out-of-plane (ρ_c) dc resistivity for different values of the doping concentration [9]. It is well known that the easiest way to suppress the superconductivity at low temperatures without deliberate chemical substitution is to apply a high (pulsed) magnetic field. In such experiments the field is usually applied parallel to the *c*-axis to most effectively suppress the superconducting state, so the magnetic field is normally applied perpendicular to the CuO₂ basal plane where the ordered spins are primarily aligned [10, 11]. This alignment is usually originated by spin–orbit interaction and it has been observed for different alloys [12].

On the other hand, extensive experimental investigations show that the normal-state properties of high- T_c superconductors are not explained in terms of the Fermi-liquid (FL) theory [9,13]. Deviations from the normal FL behaviour were observed also in the normal state of different heavy-fermion compounds [14] as well as in quasi-one-dimensional materials [15]. This unexpected behaviour increased the interest in studying physical models that clearly present non-Fermi-liquid (NFL) properties. For example, Si et al [16] introduced a spinless two-band model to describe the effect of interactions in a band insulating system. By solving the model numerically in the limit of infinite spatial dimensions $(d \to \infty)$ they showed that it exhibits NFL properties. In addition, Consiglio and Gusmão [17] have shown that the main features of the optical conductivity of the Kondo alloy $Y_{1-x}U_xPd_3$ are well taken into account by the simplified periodic Anderson model. In the last few years, attention has also been paid to the simplified Hubbard (SH) model [18–22]. This is a modification of the Hubbard model, where electrons with one particular spin orientation do not hop in the lattice. This is one of the few models which have an exact solution in the limit of high dimensions [18], and it shows a metal-insulator transition both as a function of the on-site Coulomb interaction and as a function of the doping.

Of particular importance here is the work of Brandt and Urbanek [23], where the spectral properties of the heavy particles, the electrons that do not hop, are discussed in detail. In addition, some years ago the SH model in a magnetic field was studied by van Dongen and Leinung [24]. They considered the problem of the metal–insulator transition as a function of the Zeeman (*z*-direction) field. As expected, at large fields the system is a fully polarized ferromagnet; however, in the non-saturated phase a metal–insulator (MI) transition takes place as a function of the field and the local on-site Coulomb interaction (U). They showed that a magnetic field slightly reduces the critical value of the Coulomb interaction, with the result that the MI transition for non-zero field occurs at a critical U smaller than that for the transition at zero field.

It is worth noticing that, despite the great interest in strongly correlated electron systems, to the best of our knowledge there has been no investigation of the effects of transverse fields in models which explicitly show both broken spin symmetry and non-Fermi-liquid properties. In this paper, we address precisely this issue: the study of the SH model in the presence of a transverse field in the high-dimension limit. This limit, introduced originally by Metzner and Vollhardt [25], has been shown to be a very good starting point in the study of several physical systems [26]. We study the SH model because it has by construction broken spin symmetry, which is closely connected to the different dynamics of the two types of electrons. Here, we discuss the formal solution of this model in a transverse field, where the so-called *static approximation* [27] is employed to solve the related single-site problem. Comparing with the results of reference [23], we show that the *static approximation* gives a very accurate description of the T = 0 physical properties of the heavy particles for on-site Coulomb interactions above the metal–insulator transition. Next, we study the effect of the transverse field on the spectral and the optical properties of the SH model.

2. Model and perturbation method

In the usual notation, the SH model in a transverse field is described by the Hamiltonian

$$H = \sum_{k} \epsilon_{k} c_{k\uparrow}^{\dagger} c_{k\uparrow} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + (E - \mu) \sum_{i\sigma} n_{i\sigma} + \sum_{i} t (c_{i\uparrow}^{\dagger} c_{i\downarrow} + \text{h.c.})$$
(1)

where ϵ_k is the dispersion relation of the conduction electrons (\uparrow -electrons), and the \downarrow -electrons do not hop in this model. *E* is the energy level of the two particles, which are coupled through

the correlation U and a transverse field t. This field is usually a magnetic field along the x-direction, but a similar type of effect could have a different origin. One example would be a correlated hopping with spin flip originated in the spin–orbit interaction, and this type of term has already been employed [28] in the study of other strongly correlated electron systems.

In this work we are interested in the two relevant one-particle Green's functions of equation (1). The temperature-dependent one-particle Green's function for both up and down electrons is obtained, following the approach recently introduced to study the formal solution of a spinless two-band model [29], by means of a perturbative treatment around the atomic limit of the hopping and the transverse-field terms. To apply this method, we first consider the exact solution of the unperturbed Hamiltonian, given by the second and third terms of the RHS of equation (1). Next we solve the t = 0 limit of equation (1) by means of a tight-binding treatment around the atomic limit of the conduction electrons [30]. The formal solution of the complete Hamiltonian is then obtained by performing a perturbative treatment on the hybridization term [29]. Following this procedure and considering the high-dimension limit, it is straightforward to show that

$$G_{ii\uparrow}(i\omega_n) = \frac{1}{N} \sum_k \frac{1}{[\mathcal{G}_{\uparrow}(i\omega_n)]^{-1} - \epsilon_k - t^2 \mathcal{G}_{\downarrow}(i\omega_n)}$$
(2)

and

$$G_{ii\downarrow}(i\omega_n) = \mathcal{G}_{\downarrow}(i\omega_n)[1 + \mathcal{G}_{\downarrow}(i\omega_n)t^2G_{ii\uparrow}(i\omega_n)]$$
(3)

where $\mathcal{G}_{\uparrow}(i\omega_n)$ and $\mathcal{G}_{\downarrow}(i\omega_n)$ are the irreducible one-particle Green's functions for the conduction electrons and for the heavy particles, respectively. The former is irreducible in the sense that the contributing diagrams cannot be divided into two pieces by cutting a single hopping line, while the second is irreducible with respect to the cutting of a $t^2 \bar{g}_{k\uparrow}(i\omega_n)$ line [17, 29], where $\bar{g}_{k\uparrow}(i\omega_n)$ is the solution of equation (1) in the limit of t = 0. From equation (2) it becomes clear that the transverse field t acts as a hybridization term, mixing the single-site one-particle excitation of the \uparrow -electrons with the \downarrow -electrons. One should notice that in the case of the complete Hubbard model a similar equation for the \downarrow -electrons is obtained by exchanging the spin directions. The main difference between equations (2), (3) and those of reference [29] is that here they describe the formal solution of the one-band model with hybridization in the spin sector, while there we considered a two-band model with interaction and hybridization in the charge degrees of freedom of fully polarized orbitals¹.

The irreducible propagators in equations (2), (3) can be written in terms of the single-site one-particle Green's function and the dynamical mean field $A_{\sigma}(i\omega_n)$, which connects a single site with the electron bath, through the relation [27]

$$\frac{1}{\mathcal{G}_{\sigma}(\mathrm{i}\omega_n)} = \frac{1}{G_{ii\sigma}(\mathrm{i}\omega_n)} + \mathcal{A}_{\sigma}(\mathrm{i}\omega_n).$$
(4)

It is important to notice that once we turn on the transverse field, the solution of the conduction electron local problem is not trivial any longer. This is because the transverse-field term locally hybridizes the up and down electrons, so the spin-down electrons are not frozen any longer. Once we provide dynamics to the heavy electrons, the local spin-fluctuation problem also holds for the conduction electrons.

Now we proceed to analyse the solution of the single-site problem of both electrons from the point of view of the perturbation around the atomic limit [27, 29]. This method provides a direct way of solving the local problem by means of a perturbative expansion in the local

 $^{^{1}}$ The spin degeneracy can be lifted by a strong magnetic field or by a very large Hund's-rule coupling, as in the case of Fe₃O₄ [31].

mean field. This approach has been used in reference [27] to obtain the exact solution for the conduction electrons of the SH model as well as to study the problem of the spin fluctuation in the Hubbard model. For the latter case the *static approximation* has been introduced. Here, we will employ this approximation to account for the local spin fluctuations induced by the transverse field.

In our perturbation approach to the single-site problem we start with the unperturbed local Green's function $-\langle \hat{T}c_{\sigma}(\tau) c_{\sigma}^{\dagger}(0) \rangle_{0}$; each order in perturbation theory introduces a product of the type $\mathcal{A}_{\sigma_{1}}(\tau_{1} - \tau_{1}')c_{\sigma}(\tau_{1})c_{\sigma}^{\dagger}(\tau_{1}')$, so in general one has to calculate averages of the form $\langle c_{\sigma_{1}}(\tau_{1})c_{\sigma_{1}}^{\dagger}(\tau_{1}')c_{\sigma_{2}}(\tau_{2})c_{\sigma_{2}}^{\dagger}(\tau_{2}')\rangle_{0}$. To calculate this averages we rewrite the fermion operators in terms of the Hubbard operators [30], and utilize the standard algebra for the latter. This allows us to perform all possible direct contractions, in the sense of Wick's theorem. We have applied this procedure in references [27, 30] to evaluate explicitly a four-operator average that appears in the one-loop approximation. In addition, in reference [27] the *static approximation* for the single-site one-particle Green's function has been obtained by neglecting all terms that involve non-zero bosonic frequencies originated by local contractions between boson-like Hubbard operators. Since the averages that we need to consider here are exactly the same as in the case of the Hubbard model, we refer the reader to references [27, 30] for their calculation.

In terms of the *static approximation*, the single-site one-particle Green's function is given by

$$G_{ii\sigma}(\mathbf{i}\omega_n) = \bar{G}_{ii\sigma}(\mathbf{i}\omega_n) + \Delta_{\sigma}(\mathbf{i}\omega_n)$$
(5)

where

$$\bar{G}_{ii\sigma}(i\omega_n) = (1 - \langle n_{\bar{\sigma}} \rangle)\bar{g}_{0\sigma}(i\omega_n) + \langle n_{\bar{\sigma}} \rangle\bar{g}_{\bar{\sigma}2}(i\omega_n)$$
(6)

is the well known exact solution for the conduction electrons of the SH model (the t = 0 limit of equation (1)) and

$$\Delta_{\sigma}(\mathrm{i}\omega_{n}) = (g_{0\sigma} - g_{\bar{\sigma}2})\mathcal{A}_{\bar{\sigma}} \bigg[\frac{(1 - \langle n_{\bar{\sigma}} \rangle)\bar{g}_{0\sigma}}{1 - \mathcal{A}_{\sigma}g_{0\sigma} - \mathcal{A}_{\bar{\sigma}}(g_{0\sigma} + g_{\bar{\sigma}2})} - \frac{\langle n_{\bar{\sigma}} \rangle \bar{g}_{\bar{\sigma}2}}{1 - \mathcal{A}_{\sigma}g_{\bar{\sigma}2} - \mathcal{A}_{\bar{\sigma}}(g_{0\sigma} + g_{\bar{\sigma}2})} \bigg].$$
(7)

 $g_{0\sigma}(i\omega_n)$ and $g_{\bar{\sigma}2}(i\omega_n)$ in equations (6), (7) are the fermionic Green's functions of Hubbard operators [30], while $\bar{g}_{0\sigma}(i\omega_n)$ and $\bar{g}_{\bar{\sigma}2}(i\omega_n)$ describe the single-site one-particle excitations renormalized by the dynamical mean field². Note that even for the lowest order in the dynamical mean field, $\Delta_{\sigma}(i\omega_n)$ is obtained from local contractions between *one-band* operators with different spin orientations. This means that $\Delta_{\sigma}(i\omega_n) = 0$ for systems where local spin fluctuations are absent³.

3. Results

Let us consider first the t = 0 limit of equation (1). $\mathcal{A}_{\downarrow}(i\omega_n) = 0$ in this limit, because \mathcal{A}_{\downarrow} is proportional to the hybridization term. This can be easily seen from equations (3) and (4). Therefore, in this limit the single-site one-particle Green's function of the heavy electrons $G_{ii\downarrow}(i\omega_n)$ is only a function of the dynamical mean field of the conduction electrons; see equations (5)–(7). In figure 1 the density of states (DOS) of the heavy electrons is shown for t = 0 and different values⁴ of U. For U = 0.9 we obtain a sharp peak around the Fermi level

² More precisely, $\bar{g}_{0\sigma}(i\omega_n) \equiv 1/(i\omega_n - E + \mu - A_{\sigma}(i\omega_n))$ and $\bar{g}_{\bar{\sigma}2}(i\omega_n) \equiv 1/(i\omega_n - E - U + \mu - A_{\sigma}(i\omega_n))$.

³ The spin degeneracy can be lifted by a strong magnetic field or by a very large Hund's-rule coupling, as in the case of Fe_3O_4 [31].

⁴ The calculations were performed for the symmetric case with a Gaussian DOS.



Figure 1. Zero-temperature densities of states for the heavy electrons of the simplified Hubbard model at t = 0 for different values of U.

 $(\omega = 0)$. On increasing U, the height of the central peak is reduced, and a small tendency to form a gap is observed for U = 1. From the comparison between our results with those of reference [23], it becomes clear that the *static approximation* is able to recover the main features of the spectral properties of the heavy particles in the metallic phase of the SH model. Indeed, in the regime of strong on-site interaction U we observe a very good agreement between our results and those obtained by Brandt and Urbanek [23]. Hence, one can conclude that the *static approximation* is very accurate in describing the \downarrow -electron properties of the SH model in the strong-coupling limit.

From this result it is possible to conclude that for the half-filled and symmetric SH model at T = 0 none of the terms that involve non-zero bosonic frequencies [23, 27, 30] in the local Green's functions play an important role in the limit of large values of the Coulomb on-site interaction. Indeed, figure 1 shows that the perturbation treatment around the atomic limit is very accurate in the large-U limit. Note that, in our treatment for the corrections due to spin fluctuations (equation (7)), an infinite series of diagrams for the site-diagonal Green's function as well as for the irreducible propagators are considered. Furthermore, from the results of figure 1 it becomes clear that our solution for the single-site problem is a good approximation, and we do not need to consider any small parameter to justify equation (7).

As our method describes correctly the spectral properties of the SH model in the large-U limit, we shall employ this limit to study the spectral properties of the SH model in the presence of the transverse magnetic field, expecting to obtain realistic results. In figure 2 the DOS is shown for both types of electrons for U = 2 and different values of the transverse field t. Let us consider once more the t = 0 limit. In the dashed line of figure 2 one can clearly see that the gap sizes for the two particles coincide. Hence, it is clear from this behaviour that the DOS at the Fermi level vanishes at the same value of U for the two spin directions. Furthermore, the DOSs of the two particles show very strong similarities. One can expect these similarities to increase with U, and the two particles to behave in almost the same way in the half-filled case for $U \to \infty$.



Figure 2. Zero-temperature densities of states for the SH model for U = 2 and different values of *t*. (a) and (b) show the DOSs of \downarrow - and \uparrow -electrons, respectively.

According to our results in figure 2, the charge Mott gap is strongly affected by the transverse field. In the case of U = 2, this gap persists up to t = 0.3, where the insulator-metal transition takes place. It is instructive to note that for both spin directions we observe spectral transfer from the high to the low energies. The most interesting behaviour of the metallic phase occurs for t = 0.5, where a sharp peak around the Fermi level is observed in the DOS of the heavy particles. This peak is related to a self-consistent modification of the electron bath, where a partial decoupling of the local degrees of freedom takes place [16]. Note that, for both non-zero values of the transverse field in figure 2, the two atomic-like poles of the $G_{ii\uparrow}$ remain in almost the same position, while the internal pole of the $G_{ii\downarrow}$ is shifted to zero energy for t = 0.5. This is because the transverse field strongly mixes the low-energy excitations of the two types of electrons by the spin-flip process.

To provide a complete description of the insulator-metal transition of the SH model in a transverse field we study in figure 3 the single-particle density of states away from half-filling, at a fixed n = 0.8. For t = 0 one can see that our results for the DOS of the conduction electrons agrees with those obtained by Möller *et al* [32]. As in figure 2, the gaps in the DOSs of the two particles coincide in this limit. However, the upper Hubbard band of the heavy electrons is higher than the one for the conduction electrons, and this behaviour is related to the atomic-like character of the heavy particles at large U. Another interesting feature to be seen in figure 3 is the presence of a second sharp peak at high energies in the DOS of the \downarrow -electrons for non-zero t. This peak reduces on increasing the transverse field. Finally, the DOS of the conduction electrons also shows interesting new structures, in particular for t = 0.5. We believe that these structures are related to the asymmetric behaviour in the DOS of the heavy electrons together with the large hybridization between the two types of electrons.

To further confirm the insulator-metal transition we calculate the optical conductivity for the half-filled case with the same parameters as were employed in figure 2. It is known that in the infinite-dimension limit the vertex corrections drop out in the two-particle equation, and



Figure 3. Zero-temperature densities of states for the SH model for U = 2, n = 0.8 and different values of *t*. (a) and (b) show the DOSs of \downarrow - and \uparrow -electrons, respectively.

the optical conductivity assumes the simple form [26]

$$\sigma(\omega) = \pi \sum_{\sigma} \int d\epsilon \ \rho_0(\epsilon) \int d\omega' A_{\sigma}(\epsilon, \omega') A_{\sigma}(\epsilon, \omega' + \omega) \frac{[f(\omega') - f(\omega' + \omega)]}{\omega}$$
(8)

where $\rho_0(\epsilon)$ is the uncorrelated density of states of the conduction band, $f(\epsilon)$ is the Fermi function and $A_{\sigma}(\epsilon, \omega')$ is the one-particle spectral density of the total conduction electron Green's function.

Our results for the optical conductivity are shown in figure 4. For t = 0 we have a very good agreement with those of reference [32]. As one can see, the system is an insulator with a large gap in the optical conductivity and the maximum value of $\sigma(\omega)$ coincides with the value of the Hubbard interaction. Once we turn on the transverse field, we observe a spectral transfer from high to low energies, as in the DOS. The spectral transfer closes the gap and increases the conductivity at low frequencies. As we expect, the system is an incoherent metal (no Drude peak feature is found), mainly because the transverse field is not able to completely restore the dynamics of the heavy particles.

Now we turn our attention to figure 5 where we show our results for the dc resistivity at half-filling as a function of the temperature. For $d = \infty$ this quantity is given by the inverse $(1/\sigma(0))$ of the static limit ($\omega = 0$) of equation (8):

$$\sigma(0) = \frac{\pi}{T} \int d\epsilon \ \rho_0(\epsilon) \int d\omega' \ A_{\uparrow}^2(\epsilon, \omega') f(\omega') [1 - f(\omega')]$$
(9)

where T is the temperature.

At t = 0 and U = 2 the dc resistivity shows a semiconducting-like behaviour with temperature. Above T = 0.6, not shown, it starts to increase with T as in a metal. In accordance with our previous results for the insulator-metal transition, the static resistivity decreases as a function of the transverse field. One can clearly see in figure 5 the presence



Figure 4. The zero-temperature optical conductivity for the SH model in the half-filled case for U = 2, and three different values of the applied transverse magnetic field.



Figure 5. The temperature dependence of the static resistivity in the half-filled SH model for U = 2 and different values of t.

of an isosbectic point, where all the curves cross at the same temperature. It is important to mention that a similar behaviour for the static resistivity to the one that we obtain for 0.45 < t < 0.5 has been observed in the normal state of Bi₂Sr₂CuO_y.

In reference [8] the in-plane (ρ_{ab}) and out-of-plane (ρ_c) dc resistivities of Bi₂Sr₂CuO_y have been measured for different values of the magnetic field. The experiment shows completely different behaviours for the in-plane and out-of-plane measurements: ρ_{ab} increases to a certain saturation value, while ρ_c strongly decreases (by a factor of 10⁴) for the same values of the magnetic field. One can understand this contrasting behaviour by considering our results and those of reference [24]. As mentioned before, it was shown in reference [24] that the critical U for the metal–insulator crossover is reduced by the effect of a z-component magnetic field. Thus for the same value of U the system loses its metallic phase as a function of the field and the resistivity increases with the Zeeman field. On the other hand, we show here that a field applied along to the x-direction (in the spin space) drives an insulator-to-metal transition in the system. Since both theoretical results agree with what was observed in the measurements of Ando *et al*, one can conclude that the direction along which the field is applied is crucial for systems with broken spin symmetry.

4. Conclusions

We report the results of the first systematic study of a strongly correlated electron system in transverse fields, undertaken to understand the interplay between on-site correlations and local spin fluctuations. To make contact with experiment we consider the simplified Hubbard (SH) model, a model Hamiltonian with broken spin symmetry. The relevant one-particle Green's functions for this model in the presence of a transverse field t are obtained by means of a perturbative treatment of the hopping and the field around the atomic limit. We employ the *static approximation* to study the insulator-metal transition as a function of t. At intermediate values of the field the metallic phase shows very interesting features. In this regime we observe the presence of sharp peaks in the spectral function of the heavy electrons at the Fermi level. We show that the *static approximation* is very accurate in describing the dynamics of the heavy particles for intermediate and strong values of U.

We have also studied the optical properties of the SH model as a function of the transverse field. Our results for the optical conductivity and static resistivity confirm the insulator-metal crossover. We found good qualitative agreement between our results for the latter quantity and those observed for the out-of-plane resistivity of $Bi_2Sr_2CuO_y$ [8]. In both theoretical and experimental investigations the resistivity decreases as a function of the magnetic field. In addition, we observe in our results the presence of an *isosbectic* point, where all curves cross at the same temperature. This crossing point seems to appear also in the experiment, although it could not be clearly observed because the measurements were done for temperatures slightly below that at which the crossing occurs.

To further our understanding of the semiconducting behaviour along the *c*-axis in cuprates [33], we should mention that in the non-magnetic phase the SH model has an intrinsic disorder built into it. Such disorder is responsible for the non-Fermi-liquid properties of the conduction electrons, since the heavy electrons act as randomly distributed scattering centres. For large values of disorder (*U* in the present model), the motion of the conduction electrons is totally suppressed and the system behaves as a semiconductor, as shown in figure 5 for small values of *t*. According to our results, the semiconducting behaviour can be partially suppressed by enhancing the local spin degrees of freedom through a transverse field. Following this scenario and the measurements of the dc resistivity of $Bi_2Sr_2CuO_y$, one can suggest that the low-temperature semiconducting behaviour in cuprates along the *c*-direction might result from conventional random disorder.

Finally, as a possible extension of this work we should consider in the future the possibility of extending our approach to the case of the one-band Hubbard model. In this case it would be interesting to analyse the effect of the transverse field on the well known Fermi-liquid properties of this model. Furthermore, inspired by the results of figure 1 it would be interesting to analyse whether our perturbation method for the local problem is also accurate in describing the

single-particle properties of the Hubbard model in the large-U limit. Unfortunately, apparently there are no exact results for this model at T = 0 for $d = \infty$, but one can follow the spirit of reference [29] and compare our results for the Matsubara Green's functions with those of finite-temperature quantum Monte Carlo simulations [26]. We believe that the *static approximation* (equation (5)) is an effective approximation for the Hubbard model if we consider that the *local* spin fluctuations are irrelevant in the strong-coupling limit.

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