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ON THE KINETIC EXCHANGE INTERACTIONS IN THE HUBBARD MODEL

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ABSTRACT

We use the canonical transformation method in the Hubbard model to derive the general form of the effective Hamiltonian which includes the virtual hopping from single- to double-occupied sites. The correspondence with the Anderson kinetic exchange Hamiltonian is briefly discussed.

I. INTRODUCTION

The Hubbard model is very useful for the description of two kinds of phenomena due to correlations in narrow bands: band ferromagnetism of metals and alloys, and metal-nonmetal transition[1]. The Hubbard Hamiltonian is:

$$H = \sum_{i \neq j, \sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

with $t_{ij} = t_{ji}^*$. Indices i and j represent lattice sites, while $\sigma = \pm 1$ is a spin quantum number. The operator $a_{i\sigma}^+$ ($a_{i\sigma}$) creates (destroys) an electron with the diagonal spin component $S^z = \sigma/2$ on site i, so $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$ is the operator of particle number on the site i. The first sum in Eq. (1) is usually called the hopping term and expresses the movement of an electron with $S^z = \sigma/2$ from site j to site i. The hopping term is written in the Wannier representation and it stands for the kinetic energy of electrons plus the energy due to the attractive periodic potential. The larger the contribution of this sum to the total energy of the system, the more freely the electrons move through the lattice and form proportionally wider bands. In the tight binding approximation we limit ourselves to the hopping between the nearest neighbours $\langle i,j \rangle$ and then we put $t_{\langle i,j \rangle} = t < 0$.

The second sum in Eq. (1) describes the Coulomb repulsion between electrons with opposite spins on the same lattice site. In the nondegenerate Hubbard model each atom has only single orbital atomic state available for electrons (i.e. of 1s type), which can hold up to two electrons

with opposite spins, as it can be seen from Eq. (1).

The Coulomb and exchange interactions between electrons located on different sites are neglected in the traditional Hubbard treatment[1]. However, the intersite interactions come out also from the Hubbard Hamiltonian (1) if the Coulomb repulsion U is strong enough. A part of them is a spin-spin interaction of the Heisenberg form (i.e. $\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j$), and after Anderson[2] is called the kinetic exchange interaction. The concept of the kinetic exchange interaction is shortly summarized in Sec.II.

In Sec.III we obtain an explicit form of the effective Hamiltonian with the virtual hopping from single- to double-occupied sites included in it, using the canonical transformation method.

Sec.IV consists of conclusions.

II. THE CONCEPT OF THE KINETIC EXCHANGE INTERACTIONS

It could have been expected that even for small t and for the case of one electron per atom (i.e. for n = 1), the band is half-filled. In fact, the situation is more complex. In the atomic limit, i.e. for noninteracting atoms (t = 0), each atom has two energy levels which are split by U. So in the ground state for n = 1 only lower levels are filled. Similarly, when $|t| \ll U$ electrons fill only the lower energy level which is broadened by the interaction and forms a narrow band. Thus a system at the temperature T = 0 can remain an insulator, due to an increase of the electrostatic energy by the amount pU, where p is a number of double occupied sites. Such an insulating

system, while $t \neq 0$, is called the Mott insulator[3]. It is important then to ask about the spin configuration of this system. From that reason our aim in this paper is to construct an effective Hamiltonian in which the spin degeneracy existing in the atomic limit is removed. The method adopted to the problem is also applicable if $n \neq 1$, i.e. for a partially filled band. As we shall see it gives results which are more general than the approach based on the perturbation theory[2,4]. In fact, in the latter case the Heisenberg-type interaction was derived from the Hubbard model for $n=1$[2] and thus the total Hamiltonian is of the form:

$$ H = \sum_{\substack{\langle i,j \rangle \\ \sigma}} t\, a^{+}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{2t^2}{U} \sum_{\langle i,j \rangle} \underset{\sim}{S_i} \cdot \underset{\sim}{S_j} , \tag{2}$$

where $S_i = (S^{+}_i, S^{-}_i, S^{z}_i)$, $S^{+}_i = a^{+}_{i\uparrow} a_{i\downarrow}$, $S^{-}_i = a^{+}_{i\downarrow} a_{i\uparrow}$, and $S^{z}_i = (n_{i\uparrow} - n_{i\downarrow})/2$. The last term in Eq. (2) is called the kinetic exchange interaction and is only a part of the Heisenberg Hamiltonian[2]. The case of the Mott insulator, when the operator $n_i = n_{i\sigma} + n_{i-\sigma} = 1$, is not easily visible in Eq. (2) since the hopping term is always present whenever $t \neq 0$. We will show that in the case of the Mott insulator our effective Hamiltonian reduces strictly to the Hamiltonian of the Anderson kinetic exchange[2]. In a perturbative approach the Mott insulator was discussed taking the whole hopping term as a perturbation. With the help of the canonical transformation method we remove the part of it connected with transitions from single- to double-occupied sites only, and we replace it by the spin-dependent inter-

site interactions between electrons.

III. THE EFFECTIVE HAMILTONIAN

The essential feature of the theory which we would like to develop now is that we take into account ab initio the fact that intra-atomic forces are sufficiently strong ($|t| \ll U$), to prevent two electrons of opposite spins from occupying the same atomic site, except in virtual transitions[4]. To start with we divide the site-occupation number Hilbert space into two subspaces: the first one which includes states with occupation number $n_i = 0$ and 1 in each lattice site i, and the hopping between them, and the second one - the subspace of double-occupied sites $(n_{i\sigma} = n_{i-\sigma} = 1)$, and the hopping between them. Next we treat the hopping between these subspaces as a perturbation which we want to eliminate by the properly chosen unitary transformation of the Hamiltonian. Such a transformation has been recently considered by Stevens[5]. Following his concept, and with the help of the identity:

$$t\sum_{\substack{\langle i,j \rangle \\ \sigma}} a_{i\sigma}^{+} a_{j\sigma} = t\sum_{\substack{\langle i,j \rangle \\ \sigma}} a_{i\sigma}^{+}\left(1 - n_{i\sigma} + n_{i-\sigma}\right) a_{j\sigma}\left(1 - n_{j-\sigma} + n_{j-\sigma}\right),$$

$$(3)$$

we divide the hopping part of the Hamiltonian (1) into terms which operate in particular subspaces or transform the electron from one to the other. For convenience we write the full Hamiltonian as four terms: a projection of it onto the first subspace $(P_O H P_O)$, onto the second subspace $(P_N H P_N)$, and the mixing term $(P_O H P_N + P_N H P_O)$, where P_O and P_N are

projection operators of the first and second subspaces, respectively $(P_O + P_N = 1)$:

$$H = P_O H P_O + P_N H P_N + P_O H P_N + P_N H P_O , \tag{4}$$

where:

$$P_O H P_O = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ (1 - n_{i-\sigma}) a_{j\sigma} (1 - n_{j-\sigma}) , \tag{4a}$$

$$P_N H P_N = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ n_{i-\sigma} a_{j\sigma} n_{j-\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} , \tag{4b}$$

$$P_O H P_N = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ (1 - n_{i-\sigma}) a_{j\sigma} n_{j-\sigma} , \tag{4c}$$

and

$$P_N H P_O = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ n_{i-\sigma} a_{j\sigma} (1 - n_{j-\sigma}) . \tag{4d}$$

Let us define the operator:

$$H_\epsilon = H_O + \epsilon H_1 , \tag{5}$$

where $H_O = P_O H P_O + P_N H P_N$, $H_1 = H - H_O$, and which reproduces the Hamiltonian H for $\epsilon = 1$. We look for a transformation:

$$H_\epsilon \rightarrow \mathcal{H}_\epsilon = e^{-i\epsilon S} H_\epsilon e^{i\epsilon S} , \tag{6}$$

with $S = S^+$, such that $\mathcal{H}_\epsilon$ has all its off-diagonal elements of order less than ϵ . Of course, the effective Hamiltonian $\mathcal{H} = \mathcal{H}_{\epsilon=1}$. Assuming that:

$$e^{i\epsilon S} \simeq 1 + i\epsilon S - \frac{1}{2}\epsilon^2 S^2, \qquad (7)$$

we obtain terms up to order $\sim \epsilon^2$:

$$\mathcal{H}_\epsilon \simeq H_o + \epsilon \left(H_1 + i[H_o, S] \right) +$$
$$- \frac{1}{2}\epsilon^2 \left(2i[H_1, S] - [[H_o, S], S] \right). \qquad (8)$$

The linear term $\sim \epsilon$ is absent when:

$$H_1 + i[H_o, S] = 0. \qquad (9)$$

This condition substituted into Eq. (8) gives:

$$\mathcal{H}_\epsilon \simeq H_o + \frac{1}{2} i\epsilon^2 [H_1, S]. \qquad (10)$$

Eq. (9) may be solved with respect to S. It can be projected onto subspaces and thus can be written as:

$$P_o H_1 P_N + i P_o [H_o, S] P_N = 0, \qquad (9a)$$

$$P_o (H_o S - S H_o) P_o = 0, \qquad (9b)$$

$$P_N (H_o S - S H_o) P_N = 0. \qquad (9c)$$

Eq. (9b) and (9c) are satisfied if we put $P_o S P_o = P_o$ and $P_N S P_N = P_N$. It is the only solution of these equations because $P_o [H_o, S] P_N \neq 0$ and thus S is not a function

of H_0, but commutes with it when projected onto subspaces. With regard to that we have:

$$P_0 S P_N = \left[-i\, P_0 H_1 P_N + (P_0 H P_0)(P_0 S P_N) \right] (P_N H P_N)^{-1}. \qquad (11)$$

One may solve this equation by the following iteration procedure. Assuming that on the r.h.s. of Eq. (11) $P_0 S^{(0)} P_N = 0$ we get an expression for $P_0 S^{(1)} P_N$; next substituting $P_0 S^{(1)} P_N$ to the r.h.s. of Eq. (11) we obtain an expression for $P_0 S^{(2)} P_N$, etc. Iterating up to infinite order we construct a geometric progression, which leads to the final formula for $P_0 S P_N$ of the form: $\qquad (12)$

$$P_0 S P_N = -i\, P_0 H P_N \left(P_N H P_N - P_0 H P_0 \right)^{-1}.$$

The simplest approximation of $(P_N H P_N - P_0 H P_0)$ is the replacement of it by the energy difference between centers of gravity of two subbands which is equal $\Delta \simeq U$. So from Eq. (11):

$$P_0 S P_N \simeq -i\, U^{-1} \left(P_0 H P_N \right), \qquad (13)$$

and with regard to Eq. (10) we have:

$$\mathcal{H} = P_0 \mathcal{H} P_0 + P_N \mathcal{H} P_N , \qquad (14)$$

where:

$$P_0 \mathcal{H} P_0 = P_0 H P_0 - U^{-1} P_0 H P_N H P_0 , \qquad (15a)$$

$$P_N \mathcal{H} P_N = P_N H P_N + U^{-1} P_N H P_o H P_N .$$

(15b)

Substituting Eq. (4c) and Eq. (4d) to Eq. (15a) and (15b), we get after some manipulations and neglecting terms connecting more than two lattice sites:

$$P_o \mathcal{H} P_o = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ (1 - m_{i-\sigma}) a_{j\sigma} (1 - m_{j-\sigma}) +$$

$$+ \frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma} \left[S_i^\sigma S_j^{-\sigma} - m_{i\sigma}(1 - m_{i-\sigma}) n_{j-\sigma}(1 - m_{j\sigma}) \right],$$

(16)

$$P_N \mathcal{H} P_N = t \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^+ m_{i-\sigma} a_{j\sigma} n_{j-\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} +$$

$$+ \frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma} n_{i\sigma} m_{i-\sigma} (1 - m_{j-\sigma})(1 - m_{j\sigma}) ,$$

(17)

where $S_i^\sigma = S_i^\pm$ for $\sigma = \pm 1$, respectively. The part (17) of the effective Hamiltonian does not influence the magnetic state in the case $|t| \ll U$ and $|t| \gg k_B T$ (which means that $\langle n_{i\sigma} \rangle \simeq \langle \nu_{i\sigma} \rangle$), and thus can be neglected. So the effective magnetic Hamiltonian H_M can be rewritten with new operators introduced:

(18)

$$b_{i\sigma} = a_{i\sigma} (1 - m_{i-\sigma}), \quad \nu_{i\sigma} = b_{i\sigma}^+ b_{i\sigma} ,$$

in the final form as:

$$H_M = t \sum_{\langle i,j \rangle, \sigma} b_{i\sigma}^+ b_{j\sigma} + \frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma} \left[S_i^\sigma S_j^{-\sigma} - \nu_{i\sigma} \nu_{j-\sigma} \right].$$ (19)

The new operators $b_{i\sigma}^+$ and $b_{i\sigma}$ fulfill anticommutation relations:

Correction

$$[b_{i\sigma}, b_{j\sigma'}^+]_+ = \delta_{ij}\left[\delta_{\sigma\sigma'}(1-n_{i-\sigma}) + S_i^{\bar{\sigma}}(1-\delta_{\sigma\sigma'})\right)$$

$$[b_{i\sigma}, b_{j\sigma'}^+] = 0. \tag{20}$$

In the particular case of the Mott insulator $n_{i\sigma} = 1-n_{i-\sigma}$, and H_M reduces to the Heisenberg Hamiltonian with positive exchange interactions due to the kinetic exchange. Therefore, the derived here Hamiltonian (19) can be considered as a generalization of the Anderson kinetic exchange Hamiltonian to the case $n_i \neq 1$.

IV. CONCLUSIONS

Let us summarize shortly the main points of this paper. We have applied the canonical transformation method in a nonstandard situation, namely we have not assumed that H_0 is diagonal. The canonical transformation has been used to construct the effective Hamiltonian in which the spin degeneracy of the Hubbard model is removed. For this purpose we have divided (projected) the hopping term in Eq. (1) into four parts connected with hopping from single- to double-occupied sites and vice-versa by the spin-dependent intersite interactions. The obtained formula (19) for these interactions reduces to the Anderson kinetic exchange[2] for the Mott insulator which is not the case in the perturbational approach[4]. Moreover, the canonical transformation method is more universal than the perturbation theory in this sense that it renormalizes the ground state of the sys-

tem. It means that we replace interactions between bare
particles by interactions between quasiparticles. The same
method has been applied in the theory of superconductivity
where attractive interactions between electrons are con-
structed from electron-photon interaction[6].

However, we have considered here the case when
$|t| \ll U$ only, so the metallic phase, after the Mott
transition, is beyond the scope of this paper. It requires
the inclusion of real hopping from single- to double-oc-
cupied sites which has been here discarded by the canoni-
cal transformation. Analogical problem occurs in the BCS
theory[6] which is not appropriate for the description of
a normal metallic phase above the critical temperature T_c.
Since we have replaced the hopping between single- and
double-occupied sites by the virtual hopping, the only con-
clusion about nonmetal-metal transition which can be drawn
from the theory presented here is that transition to the
metallic state cannot occur in a magnetically ordered
state.

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APPENDIX

The closed form of our Hamiltonian (19)

$$\nu_{i\sigma} = \frac{\nu_i}{2} + \sigma S_i^z$$

$$S_i^+ S_j^- + S_i^- S_j^+ \cdot \sum_\sigma \nu_{i\sigma}\, \nu_{j-\sigma} \; =$$

$$\nu_{i\uparrow} + \nu_{i\downarrow} = \nu_i$$

$$\frac{(\nu_{i\uparrow} - \nu_{i\downarrow})}{2} = S_i^z$$

$$S_i^- S_j^+ + S_i^+ S_j^- \cdot \sum_\sigma \left(\frac{\nu_i}{2} + \sigma S_i^z\right)\left(\frac{\nu_j}{2} - \sigma S_j^z\right)$$

$$= S_i^+ S_j^- + S_i^- S_j^+ \cdot 2\frac{\nu_i \nu_j}{4} + 2 S_i^z S_j^z$$

$$= 2\left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) - \frac{\nu_i \nu_j}{4}\right]$$

$$= 2\left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}\nu_i \nu_j\right)$$

$$\boxed{\tilde{\mathcal{H}}_M = t \sum_{\langle ij\rangle\sigma} b_{i\sigma}^+ b_{j\sigma} + \frac{2t^2}{U} \sum_{\langle ij\rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}\nu_i \nu_j\right)}$$

$$- \frac{t^2}{U} \sum_{\substack{ik \\ j(i,k)}} n_{k-\sigma} a_{k\sigma}^\dagger a_{j\sigma} a_{j\sigma}^\dagger (1 - n_{j-\sigma}) a_{i\sigma}(1 - n_{i-\sigma})$$

will produce hopping of Anderson singlet pairs (a 1987)

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