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Derivation of the *t*-*J* model: Electron spectrum and exchange interactions in narrow energy bands

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A derivation of the *t*-*J* model of a highly-correlated solid is given starting from the general many-electron Hamiltonian with explicit picking out of the corrections owing to the nonorthogonality of atomic wave functions. Asymmetry of the Hubbard subbands (i.e., of ''electron'' and ''hole''cases) for a nearly half-filled bare band is demonstrated. The nonorthogonality effects are shown to lead to strong modifications of indirect antiferromagnetic exchange interaction in the limit of large on-site Coulomb repulsion. Consequences of this treatment for the magnetism formation in narrow energy bands are discussed. Peculiarities of the case of ''frustrated'' lattices, which contain equilateral triangles of nearest neighbors, are considered. [S0163-1829(98)02818-5]

The problem of strong correlations and magnetism in many-electron (ME) systems is one of the most important in solid state theory. Derivation of the simplest ME model describing these phenomena in the case of narrow energy bands (strong Coulomb interaction) was proposed by Hubbard.[1] This model was studied in a great number of papers.

A detailed investigation of ferromagnetism in the Hubbard model in the limit of the infinite on-site Coulomb repulsion U was performed by Nagaoka.[2] He proved rigorously that the ground state for the simple cubic and bcc lattices in the nearest-neighbor approximation with the number of electrons $N_e = N \pm 1$, N being the number of lattice sites, possesses maximum total spin, i.e., is saturated ferromagnetic (FM), since this ordering provides the maximum kinetic energy gain for an excess electron (hole). (The same statement holds for the fcc and hcp lattices with the transfer integral $t<0$, $N_e = N+1$, or $t>0$, $N_e = N-1$.) The picture of saturated ferromagnetism is preserved at small, but finite concentrations of current carriers $c = |N_e/N - 1|$. In the case of a half-filled band ($N_e = N$), $|t| \ll U$ the ground state is antiferromagnetic (AFM) because of the Anderson's kinetic exchange (superexchange) interaction[3] which occurs in the second order in $|t|/U$. This interaction is due to the gain in the kinetic energy at virtual transitions of an electron to a neighbor site, which are possible provided that the electron at that site has an opposite spin direction. In systems with a large finite U and $N_e \neq N$, a competition between FM and AFM ordering occurs. Nagaoka[2] has put forward a criterion of ferromagnetism, which was based on the condition of the spin-wave spectrum stability. This criterion has the form

$$\alpha c > |t|/U, \tag{1}$$

where the constant α of the order of unity depends on the lattice structure, $\alpha = 0.246$ for the simple cubic lattice. At the same time, pure antiferromagnetism is stable at $N_e = N$ only, and a phase separation[4] takes place provided that the condition (1) is violated. Although other points of view concerning stability of ferromagnetism in the thermodynamic limit at $U = \infty$ are discussed now (see, e.g., Ref. 5), Nagaoka's picture seems to be reasonable (in particular, the magnon spectrum can be calculated also from the spin Green's function, see, e.g., Ref. 6).

A version of the Hubbard model in the limit $U \to \infty$ with inclusion of the AFM exchange interaction J, the t-J model, is widely applied now to describe copper-oxide high-T_c superconductors and related systems (see the review[7]). The quantity J is usually related to the Anderson's exchange ($J = -2t^2/U$), but sometimes it is considered as an independent phenomenological parameter. Recently the difference between the t-J model and large-U expansion of the Hubbard model has been discussed.[8]

At derivation of his model[1] Hubbard used the orthogonal Wannier functions. At the same time, in the limit of large U it is more natural to use well-localized atomic wavefunctions and the atomic representation,[9] so that effects of nonorthogonality of atomic wave functions occur (in the first paper[1] Hubbard neglected the difference between the Wannier and atomic wave functions at constructing the interpolation solution starting from the atomic limit). In the present paper we discuss a consistent formulation of a general ME model with strong correlations with explicit account of nonorthogonality effects and treat the electron spectrum picture and magnetism formation in this model.

We start from the general Hamiltonian of the ME system in a crystal

$$\mathcal{H} = \sum_i \left(-\frac{\hbar^2}{2m} \Delta_{\mathbf{r}_i} + V(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{2}$$

where

$$V(\mathbf{r}) = -\sum_\nu \frac{Ze^2}{|\mathbf{r} - \mathbf{R}_\nu|} = \sum_\nu v(\mathbf{r} - \mathbf{R}_\nu) \tag{3}$$

is the periodic crystal potential. For simplicity, we consider a single nondegenerate band that is formed by s-type wave functions, although this set is incomplete. The atomic states with different principal and orbital quantum numbers can be included in a similar way.[10,11] However, the case, where additional orbital-degenerate bands are present, is not expected to yield qualitatively different results (effects of hybridization with p, d, . . . -like states are irrelevant for the Hubbard model situation).

To pass to the second quantization representation we have to use orthogonal wave functions. However, the atomic wave functions $\varphi_\sigma(\mathbf{r},s)=\varphi(\mathbf{r})\chi_\sigma(s)$ (s is the spin coordinate) do not satisfy this condition at different sites ν, which can lead to some difficulties.[3,12–14] We apply the orthogonalization procedure developed by Bogoliubov[12] (see also Ref. 14), which enables one to construct perturbation theory in the overlap of atomic wavefunctions belonging to different lattice sites. To lowest order in this parameter the orthogonalized functions read

$$\psi_\nu(\mathbf{r})=\varphi_\nu(\mathbf{r})-\frac{1}{2}\gamma\sum_{\nu'\neq\nu}\varphi_{\nu'}(\mathbf{r}), \tag{4}$$

where the sum goes over the nearest neighbors,

$$\gamma=\gamma_{\nu\nu'}=\int d\mathbf{r}\varphi^*_{\nu'}(\mathbf{r})\varphi_\nu(\mathbf{r}) \tag{5}$$

is the nonorthogonality integral. Using the orthogonality of the spin wave functions $\chi_\sigma(s)$ and calculating the matrix elements of the Hamiltonian (2) for the functions (4) we obtain the ME Hamiltonian of the ‘‘polar model’’ (Refs. 15,12,16)

$$\begin{aligned}\mathcal{H}=\varepsilon\sum_{\nu\sigma}a^\dagger_{\nu\sigma}a_{\nu\sigma}+&\sum_{\nu_1\neq\nu_2,\sigma}t_{\nu_1\nu_2}a^\dagger_{\nu_1\sigma}a_{\nu_2\sigma}\\&+\frac{1}{2}\sum_{\nu_i\sigma_1\sigma_2}I_{\nu_1\nu_2\nu_3\nu_4}a^\dagger_{\nu_1\sigma_1}a^\dagger_{\nu_2\sigma_2}a_{\nu_4\sigma_2}a_{\nu_3\sigma_1},\end{aligned} \tag{6}$$

where

$$\varepsilon=\int d\mathbf{r}\phi^*_\nu(\mathbf{r})\left[-\frac{\hbar^2}{2m}\Delta+v(\mathbf{r}-\mathbf{R}_\nu)\right]\phi_\nu(\mathbf{r}) \tag{7}$$

is the one-electron level in the central potential of a given site $v(\mathbf{r})$,

$$\begin{aligned}t_{\nu_1\nu_2}&=\int d\mathbf{r}\psi^*_{\nu_1}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\Delta+V(\mathbf{r})\right)\psi_{\nu_2}(\mathbf{r})\\&\simeq\int d\mathbf{r}\phi^*_{\nu_1}(\mathbf{r})v(\mathbf{r}-\mathbf{R}_{\nu_1})\phi_{\nu_2}(\mathbf{r})\end{aligned} \tag{8}$$

are the transfer matrix elements between the sites ν_1 and ν_2, and

$$I_{\nu_1\nu_2\nu_3\nu_4}=\int d\mathbf{r}d\mathbf{r}'\psi^*_{\nu_1}(\mathbf{r})\psi^*_{\nu_2}(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\psi_{\nu_3}(\mathbf{r})\psi_{\nu_4}(\mathbf{r}') \tag{9}$$

are the matrix elements of interelectron Coulomb repulsion. We have neglected in (7) and (8) the influence of potentials of the sites $\nu'\neq\nu$ and $\nu'\neq\nu_1,\nu_2$, respectively, since the corresponding terms contain extra factors $v(\mathbf{r}-\mathbf{R}_{\nu'})\psi_\nu(\mathbf{r})$ with $\nu'\neq\nu$ which are small due to the decrease of the potential $v(\mathbf{r})$ with increasing r (in other words, the crystal potential is small in the region between the lattice sites). We have also dropped in (8) small integrals which contain $v(\mathbf{r}-\mathbf{R}_{\nu'})|\psi_\nu(\mathbf{r})|^2$.

Further we retain in (6) only one- and two-site terms and pass to the representation of the Hubbard operators $X_\nu(\lambda',\lambda)$,[9] which transform the state $|\lambda\rangle$ ($\lambda=0,\sigma,2$) at the site ν into $|\lambda'\rangle$,

$$a^\dagger_{\nu\sigma}=X_\nu(\sigma,0)+\sigma X_\nu(2,-\sigma). \tag{10}$$

Then we derive

$$\begin{aligned}\mathcal{H}=\varepsilon\sum_{\nu\sigma}X_\nu(\sigma,\sigma)&+U\sum_\nu X_\nu(2,2)\\&+\sum_{\nu_1\neq\nu_2,\sigma}\{t^{(00)}_{\nu_1\nu_2}X_{\nu_1}(\sigma,0)X_{\nu_2}(0,\sigma)\\&+t^{(22)}_{\nu_1\nu_2}X_{\nu_1}(2,\sigma)X_{\nu_2}(\sigma,2)+\sigma[t^{(02)}_{\nu_1\nu_2}X_{\nu_1}(\sigma,0)X_{\nu_2}(-\sigma,2)\\&+X_{\nu_1}(2,-\sigma)X_{\nu_2}(0,\sigma)]\}+\sum_{\nu_1\neq\nu_2}\left\{Q_{\nu_1\nu_2}n_{\nu_1}n_{\nu_2}\right.\\&\left.-J_{\nu_1\nu_2}\left[\frac{1}{2}+2(\mathbf{S}_{\nu_1}\mathbf{S}_{\nu_2})\right]\right\},\end{aligned} \tag{11}$$

where $U=I_{\nu\nu\nu\nu}$ and $Q_{\nu_1\nu_2}=I_{\nu_1\nu_2\nu_1\nu_2}$are the Hubbard parameter and the Coulomb integral at different lattice sites,

$$t^{(00)}_{\nu_1\nu_2}=t_{\nu_1\nu_2}, \tag{12}$$

$$t^{(22)}_{\nu_1\nu_2}=t_{\nu_1\nu_2}+2I_{\nu_1\nu_1\nu_2\nu_1}, \tag{13}$$

$$t^{(02)}_{\nu_1\nu_2}=t^{(20)}_{\nu_1\nu_2}=t_{\nu_1\nu_2}+I_{\nu_1\nu_1\nu_2\nu_1} \tag{14}$$

are the transfer integrals for empty states (holes) $|0\rangle$ and doubly occupied states (doubles) $|2\rangle$, and the integral of the double-hole pair creation,

$$n_\nu=\sum_\sigma n_{\nu\sigma}=\sum_\sigma a^\dagger_{\nu\sigma}a_{\nu\sigma}=\sum_\sigma[X_\nu(\sigma,\sigma)+X_\nu(2,2)].$$

Note that the quantity $t^{(02)}$, which enters the expression for the superexchange parameter, coincides with the Hartree-Fock value of the transfer integral for a half-filled band in the AFM state.

Hierarchy of the parameters of the Hamiltonian (6) is discussed in Ref. 1. In the expressions for ε, U, and Q the nonorthogonality corrections are small in the overlap and do not play a role. On the other hand, at calculating other parameters in (11) we have to take into account the second term in (4). We obtain for the integral of the ‘‘direct’’ exchange

$$J_{\nu_1\nu_2}=I_{\nu_1\nu_2\nu_2\nu_1}=\tilde{J}_{\nu_1\nu_2}-2\gamma_{\nu_1\nu_2}L_{\nu_1\nu_2}+\frac{1}{2}(U+Q_{\nu_1\nu_2})\gamma^2_{\nu_1\nu_2}, \tag{15}$$

where

$$\tilde{J}_{\nu_1\nu_2}=\tilde{I}_{\nu_1\nu_2\nu_2\nu_1},\quad L_{\nu_1\nu_2}=\tilde{I}_{\nu_1\nu_1\nu_2\nu_1}, \tag{16}$$

the integrals $\tilde{I}$ being calculated for the atomic functions φ. The expressions (12)–(14) take the form

$$t_{\nu_1\nu_2}^{(00)}=t_{\nu_1\nu_2}, \tag{17}$$

$$t_{\nu_1\nu_2}^{(22)}=t_{\nu_1\nu_2}+2L_{\nu_1\nu_2}-(U+Q_{\nu_1\nu_2})\gamma_{\nu_1\nu_2}, \tag{18}$$

$$t_{\nu_1\nu_2}^{(02)}=t_{\nu_1\nu_2}+L_{\nu_1\nu_2}-\frac{1}{2}(U+Q_{\nu_1\nu_2})\gamma_{\nu_1\nu_2}. \tag{19}$$

All the terms in (15), as well as in (17)–(19), are of the same (first) order in the overlap. Moreover, the quantity $U\gamma$ should be larger than $L,Q\gamma,\tilde{J}/\gamma$, and $|t|$. Indeed, in the case of narrow bands the interelectron repulsion (which determines $U,Q,\tilde{J}$, and L) and the crystal potential (which determines ε and t) are of the same order of magnitude, although the crystal potential is expected to be somewhat larger. At the same time, as follows from (8), (9), t (or $Q,\tilde{J}$, and L) contain another small factor that was considered above: these integrals include the product of the function $\phi_\nu(\mathbf{r})$ by the potential $v(\mathbf{r}-\mathbf{R}_{\nu'})$ (or the Coulomb repulsion) corresponding to another lattice site, which ‘‘cuts’’ a rather small region $\mathbf{r}\simeq\mathbf{R}_{\nu'}$. Thus the ‘‘on-site Coulomb’’ (nonorthogonality) contributions should dominate in (18) and (19).

It should be noted that in fact the transfer integrals (18) and (19) are to be calculated with the use of many-electron wave functions (see the review[10]) which are not, generally speaking, reduced to the Slater determinants and factorized into one-electron ones. For example, the general Hartree-Fock approximation in the atom theory (see Ref. 17) uses the radial ‘‘one-electron’’ wave functions which depend explicitly on the ME atomic term $|\Gamma\rangle$. The transfer integrals are expressed through the corresponding ME wave functions as[10]

$$t_{\nu_1\nu_2}(\Gamma\Gamma',\Gamma''\Gamma''')=\int\prod d\{\mathbf{r}_is_i\}\Psi^*_{\nu_1\Gamma}\Psi^*_{\nu_2\Gamma''}\times\sum_i\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i}+V(\mathbf{r}_i)\right)\Psi_{\nu_1\Gamma'}\Psi_{\nu_2\Gamma'''}. \tag{20}$$

Therefore the integrals (17) and (19) can be different even at neglecting interatomic Coulomb interactions and nonorthogonality.

The electron spectrum of the model (11) in the simplest ‘‘Hubbard-I’’ approximation[1] (which corresponds to a ‘‘mean-field approximation’’ in the electron hopping, the on-site Coulomb repulsion being taken into account in the zero-order approximation) is given by[10]

$$\begin{aligned}E_{\mathbf{k}\sigma}^{(1,2)}&=\varepsilon+\frac{1}{2}[t_{\mathbf{k}}^{(22)}\langle n_{-\sigma}\rangle+t_{\mathbf{k}}^{(00)}(1-\langle n_{-\sigma}\rangle)+U]\\&\mp\frac{1}{2}\{[t_{\mathbf{k}}^{(22)}\langle n_{-\sigma}\rangle-t_{\mathbf{k}}^{(00)}(1-\langle n_{-\sigma}\rangle)-U]^2\\&+4(t_{\mathbf{k}}^{(02)})^2\langle n_{-\sigma}\rangle(1-\langle n_{-\sigma}\rangle)\}^{1/2}.\end{aligned} \tag{21}$$

One can see that, unlike the standard consideration,[1] the Hubbard subbands (21) turn out to have quite different widths even in the paramagnetic case for a nearly half-filled band ($\langle n_+\rangle=\langle n_-\rangle\simeq 1/2$). In particular, in the large-U limit we have

$$E_{\mathbf{k}\sigma}^{(1)}=\varepsilon+(1-\langle n_{-\sigma}\rangle)t_{\mathbf{k}}^{(00)},\quad E_{\mathbf{k}\sigma}^{(2)}=\varepsilon+t_{\mathbf{k}}^{(22)}\langle n_{-\sigma}\rangle+U \tag{22}$$

so that, according to (17),(18), the bare hopping integral t determines the bandwidth of ‘‘holes,’’ and the bandwidth of ‘‘doubles’’ is mainly (in the above-discussed sense) determined by the intrasite Coulomb interaction and nonorthogonality integral (5). Thus an appreciable asymmetry of the cases $N_e<N$ and $N_e>N$ can occur, the bandwidth in the case of hole conductivity being considerably smaller than in the electron (double) case. This circumstance may be important, e.g., for copper-oxide high-T_c superconductors (note that an asymmetry can occur due to other reasons in the case of degenerate d bands; see, e.g., Ref. 18). Of course, the approximation (21) yields a very rough description of the electron spectrum, and more advanced approximations should be used in the AFM state, especially in the two-dimensional case. In the latter situation, the low-energy electron spectrum is determined by the scale J rather than t (see Ref. 19).

Generally speaking, we have to take into account in (11) also three-site ‘‘operator’’ Coulomb contributions to the transfer integrals,

$$\delta t_{\nu_1\nu_2}^{(\lambda\mu)}=\sum_{\nu'\neq\nu_1,\nu_2}I_{\nu_1\nu'\nu_2\nu'}n_{\nu'}. \tag{23}$$

The quantity $\tilde{I}_{\nu_1\nu'\nu_2\nu'}$ is small in comparison with $L_{\nu_1\nu_2}=\tilde{I}_{\nu_1\nu_1\nu_2\nu_1}$ due to the decrease of the Coulomb interaction with distance. A peculiar situation occurs in the case of a ‘‘frustrated’’ lattice where equilateral triangles of nearest neighbors are present (e.g., the triangular, fcc, and hcp lattices), so that the site ν' can be the nearest neighbor for both the sites ν_1 and ν_2. Then substituting (9) into (23) yields the nonorthogonality correction of order of $U\gamma$. Such corrections are important for the calculation of electron spectrum (e.g., in the ‘‘Hubbard-I’’ approximation) and yield a suppression of the above-considered asymmetry of the hole and double subbands. In such situations, additional three-site ‘‘exchange’’ terms also arise.[11]

The kinetic exchange (Anderson's superexchange) interaction occurs in the second order in $t_{\nu_1\nu_2}^{(02)}$. Performing the canonical transformation which excludes the double-hole pair creation and annihilation terms from the Hamiltonian (11) we derive

$$\mathcal{H}^{(2)}=\sum_{\nu_1\nu_2}\frac{(t_{\nu_1\nu_2}^{(02)})^2}{U}\{4(\mathbf{S}_{\nu_1}\mathbf{S}_{\nu_2})-1\}. \tag{24}$$

As follows from (19), the numerator in (24) is determined not only by the bare hopping, but also by the Coulomb interaction. The kinetic exchange interaction survives even in the limit $U\rightarrow\infty$ owing to the nonorthogonality contributions (of course, this limit can be treated only as a formal one, since in fact γ vanishes for $U\rightarrow\infty$). Combining (24) and (15) we obtain the expression for the total effective exchange parameter in the case of a half-filled band ($c=0$)

$$J_{\mathrm{eff}}=J-2(t^{(02)})^2/U=\tilde{J}-\gamma^2 Q+2\gamma t-2(t+L)^2/U. \tag{25}$$

Note that the terms of the order of $\gamma^2 U$ are canceled in J_{eff}. First three terms in (25) coincide with the corresponding result for the two-site problem (hydrogen molecule) (Ref. 20) and yield an AFM exchange interaction. As mentioned above, the crystal potential should be somewhat larger than the Coulomb interaction, and in the large-U limit the main contribution to J_{eff} reads

$$J_{\mathrm{eff}}\simeq -2\gamma|t|, \tag{26}$$

where t is assumed to be negative. We see that in the case $N_e<N$ the ratio of J_{eff} to bandwidth is proportional to the overlap parameter (rather than to $|t|/U\ll\gamma$ as in the standard consideration). High values of the Néel temperature, which are typical for the layered copper-oxide systems, may be related to this fact.

By analogy with the consideration of Ref. 2 we have the criterion of ferromagnetism

$$2\alpha c|t^{(\lambda\lambda)}|>-J_{\mathrm{eff}}, \tag{27}$$

where $\lambda=0$ for $N_e<N$ and $\lambda=2$ for $N_e>N$. Under the assumption $\gamma\gg|t|/U\gg\gamma^2$ the criterion (27) takes the form

$$\alpha c>\begin{cases}-J_{\mathrm{eff}}/(2|t|)\simeq\gamma, & N_e<N\\ -J_{\mathrm{eff}}/(\gamma U)\simeq 2|t|/U, & N_e>N,\end{cases} \tag{28}$$

which is quite different from (1) for $N_e<N$. In the case $N_e>N$ the result (28) is formally similar to (1), but has a different origin.

We see that a strong indirect AFM interaction occurs in narrow energy bands, the FM exchange owing to the motion of current carriers being more strongly suppressed in the case of ‘‘hole’’ conductivity ($N_e<N$) than in the ‘‘electron’’ case. The situation may change considerably in the case of a degenerate energy band where the indirect interaction can be ferromagnetic owing to the intraatomic Hund exchange.[23,10] Note that the degeneracy effects are often assumed to be essential also for the usual itinerant magnetism (see, e.g., Ref. 20).

From the experimental point of view, the narrow-band ferromagnetism is not a too wide-spread phenomenon. It takes place, e.g., in the systems $\mathrm{Fe}_{1-x}\mathrm{Co}_x\mathrm{S}_2$,[21] CoS_2, and CrO_2.[22] However, degeneracy of the conduction band plays an important role in the electron structure of these systems. At the same time, ferromagnetism is not observed in the copper-oxide systems. The above-discussed modifications (in comparison with the original Hubbard's treatment[1]) in formulation of the simplest s-band model and similar considerations of more realistic models (see, e.g., Refs. 7,24) may be useful for explaining this fact.

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