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GENERALIZED TIGHT BINDING METHOD FOR SCES AS A PERTURBATIVE REALIZATION OF THE EXACT LEHMANN REPRESENTATION*

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Both perturbation approach in the Hubbard operator representation and the exact Lehmann representation proves that the electron quasiparticle in SCES has spin $S = 1/2$, electric charge e, QP energy and QP spectral weight split over various QP bands. General theory and its application to the hole doped $\mathrm{CuO_2}$ layer are considered.

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1. Introduction

Conventional single electron approach (LDA-like) fails to describe electron properties of strongly correlated electron systems (SCES). Several perturbation approaches on t/U starts from the Hubbard papers [1] use projection operators or the Hubbard X-operators technique. This approaches include strong Coulomb interactions in the Hamiltonian H_0 and treat the interatomic hopping by a perturbation method. The main conclusion of these perturbation methods is that electron in SCES is considered as a sum of quasiparticles (QP) with charge e, spin $1/2$, renormalized energy and spectral weight [2]. Application of Hubbard ideas to realistic multiorbital models of transition metal oxides results in a generalized tight-binding (GTB) method [3] that combines exact diagonalization of the intracell part of H with the perturbation treatment of the intercell part. In this paper we use the exact Lehmann representation for a single electron Green function (GF)

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to compare the notion of the quasiparticle in SCES developed in the perturbation approach to the exact one. The Lehmann representation treats an electron as a sum of QP with spin $S = 1/2$, charge e and renormalized energy and spectral weight without any indications on spin–charge separation. We show that the GTB method gives the practical realization of the Lehmann representation. Some results of GTB calculations of the QP energy spectra for copper oxides and ARPES data are given in [4, 5].

2. Lehmann representation and GTB method

Single electron GF $G_\sigma = \langle\langle a_{k\sigma} \mid a^{+}_{k\sigma}\rangle\rangle_\omega$ can be written as [6]

$$G_\sigma(k,\omega) = \sum_m \left(\frac{A_+(k,\omega)}{\omega - \Omega^+_m} + \frac{B_m(k,\omega)}{\omega - \Omega^-_m} \right) , \tag{1}$$

where the QP energies are given by

$$\Omega^+_m = E_m(N+1) - E_0(N) - \mu,\ \Omega^-_m = E_0(N) - E_m(N-1) - \mu,$$

and the QP spectral weight is equal to

$$A_m(k,\omega) = \left|\langle 0,N|\, a_{k\sigma}\, |m,N+1\rangle\right|^2,\ B_m(k,\omega) = \left|\langle m,N-1|\, a_{k\sigma}\, |0,N\rangle\right|^2 .$$

Here $|m,N\rangle$ is the m-th eigenstate of the system with N electrons, $H\,|m,N\rangle = E_m\,|m,N\rangle$. The index m numerates QP with spin $S = 1/2$, electrical charge e, energy Ω^+_m (Ω^-_m), and spectral weight A_m (B_m). The Eq. (1) may be considered as a sum over different QP bands with m being a QP band index. In practical calculations the Lehmann representation is useless because the multielectron eigenstates $|m,N\rangle$ for the crystal are not known.

Let write the multiorbital generalized Hubbard model (or p–d model for oxides) in the form

$$H = H_0 + H_1,\ H_0 = \sum_i H_{\rm c}(i),\ H_1 = \sum_{i,j} H_{\rm cc}(i,j)\,, \tag{2}$$

where $H_{\rm c}(i)$ is the intracell part of H with the unit cell index i, $H_{\rm cc}(i,j)$ is the intercell hopping and interaction between cells i and j. The GTB method consists of the 3 steps:

(a) the intercell multielectron molecular orbital $|p\rangle = |m, N_{\rm c}\rangle$ is calculated by the exact diagonalization of $H_{\rm c}(i)$ for different sectors of Hilbert space numerated by the number of electrons in the cell $N_{\rm c}$.

(b) the intracell Hubbard X-operators are constructed,

$$X^{pq}_i = |p\rangle\langle q| = |m,N_{\rm c}\rangle \left\langle m',N'_{\rm c}\right| . \tag{3}$$

We assume here that the eigenstates $|p\rangle$ of neighboring cells are orthogonal. If not, for example in cuprates where two CuO_6 cells share a common oxygen ion, the special procedure of orthogonalization is required. For cuprates in the 3-band p–d model it has been done in [7–9] and for the 6-band p–d model see [4]. To simplify the notations of X-operators we relate each pair of initial and final states in Eq. (3) to root vector [10], a set of these root vectors is discrete, so we just numerate them by index n:

$$X_i^{pq} \leftrightarrow X_i^{\vec{\alpha}(p,q)} \leftrightarrow X_i^{\vec{\alpha}_n(p,q)} \leftrightarrow X_i^{n} \,. \tag{4}$$

With this notation we can write the exact representation

$$a_{i\sigma} = \sum_n \gamma_\sigma(n) X_i^n \,, \; \gamma_\sigma(n) = \langle p | a_{i\sigma} | q \rangle = \left\langle m, N_\mathrm{c} \right| a_{i\sigma} \left| m', N_\mathrm{c}+1 \right\rangle \,. \tag{5}$$

The exact intracell electron GF in X-representation is equal to

$$G_\sigma^{(0)}(k,\omega) = \sum_n |\gamma_\sigma(n)|^2 \frac{F(n)}{\omega - \Omega_n} \,, \tag{6}$$

where local QP energy $\Omega_n = E_{m'}(N_\mathrm{c}+1) - E_m(N_\mathrm{c})$, $F(n)$ is a filling factor, $F(n) = \langle X_i^{pp} \rangle + \langle X_i^{qq} \rangle$. Thus n is the QP band index, and $\left|\gamma_\sigma(n)\right|^2 F(n)$ is the QP spectral weight.

(c) in the X-representation the total Hamiltonian has the form

$$H = \sum_{i,p} E_p X_i^{pp} + \sum_{ij} \sum_{nn'} t_{ij}^{nn'} \overset{+}{X}{}_i^{n} X_j^{n'} \,, \tag{7}$$

and looks similar to the Hubbard model in the X-representation. All perturbation methods in $t/U \ll 1$ known for the Hubbard model can be used. These methods are considered in detail in [11]. The Hartree–Fock approximation in the diagram technique is equivalent to the Hubbard-I decoupling for the intercell hopping and results in the following dispersion equation for the QP bands

$$\det \left\| \delta_{nn'} (\omega - \Omega_n)/F(n) - t_{nn'}(k) \right\| = 0 \,. \tag{8}$$

The structure of the Eq. (8) is similar to the tight-binding dispersion equation with the following differences: *(i)* local QP energy Ω_n includes exactly the Coulomb interaction inside the cell. *(ii)* n is not a number of atomic or molecular single electron orbital, it is a band index of QP, *(iii)* filling factor $F(n)$ is absent in the single electron theory. In the Eq. (8) the fitting factor provides dependence of the QP bands on temperature, doping, external fields. There is no rigid band situation for the QP bands in SCES.

The QP bands of undoped and hole doped CuO_2 layer has been calculated by GTB method in [4] using CuO_6 unit cell (CuO_4Cl_2 for $Sr_2CuO_2Cl_2$). In the undoped antiferromagnetic insulator there is a charge transfer gap, the dispersion of the top of the valence band is in a good agreement with ARPES data on $Sr_2CuO_2Cl_2$ [12]. At the top of the valence band an impurity-like band appears due to spin fluctuations and doping. A pseudogap between the impurity-like band and the main valence band has a dispersion similar to "remnant Fermi surface" in $Sr_2CuO_2Cl_2$ and to a pseudogap in the underdoped Bi-2212 samples [5]. The Fermi level is pinned inside the impurity-like band and very weakly depends on doping in the underdoped region.

3. Conclusion

In the perturbation approach of GTB the structure of GF is the same as in the exact Lehmann representation. There is a splitting of electron given by the Eq. (5) on different QP bands characterized by spectral weight redistribution over QP bands. Only summing all QP spectral weights one gets free electron spectral weight. Thus spectral weight splitting and removing its large part far away from the Fermi level is the most essential effect of strong correlations.

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REFERENCES

[1] J.C. Hubbard, *Proc. R. Soc.* **A285**, 542 (1965).
[2] P. Fulde, *Electron Correlations in Molecules and Solids*, Springer Verlag, Berlin-Heidelberg 1991.
[3] S.G. Ovchinnikov, I.S. Sandalov, *Physica C* **161**, 607 (1989).
[4] V.A. Gavrichkov, S.G. Ovchinnikov, A.A. Borisov, E.G. Goryachev, *Sov. Phys. JETP* **91**, 369 (2000).
[5] V. Gavrichkov, A. Borisov, S.G. Ovchinnikov, *Phys. Rev.* **B64**, 235124 (2001).
[6] H. Lehmann, *Nuovo Cimento* **11**, 342 (1954).
[7] S.V. Lotsov, V.Yu. Yushankhai, *Physica C* **179**, 159 (1991).
[8] J.H. Jefferson, H. Eskes, L.F. Feiner, *Phys. Rev.* **B45**, 7959 (1992).
[9] H.B. Schutler, A.J. Fedro, *Phys. Rev.* **B45**, 7588 (1992).
[10] R.O. Zaitsev, *Zh. Eksp. Teor. Fiz.* **70**, 1100 (1976) (in Russian).
[11] V.V. Val'kov, S.G. Ovchinnikov, Quasiparticles in strongly correlated systems, Siberian Branch of RAS, Novosibirsk 2001 (in Russian).
[12] B.O. Wells, Z.-X. Shen, A. Matsuura, *et al.*, *Phys. Rev. Lett.* **74**, 964 (1995).