

## ELECTRON - PHONON INTERACTION IN STRONGLY CORRELATED SYSTEMS. ACOUSTICAL PHONON CASE

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We investigate the interaction of strongly correlated electrons with acoustical phonons in the frame of Hubbard-Holstein model. The electron-phonon interaction and on-site Coulomb repulsion are considered to be strong. By using the Lang-Firsov canonical transformation this problem has been transformed to the problem of mobile polarons. A new diagram technique is used in order to handle the strong Coulomb repulsion of the electrons and the existence of phonon clouds surrounding the electrons. The generalized Wick theorems for chronological products of electron and phonon-clouds operators have been formulated. We have found the collective mode of phonon clouds that surround electrons and discussed the physics of the emission and absorption of this mode by the polarons. We have also discussed the difference in the behaviour of optical and acoustical phonon-clouds surrounding polarons during their movement through the crystal lattice.

The aim of the present paper is to gain further insight into the mutual influence of strong on-site Coulomb repulsion and strong electron-phonon interaction using the single-band Hubbard-Holstein model [1,2] and a recently developed diagram approach [3-5].

We consider now the most interesting case as regards superconductivity of coupling of correlated electrons with dispersive acoustical phonons.

The initial Hamiltonian of the correlated electrons coupled to acoustical phonons has the form

$$H = H_e + H_{ph}^0 + H_{e-ph},$$

where

$$H_e = \sum_{i,j,\sigma} [t(j-i) + \varepsilon_0 \delta_{ij}] a_{j\sigma}^+ a_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} V_{i,j}^c n_i n_j,$$

$$H_{ph}^0 = \sum_k \hbar \omega_k \left( b_k^+ b_k + \frac{1}{2} \right),$$

$$H_{e-ph} = \sum_{i,j} g(i-j) q_i n_j,$$

$$n_i = \sum_{\sigma} n_{i\sigma}, \quad n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}.$$

Here  $a_{i\sigma}$  ( $a_{i\sigma}^+$ ) annihilation (creation) operators of the electrons at lattice site  $i$  and with spin  $y$ ,  $b_k$  ( $b_k^+$ ) phonon operators with vector  $\mathbf{k}$ ,  $q_i(p_i)$  is the phonon's coordinate (momentum) in site  $i$ , which is related with phonon operations by the equations:

$$q_i = \frac{1}{\sqrt{2}}(b_i + b_i^+); \quad p_i = \frac{i}{\sqrt{2}}(b_i^+ - b_i)$$

In this Hamiltonian  $U$  and  $V_{i,j}^c$  are the on-site and inter-site Coulomb interactions,  $t(j-i)$  is two center transfer integral,  $g(i-j)$  is the matrix-element of electron-phonon interaction,  $\varepsilon_0 = \bar{\varepsilon}_0 - \mu$  where  $\bar{\varepsilon}_0$  is the local electron energy and  $\mu$  is the chemical potential of the system. The Fourier representation of  $g(\mathbf{R})$  will be used as  $g(\mathbf{k})$ .

After applying the Lang-Firsov displacement transformation [6]:

$$H_p = e^S H e^{-S}, \quad c_{i\sigma} = e^S a_{i\sigma} e^{-S}, \quad c_{i\sigma}^+ = e^S a_{i\sigma}^+ e^{-S}$$

with

$$S = \frac{-i}{\sqrt{N}} \sum_{\mathbf{k}, i} S(\mathbf{k}) p_{\mathbf{k}} n_i e^{i\mathbf{k}\mathbf{R}_i}, \quad p_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i p_i \exp(-i\mathbf{k}\mathbf{R}),$$

$$S(\mathbf{k}) = \frac{g(\mathbf{k})}{\hbar\omega_{\mathbf{k}}} \equiv \bar{g}(\mathbf{k}),$$

we obtain the polaron Hamiltonian. The problem is now to deal properly with the impact of electronic correlations on the polaron problem. This can be done best by using the Green's functions provided one finds the key to deal with the spin and charge degrees.

We define the temperature Green's function for the electrons and polarons in the interaction representation correspondingly by

$$G_e(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T a_{\mathbf{x}\sigma}(\tau) \bar{a}_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c, \quad G_p(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T c_{\mathbf{x}\sigma}(\tau) \bar{c}_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c,$$

with operators  $a_{\mathbf{x}\sigma}$  and  $c_{\mathbf{x}\sigma}$  in interaction representation.

Here  $H^0 = H_p^0 + H_{ph}^0$  with

$$H_p^0 = \sum_i H_{ip}^0, \quad H_{ip}^0 = \varepsilon \sum_{\sigma} n_{i\sigma} + \tilde{U} n_{i\uparrow} n_{i\downarrow}, \quad H_{int} = \sum_{i,j,\sigma} t(j-i) c_{j\sigma}^+ c_{i\sigma} + \frac{1}{2} \sum_{i \neq j} V_{ij} n_i n_j,$$

where

$$\varepsilon = \bar{\varepsilon}_0 - \tilde{\mu}, \quad V_{ij} = V_{ij}^c - V_{ij}^{ph}, \quad V_{ij}^{ph} = \frac{1}{N} \sum_{\mathbf{k}} \frac{|\bar{g}(\mathbf{k})|^2}{\hbar\omega_{\mathbf{k}}} \exp(-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)),$$

$H_p^0$  is equal to the local part of  $H_e$  with renormalized parameters  $\tilde{U}$  and  $\tilde{\mu}$

$$\tilde{U} = U - 2\hbar\omega_c, \quad \tilde{\mu} = \mu + \hbar\omega_c.$$

$H_{int}$  contains two parts: the tunneling of the polarons and direct intersite interaction of polarons. The evolution operator is given by

$$U(\beta) = T \exp\left(-\int_0^{\beta} d\tau H_{int}(\tau)\right).$$

One-phonon zero order Matsubara Green's function has the form:

$$\sigma(x|x') = \sigma(\mathbf{x} - \mathbf{x}' | \tau - \tau') = \langle T \pi_{\mathbf{x}}(\tau) \pi_{\mathbf{x}'}(\tau') \rangle_0 = \frac{1}{2N} \sum_{\mathbf{k}} |\bar{g}(\mathbf{k})|^2 \cos \mathbf{k}(\mathbf{x} - \mathbf{x}') \frac{\cosh \hbar\omega_{\mathbf{k}} \left(\frac{\beta}{2} - |\tau - \tau'|\right)}{\sin \hbar\omega_{\mathbf{k}} \beta / 2}$$

where

$$\pi_{\mathbf{x}}(\tau) = \sum_j p_j(\tau) \bar{g}(\mathbf{R}_j - \mathbf{R}_{\mathbf{x}}), \quad \bar{g}(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \bar{g}(\mathbf{k}) \exp(-i\mathbf{k}\mathbf{R}).$$

In superconducting state, discussed by us, there are additional anomalous Green's functions for electrons and polarons:

$$F_e(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T a_{\mathbf{x}\sigma}(\tau) a_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c; \quad F_p(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T c_{\mathbf{x}\sigma}(\tau) c_{\mathbf{x}'\sigma'}(\tau') U(\beta) \rangle_0^c;$$

Here  $\mathbf{x}$  denotes position and  $\phi$  -imaginary time.

There are two different phonon-cloud propagators given by:

$$\Phi(x | x') = \langle T \exp(i\pi_{\mathbf{x}}(\tau) - i\pi_{\mathbf{x}'}(\tau')) \rangle_0; \quad \varphi(x | x') = \langle T \exp(i\pi_{\mathbf{x}}(\tau) + i\pi_{\mathbf{x}'}(\tau')) \rangle_0$$

The Fourier representation of them is the Lorentzian and Gaussian correspondingly:

$$\widehat{\Phi}(i\Omega) = \frac{2\hbar\omega_c}{(i\hbar\Omega)^2 - (\hbar\omega_c)^2};$$

$$\widehat{\varphi}(i\Omega) = \sqrt{\frac{2\pi}{\sigma_2}} \exp\left[ \frac{i\beta\hbar\Omega}{2} - \sigma(0|0) - \sigma\left(0\left|\frac{\beta}{2}\right.\right) - \frac{(\hbar\Omega)^2}{2\sigma_2} \right]$$

where  $\hbar\omega_c = -\sigma'(0|\tau)|_{\tau=0}$  is the collective frequency of phonon cloud and

$$\sigma_2 = \sigma''\left(0\left|\frac{\beta}{2}\right.\right)$$

The analysis of the diagram structure of the thermodynamical perturbation theory permits us to formulate the following exact Dyson equations for polaron renormalized Green's functions:

$$G_{p\sigma\sigma}(\mathbf{k} | i\omega) = \frac{\Lambda_{p\sigma\sigma}(\mathbf{k} | i\omega)}{[1 - \varepsilon(\mathbf{k})\Lambda_{p\sigma\sigma}(\mathbf{k} | i\omega)]}$$

$$F_{p\sigma\bar{\sigma}}(\mathbf{k} | i\omega) = \frac{Y_{p\sigma\bar{\sigma}}(\mathbf{k} | i\omega)}{[1 - \varepsilon(\mathbf{k})\Lambda_{p\sigma\sigma}(\mathbf{k} | i\omega)] [1 - \varepsilon(-\mathbf{k})\Lambda_{p\bar{\sigma}\bar{\sigma}}(-\mathbf{k} | -i\omega)]}$$

where  $\Lambda_{p\sigma\sigma}(\mathbf{k} | i\omega) = G_{p\sigma}^0(i\omega) + Z_{p\sigma\sigma}(\mathbf{k} | i\omega)$

$Z_{p\sigma\sigma}(\mathbf{k} | i\omega)$  and  $Y_{p\sigma\bar{\sigma}}(\mathbf{k} | i\omega)$  are the correlation functions characteristic of diagram technique [3-5]. They take into account all the correlation effects caused by the Coulomb interaction and presence of phonon clouds. Here  $\bar{\sigma} = -\sigma$ .

In this equation  $\varepsilon(\mathbf{k})$  is the bare energy of band electrons equal to the Fourier representation of tunneling matrix element. The anomalous quantities  $Y_p$  and  $F_p$  are proportional to the anomalous phonon-cloud propagator  $\varphi$  which, in strong coupling limit discussed by us, is exponentially small quantity. Therefore we investigate the properties of electron propagators in the environment of phonon clouds and obtain the following exact Dyson equations [ $k = \mathbf{k}, i\omega$ ]:

$$G_{e\sigma}(-k) = \frac{1}{d_{\sigma}(k)} \left\{ \Lambda_{e\sigma}(-k) + \Sigma_{e\sigma}(k) \left[ \Lambda_{e\sigma}(k) \Lambda_{e\sigma}(-k) + Y_{e\sigma\bar{\sigma}}(k) \bar{Y}_{e\sigma\bar{\sigma}}(k) \right] \right\}$$

$$F_{e\sigma\bar{\sigma}}(k) = \frac{1}{d_{\sigma}(k)} \left\{ Y_{e\sigma\bar{\sigma}}(k) + \Xi_{e\sigma\bar{\sigma}}(k) \left[ Y_{e\sigma\bar{\sigma}}(k) \bar{Y}_{e\sigma\bar{\sigma}}(k) + \Lambda_{e\sigma}(k) \Lambda_{e\bar{\sigma}}(-k) \right] \right\}$$

$$d_{\sigma}(k) = 1 - \Lambda_{e\sigma}(k) \Sigma_{e\sigma}(k) - \Lambda_{e\bar{\sigma}}(-k) \Sigma_{e\bar{\sigma}}(-k) + Y_{e\sigma\bar{\sigma}}(k) \bar{\Xi}_{e\sigma\bar{\sigma}}(k) + \bar{Y}_{e\sigma\bar{\sigma}}(k) \Xi_{e\sigma\bar{\sigma}}(k) +$$

$$+ \left[ \Lambda_{e\sigma}(k) \Lambda_{e\bar{\sigma}}(-k) + Y_{e\sigma\bar{\sigma}}(k) \bar{Y}_{e\sigma\bar{\sigma}}(k) \right] \left[ \Sigma_{e\sigma}(k) \Sigma_{e\bar{\sigma}}(-k) + \Xi_{e\sigma\bar{\sigma}}(k) \bar{\Xi}_{e\sigma\bar{\sigma}}(k) \right]$$

Here  $\Sigma_{e\sigma}(k)$ ,  $\Xi_{e\sigma\bar{\sigma}}(k)$  and complex quantity  $\bar{\Xi}_{e\sigma\bar{\sigma}}(k)$  are the exact mass operators of the system and in the simplest approximation are equal to the renormalized by phonon clouds tunneling matrix elements. The quantities  $\Lambda_{e\sigma}(k)$  are equal to

$$\Lambda_{e\sigma}(k) = G_{\sigma}^0(i\omega) + Z_{e\sigma}(k)$$

and  $Z_{e\sigma}$ ,  $Y_{e\sigma\bar{\sigma}}$  and complex quantity  $\bar{Y}_{e\sigma\bar{\sigma}}$  are characteristic of our diagram technique correlation functions. These exact equations for electron functions don't contain the small phonon cloud propagator  $\varphi$  and are the base for the next discussion of the phase transitions.

The main conclusion is the statement that superconducting pairing is realized easier by electrons without phonon clouds, but which move in the environment of such clouds, than by polaron loaded by heavy phonon clouds.

### References

- [1] J. Hubbard, Proc. Roy.Soc. A **276**, 233 (1963).
- [2] T. Holstein, Ann. Phys. (N. Y.) **8**, 325 (1959).
- [3] M.I. Vladimir and V.A. Moskalenko, Teor. Mat. Fiz. 82, 428, (1990) [Theor.Math.Phys. 82, 301(1990)].
- [4] S.I. Vacaru, M.I. Vladimir, and V.A. Moskalenko, Teor. Mat. Fiz. 85, 248 (1990), [Theor.Math.Phys. 85, 1185 (1990)].
- [5] N.N. Bogoliubov, and V.A. Moskalenko, Teor. Mat. Fiz., **86**, 16 (1991); Teor. Mat. Fiz., **92**, 182 (1992) [Theor. Math. Phys. 92, 820(1992)].
- [6] I. G. Lang and Yu. A. Firsov, Zh. Eksp. Teor. Fiz. **16**, 1301, (1963).