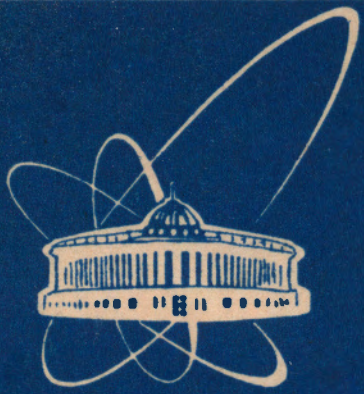

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

96-464

E17-96-464

V.A.Moskalenko, L.A.Dogotaru[1], I.G.Porcescu[2]

ELECTRON-PHONON COUPLING FOR THE SYSTEM WITH STRONG ELECTRON CORRELATIONS

Submitted to «ТМФ»

---

[1]Technical University of Moldova , Chisinau, Moldova

[2]Institute of Applied Physics, Moldova Academy of Sciences, Chisinau, Moldova

1996

The influence of electron-phonon interaction on the properties of the cuprates in the presence of strong electron correlation is studied.

The basic model is Hubbard one [1] completed with the Holstein interaction [2] between local charge fluctuations of electrons and phonon's coordinates.

The Hamiltonian of the system is the sum of Hubbard electron Hamiltonian, the Hamiltonian of free optical phonons with dispersionless frequency w_0 and electron-phonon interaction

$$H = H_e + H_{ph} + H_{e-ph} \tag{1}$$

$$H_{e-ph} = g \sum_{i\sigma} n_{i\sigma} q_i, \quad q_i = \frac{1}{\sqrt{2}} \left(b_i^+ + b_i \right)$$

where b_i^+, b_i are the operators of creation and annihilation of phonons, q_i is the phonon coordinate, $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ is the operator of number of electrons on site i with spin σ and g is the electron-phonon interaction constant.

After Lang-Firsov canonical transformation [3], a new Hamiltonian $\tilde{H} = e^S H e^{-S}$ does not contain linear phonon coordinates q_i, the chemical potential and on-site Coulomb interaction become renormalized

$$\tilde{\mu} = \mu + \frac{g^2}{2\hbar\omega_0}; \quad \tilde{U} = U - \frac{g^2}{2\hbar\omega_0} \tag{2}$$

and kinetic part of the Hubbard Hamiltonian depends on phonons

$$-\sum_{ij\sigma} t\,(i-j)\, \tilde{c}_{i\sigma}^+ \tilde{c}_{i\sigma} \tag{3}$$

where

Объединенный институт
ядерных исследований
БИБЛИОТЕКА

$$\tilde{c}_{i\sigma} = c_{i\sigma}\exp\left(i\bar{g}p_i\right),\ \tilde{c}^{+}_{i\sigma} = c^{+}_{i\sigma}\exp\left(-i\bar{g}p_i\right)$$
$$p_i = \frac{i}{\sqrt{2}}\left(b^{+}_i - b_i\right),\ \ \bar{g} = \frac{g}{\hbar\omega_0} \tag{4}$$

In such a way the intensity of electronic repulsion U is diminished and hoppings of polarons instead of electrons appear.

The renormalized Coulomb interaction $\tilde{U}$ is considered as a zero order electron Hamiltonian which is diagonalized using Hubbard operators and the role of interaction plays the hoppings of polarons (3).

We use a new diagram technique proposed in [4,5] based on the zero order localized approximation and electron irreducible Green functions or Kubo cumulants as the main structures of thermodynamic perturbation theory.

Zero order one-particle Green functions for polarons is

$$\tilde{G}^0(x\,|x') = -\left\langle T\tilde{c}_{x\sigma}(\tau)\,\bar{c}_{x'\sigma'}(\tau')\right\rangle_0 =$$
$$= -\left\langle Tc_{x\sigma}(\tau)\,\bar{c}_{x'\sigma'}(\tau')\right\rangle_0\left\langle T\exp\left(i\bar{g}\left(p(\tau)-p(\tau')\right)\right)\right\rangle_0 =$$
$$= G^0(x\,|x')\exp\left[-\frac{1}{2}\bar{g}^2\left\langle T\left(p(\tau)-p(\tau')\right)^2\right\rangle_0\right] \tag{5}$$

and the simplest irreducible Green function has the form

$$G_2^{(0)ir}(\sigma_1,\tau_1,\sigma_2,\tau_2\,|\sigma_3,\tau_3,\sigma_4,\tau_4) = \left\langle Tc_{\sigma_1}(\tau_1)\,c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\,\bar{c}_{\sigma_4}(\tau_4)\right\rangle_0 \times$$
$$\times\left\langle T\exp\left(i\bar{g}\left(p(\tau_1)+p(\tau_2)-p(\tau_3)-p(\tau_4)\right)\right)\right\rangle_0 -$$
$$-\left\langle Tc_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_4}(\tau_4)\right\rangle_0\left\langle Tc_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\right\rangle_0 \times\left\langle T\exp\left(i\bar{g}\left(p(\tau_1)-p(\tau_4)\right)\right)\right\rangle_0 \times$$
$$\times\left\langle T\exp\left(i\bar{g}\left(p(\tau_2)-p(\tau_3)\right)\right)\right\rangle_0 + \left\langle Tc_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_3}(\tau_3)\right\rangle_0\left\langle Tc_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_4}(\tau_4)\right\rangle_0 \times$$
$$\times\left\langle T\exp\left(i\bar{g}\left(p(\tau_1)-p(\tau_3)\right)\right)\right\rangle_0 \times\left\langle T\exp\left(i\bar{g}\left(p(\tau_2)-p(\tau_4)\right)\right)\right\rangle_0 \tag{6}$$

The sum of such and higher order cumulants gives us a new function $Z(x|x')$ which together with mass operator permits us to formulate Dyson equation for Matsubara one-particle Green function

$$\Lambda(x|x') = G^0(x|x') + Z(x|x')$$
$$G(x\,|x') = \Lambda(x\,|x') + \sum_{\bar{1}1}\Lambda(x\,|\,\bar{1})t(\bar{1}-1)G(1\,|x') \tag{7}$$

Here x stands for (x,σ,τ), where x is site index, σ is spin and τ is the imaginary time. The sum stands for summing over the discrete indices and integration over the τ.

Using Fourier representation for these quantities we obtain

$$G_\sigma(\mathrm{k}\,|i\omega_n) = \frac{1}{\Lambda_\sigma^{-1}(\mathrm{k}\,|i\omega_n) - \epsilon(\mathrm{k})} \tag{8}$$

where $\omega = (2n+1)\pi/\beta$, $\epsilon(\mathrm{k})$ is the electron band energy.

The first orders of the perturbation theory for the electron propagator are shown in

Fig.1. The first term is the zero order Green function (5). The dotted line denotes the hopping integral $t(i-j)$ and wave line is the phonon contribution. The first three terms are the chain diagrams of Hubbard I approximation. The last diagram

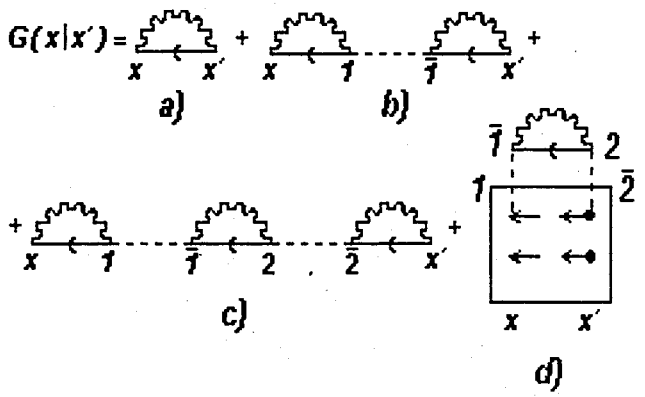

Fig. 1. The propagator's diagrams of first two orders of perturbation theory.

contains the simplest irreducible Green function (6) $G_2^{irr}(x1|\,\bar{2}x')$ drawn as a square. In such a way the simplest function $Z(x|x')$ is

$$Z^{(2)}(x\,|x') = \sum_{1\bar{1}\bar{2}} G_2^{ir}(x1|\,\bar{2}x')t(\bar{1}-1)t(\bar{2}-2)\tilde{G}^0(2|\,\bar{1})$$

Vacuum diagrams for polaron hopping processes were analysed and equation for connected diagrams was proved

$$\left\langle U(\beta)\right\rangle_0 = \exp[\left\langle U(\beta)\right\rangle_0^c]$$

where $\left\langle U(\beta)\right\rangle_0$ is statistical average of the evolution operator and $\left\langle U(\beta)\right\rangle_0^c$ is the sum of connected diagrams. The unity is not included here.

Phonon Green function is also investigated. The Dyson equation has not been established for it because the weak linked diagrams are not present.

REFERENCES

[1] J.Hubbard, Proc. Roy. Soc., 276 (1963) 233
[2] T.Holstein, Ann. of Phys., 8 (1959) 325
[3] I.G.Lang and Y.A.Firsov, Zh. Eksp. Teor. Fiz., 43 (1962) 1843
[4] M.I.Vladimir and V.A.Moskalenko, Teor. Mat.Fiz., 82 (1990) 428
[5] S.I.Vacaru, M.I.Vladimir, V.A.Moskalenko, Teor. Mat. Fiz., 85 (1990) 248

Received by Publishing Department
on December 14, 1996.