# MANY-CLOUD PHONON PROPOGATORS IN THE CASE OF ACOUSTICAL PHONONS

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In the High Temperature Superconductors we consider the system of correlated electrons which interect with phonons. In the theory of such sistems an effective way to describe correlation effects of electrons is based on the use of Green’s functions metod. A new diagram technique for the Green’s functions of the strong correlated electrons was proposed by V.A.Moskalenko et al. in [1-3]. This technique involves simpler creation and annihilation operators for electrons at all intermediate stages of the theory and Hubbard operators [4] only when evaluating final expressions. In the case when the electrons interect whith the acoustical phonons the new elements of the diagram technique appear. The aim of the present paper is to propose the mode how to calculate the such new elements of the diagram technique as the phonon-cloud propagators.

We use the Hubbard-Holstein Hamiltonian [5] to describe the sistem of correlated electrons which interect with acoustical phonons. After the canonical Lang-Firsov transformation the obtained new Hamiltonian in zero order of hoping interaction describes localized polarons and independent phonons which are vibration of ions relative to new equilibrium positions. Many-cloud phonon propagators will be present in all diagrams of the the temperature Green's function for the polarons. There are two kinds of one-cloud propagators, of which $\phi(x \mid x')$ is the normal-state and $\varphi(x \mid x')$ the anomalous one of the superconducting state, given by

$$\phi(x \mid x') = \phi(\mathbf{x}-\mathbf{x}' \mid \tau-\tau') = \langle \mathbf{T}\exp(i\pi_{\mathbf{x}}(\tau) - i\pi_{\mathbf{x}'}(\tau')) \rangle_0 = \exp[-\sigma(0 \mid 0) + \sigma(\mathbf{x}-\mathbf{x}' \mid \tau-\tau')],$$

$$\varphi(x \mid x') = \varphi(\mathbf{x}-\mathbf{x}' \mid \tau-\tau') = \langle \mathbf{T}\exp(i\pi_{\mathbf{x}}(\tau) + i\pi_{\mathbf{x}'}(\tau')) \rangle_0 = \exp[-\sigma(0 \mid 0) - \sigma(\mathbf{x}-\mathbf{x}' \mid \tau-\tau')].$$

The statistical averages $\langle ... \rangle_0$ are evaluated with respect to the zero-order density matrix of the grand canonical ensemble of free acoustical phonons. **T** is the time ordering operator.

The zero-order one-phonon Matsubara Green's function $\sigma(x, x')$ has the form

$$\sigma(x, x') = \sigma(\mathbf{x}-\mathbf{x}' \mid \tau-\tau') = \left\langle \mathbf{T}\pi_{\mathbf{x}}(\tau)\pi_{\mathbf{x}'}(\tau') \right\rangle_0$$

$$= \frac{1}{2N}\sum_{\mathbf{k}} |\bar{g}(\mathbf{k})|^2 \cos\mathbf{k}(\mathbf{x}-\mathbf{x}') \frac{\cosh\omega_{\mathbf{k}}(\beta/2 - |\tau-\tau'|)}{\sinh\omega_{\mathbf{k}}\beta/2},$$

$$\pi_{\mathbf{x}}(\tau) = \sum_j p_j(\tau)\bar{g}(\mathbf{R}_j - \mathbf{R}_x),$$

where $\mathbf{x}$ is the position and $c$ the imaginary time while $x$ stands for $(\mathbf{x}, \tau)$; $\omega_k$ is the phonon frequency with wave vector **k**; $p_j$ is the opertor of phonon momentum at site *j*; $\bar{g}(\mathbf{k}) \equiv g(\mathbf{k})/\omega_{\mathbf{k}}$; $g(\mathbf{k})$ is the Fourier representation of the the matrix element of the
electron-phonon interaction g(**R**).

The function $\sigma(x, x')$ makes an essential contribution for small values of distances $|\mathbf{x}-\mathbf{x}'|$ and $|\tau-\tau'|$ close to zero or $\beta$. For $\mathbf{x}=\mathbf{x}'$ the minimum value of this function is obtained for $|\tau-\tau'|=\beta/2$. For the strong-coupling limit of the electron-phonon interaction, we will use the series expansion of $\sigma(x, x')$ near $\tau=0$ and $\tau=\beta$ :

$$\sigma(0|\tau)=\begin{cases}\sigma(0|0)-\omega_c\tau, & \tau ? 0\\ \sigma(0|0)+\omega_c(\tau-\beta), & \tau ? \beta\end{cases}, \qquad \omega_c=\frac{1}{2N}\sum_{\mathbf{k}}|\bar{g}(\mathbf{k})|^2\,\omega_{\mathbf{k}}$$

as collective phonon cloud frequency [6,7].

For the first function $\phi(x|x')$ the maximum value of the one-phonon propagator $\sigma(\mathbf{x}|\tau)$ is favored while for the second function $\varphi(x|x')$ the corresponding minimum value is preferred.

The Fourier representations in $c$-space have the form

$$\phi(0|\tau)=\frac{1}{\beta}\sum_{\Omega}e^{-i\Omega_n\tau}\tilde{\phi}(i\Omega_n), \quad \varphi(0|\tau)=\frac{1}{\beta}\sum_{\Omega}e^{-i\Omega_n\tau}\tilde{\varphi}(i\Omega_n),$$

where

$$\tilde{\phi}(i\Omega_n)=\int_0^\beta d\tau\exp(i\Omega_n\tau)e^{-\sigma(0|0)+\sigma(0|\tau)}; \quad \tilde{\varphi}(i\Omega_n)=\int_0^\beta d\tau\exp(i\Omega_n\tau)e^{-\sigma(0|0)-\sigma(0|\tau)}.$$

Here $\Omega_n$ is the even Matsubara frequency $\Omega_n=2\pi n/\beta$.

In order to find the Fourier representations of these functions we have used the peculiarities of the $\mathcal{C}$-propagator in the strong-coupling limit of the electron-phonon interaction. The first propagator can be written as

$$\phi(\mathbf{x}|\tau')\cong\phi(\mathbf{x})\phi(\tau), \quad \phi(\mathbf{x})\approx\delta_{\mathbf{x},0}, \quad \tilde{\phi}(i\Omega_n)\approx\frac{2\omega_c}{(i\Omega_n)^2-(\omega_c)^2}, \quad \tilde{\phi}(\mathbf{q})\approx 1.$$

A more realistic value for $\tilde{\phi}(\mathbf{q})$ is obtained by using the dependence of $\sigma(\mathbf{x}|\tau)$ on small values of $\mathbf{x}$. In this more precise approximation we find

$$\tilde{\phi}(\mathbf{q})=(\frac{2\pi}{\sigma_1})^{3/2}e^{-\mathbf{q}^2/(2\sigma_1)}, \quad \phi(\mathbf{x})\approx e^{-\sigma_1\mathbf{x}^2/2}$$

where

$$\sigma_1=\frac{1}{6N}\sum_{\mathbf{k}}|\bar{g}(\mathbf{k})|^2\mathbf{k}^2\coth\frac{1}{2}\omega_{\mathbf{k}}\beta.$$

This result has been obtained by an expansion of $\cos\mathbf{kx}$ in terms of $\mathbf{x}$. We also assume that $\bar{g}(\mathbf{k})$ depends on $\mathbf{k}$ only through its modulo $|\mathbf{k}|$. Then the Fourier representation of the normal phonon cloud propagator is a Lorentzian and therefore the time dependence of this phonon cloud corresponds to that of an oscillator with the large collective frequency [illegible] . For the anomalous one-cloud propagator $\varphi(x \mid x')$ we obtain in this approximation a Gaussian representation:

$$\tilde{\phi}(i\Omega_n) = \sqrt{2\pi / \sigma_2} \exp[\frac{1}{2} i\beta\Omega_n - \sigma(0 \mid 0) - \sigma(0 \mid \beta/2) - (\Omega_n)^2 / (2\sigma_2)], \quad \sigma_2 = \sigma''(0 \mid \beta/2).$$

The space dependence of $\varphi(\mathbf{x} \mid i\Omega_n)$ is more complicated compared to the space dependence of $\phi(\mathbf{x} \mid i\Omega_n)$ because we cannot restrict the discussion to small values of $|\mathbf{x}|$ . In the following we will discuss many-cloud propagators, both in the normal and superconducting states. We start with the two-cloud propagators [as before, $x = (\mathbf{x}, \tau)$ ]:

$$\phi_2(x_1, x_2 \mid x_3, x_4) = \langle \mathbf{T} \exp[i(\pi_{\mathbf{x}_1}(\tau_1) + \pi_{\mathbf{x}_2}(\tau_2) - \pi_{\mathbf{x}_3}(\tau_3) - \pi_{\mathbf{x}_4}(\tau_4))] \rangle_0$$

$$= \exp\left( -\frac{1}{2} \langle \mathbf{T} \left[ \pi_{\mathbf{x}_1}(\tau_1) + \pi_{\mathbf{x}_2}(\tau_2) - \pi_{\mathbf{x}_3}(\tau_3) - \pi_{\mathbf{x}_4}(\tau_4) \right]^2 \rangle_0 \right) = \exp\left( \Sigma(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2 \mid \mathbf{x}_3, \tau_3; \mathbf{x}_4, \tau_4) \right),$$

$$\varphi_2(x_1, x_2, x_3 \mid x_4) = \langle \mathbf{T} \exp[i(\pi_{\mathbf{x}_1}(\tau_1) + \pi_{\mathbf{x}_2}(\tau_2) + \pi_{\mathbf{x}_3}(\tau_3) - \pi_{\mathbf{x}_4}(\tau_4))] \rangle_0$$

$$= \exp\left( -\frac{1}{2} \langle \mathbf{T} \left[ \pi_{\mathbf{x}_1}(\tau_1) + \pi_{\mathbf{x}_2}(\tau_2) + \pi_{\mathbf{x}_3}(\tau_3) - \pi_{\mathbf{x}_4}(\tau_4) \right]^2 \rangle_0 \right) = \exp\left( \Sigma(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2; \mathbf{x}_3, \tau_3 \mid \mathbf{x}_4, \tau_4) \right),$$

where

$$\sum(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2 \mid \mathbf{x}_3, \tau_3; \mathbf{x}_4, \tau_4) = \sigma(\mathbf{x}_1 - \mathbf{x}_3 \mid \tau_1 - \tau_3 |) + \sigma(\mathbf{x}_1 - \mathbf{x}_4 \mid \tau_1 - \tau_4 |) + \sigma(\mathbf{x}_2 - \mathbf{x}_4 \mid \tau_2 - \tau_4 |) + \sigma(\mathbf{x}_2 - \mathbf{x}_3 \mid \tau_2 - \tau_3 |) - \sigma(\mathbf{x}_1 - \mathbf{x}_2 \| \tau_1 - \tau_2 |) - \sigma(\mathbf{x}_3 - \mathbf{x}_4 \mid \tau_3 - \tau_4 |) - 2\sigma(0 \mid 0),$$

$$\sum(\mathbf{x}_1, \tau_1;_2, \tau_2; \mathbf{x}_3, \tau_3 \mid \mathbf{x}_4, \tau_4) = \sigma(\mathbf{x}_1 - \mathbf{x}_4 \| \tau_1 - \tau_4 |) + \sigma(\mathbf{x}_2 - \mathbf{x}_4 \| \tau_2 - \tau_4 |) + \sigma(\mathbf{x}_3 - \mathbf{x}_4 \| \tau_3 - \tau_4 |) - \sigma(\mathbf{x}_1 - \mathbf{x}_1 \| \tau_1 - \tau_2 |) - \sigma(\mathbf{x}_1 - \mathbf{x}_3 \| \tau_1 - \tau_3 |) - \sigma(\mathbf{x}_2 - \mathbf{x}_3 \| \tau_2 - \tau_3 |) - 2\sigma(0 \mid 0),$$

The following relations exist between two- and one-cloud Green's functions:

$$\begin{aligned} \phi_2(x_1, x_2 \mid x_3, x_4) &= \phi(x_1 \mid x_3)\phi(x_2 \mid x_4)\exp\left[\sigma(x_1 \mid x_4) + \sigma(x_2 \mid x_3) - \sigma(x_1 \mid x_2) - \sigma(x_3 \mid x_4)\right] \\ &= \phi(x_1 \mid x_4)\phi(x_2 \mid x_3)\exp\left[\sigma(x_1 \mid x_3) + \sigma(x_2 \mid x_4) - \sigma(x_1 \mid x_2) - \sigma(x_3 \mid x_4)\right], \end{aligned} \quad (1)$$

$$\begin{aligned} \varphi_2(x_1, x_2, x_3 \mid x_4) &= \varphi(x_1 \mid x_2)\phi(x_3 \mid x_4)\exp\left[\sigma(x_1 \mid x_4) + \sigma(x_2 \mid x_4) - \sigma(x_1 \mid x_3) - \sigma(x_2 \mid x_3)\right] \\ &= \varphi(x_1 \mid x_3)\phi(x_2 \mid x_4)\exp\left[\sigma(x_1 \mid x_4) + \sigma(x_3 \mid x_4) - \sigma(x_1 \mid x_2) - \sigma(x_2 \mid x_3)\right] \\ &= \varphi(x_2 \mid x_3)\phi(x_1 \mid x_4)\exp\left[\sigma(x_2 \mid x_4) + \sigma(x_3 \mid x_4) - \sigma(x_1 \mid x_2) - \sigma(x_1 \mid x_3)\right]. \end{aligned} \quad (2)$$

As above equations show, all sites of the diagrams are joint and appear to be connected in the presence of acoustical phonons. In order to classify the diagrams as connected and disconnected ones, it is necessary to have the analogy of Wick's theorem for many-cloud propagators similar to the theorem that has been formulated for correlated electrons [1,6]. In the absence of such a theorem we cannot prove the existence of a linked-cluster theorem for the thermodynamical potential and for other extensive quantities.

This problem has been discussed in detail in Ref. [8], however, only now it is able to present a solution. In order to obtain this solution, we observe that the two-cloud functions determined by Eqs. (1) and (2) have their maximum values when the arguments of the normal one-cloud functions $\phi(x \mid x')$ coincide ( $x = x'$ ) and the corresponding exponential factors close to these arguments approach one. There are several possibilities to achieve this and all of them have to be taken into account. We assume that as main approximation the following expressions for the two-cloud propagators will result,

$$\phi_2(x_1,x_2\,|\,x_3,x_4)=\phi(x_1\,|\,x_3)\phi(x_2\,|\,x_4)+\phi(x_1\,|\,x_4)\phi(x_2\,|\,x_3)+\phi_2^{ir}(x_1,x_2\,|\,x_3,x_4), \quad (3)$$

$$\begin{aligned}\varphi_2(x_1,x_2,x_3\,|\,x_4)&=\varphi(x_1\,|\,x_2)\phi(x_3\,|\,x_4)+\varphi(x_1\,|\,x_3)\phi(x_2\,|\,x_4)\\&+\varphi(x_2\,|\,x_3)\phi(x_1\,|\,x_4)+\phi_2^{ir}(x_1,x_2,x_3\,|\,x_4).\end{aligned} \quad (4)$$

These last equations also define the irreducible parts of the two-cloud propagators or phonon-cloud cumulants. In the strong-coupling limit the irreducible functions are small and can be omitted as shown below. The Fourier representation of the normal two-cloud propagator,

$$\begin{aligned}\phi_2(\mathbf{x}_1,i\Omega_1;\mathbf{x}_2,i\Omega_2\,|\,\mathbf{x}_3,i\Omega_3;\mathbf{x}_4,i\Omega_4)&=\int_0^\beta...\int_0^\beta d\tau_1...d\tau_4\times\exp(i\Omega_1\tau_1+i\Omega_2\tau_2-i\Omega_3\tau_3-i\Omega_4\tau_4)\\&\times\phi_2(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2\,|\,\mathbf{x}_3,\tau_3;\mathbf{x}_4,\tau_4),\end{aligned}$$

has been calculated in the strong-coupling limit leading to

$$\begin{aligned}\phi_2(\mathbf{x}_1,i\Omega_1;\mathbf{x}_2,i\Omega_2\,|\,\mathbf{x}_3,i\Omega_3;\mathbf{x}_4,i\Omega_4)&\approx\phi(\mathbf{x}_1-\mathbf{x}_2\,|\,i\Omega_1)\delta_{\Omega_1\Omega_3}\phi(\mathbf{x}_2-\mathbf{x}_4\,|\,i\Omega_2)\delta_{\Omega_2\Omega_4}\\&+\phi(\mathbf{x}_1-\mathbf{x}_4\,|\,i\Omega_1)\delta_{\Omega_1\Omega_4}\phi(\mathbf{x}_2-\mathbf{x}_3\,|\,i\Omega_2)\delta_{\Omega_2\Omega_3}\end{aligned}$$

The last equation shows that in this limit the irreducible function is not relevant and Wick's theorem has a simple form, which does no contain significant irreducible contributions. Similarly we obtain for $\varphi_2$ a form without irreducible contributions,

$$\begin{aligned}&\phi_2(\mathbf{x}_1,i\Omega_1;\mathbf{x}_2,i\Omega_2;\mathbf{x}_3,i\Omega_3\,|\,\mathbf{x}_4,i\Omega_4)=\int_0^\beta...\int_0^\beta d\mathbf{x}_1...d\mathbf{x}_4e^{-(i\Omega_1\tau_1+i\Omega_2\tau_2+i\Omega_3\tau_3-i\Omega_4\tau_4)}\\&\times\phi_2(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2;\mathbf{x}_3,\tau_3\,|\,\mathbf{x}_4,\tau_4)\approx\phi(\mathbf{x}_1-\mathbf{x}_2\,|\,i\Omega_1)\delta_{\Omega_2,-\Omega_1}\phi(\mathbf{x}_3-\mathbf{x}_4\,|\,i\Omega_3)\delta_{\Omega_3,\Omega_4}\\&+\phi(\mathbf{x}_1-\mathbf{x}_3\,|\,i\Omega_1)\delta_{\Omega_3,-\Omega_1}\phi(\mathbf{x}_2-\mathbf{x}_4\,|\,i\Omega_2)\delta_{\Omega_2,\Omega_4}+\phi(\mathbf{x}_2-\mathbf{x}_3\,|\,i\Omega_2)\delta_{\Omega_3,-\Omega_2}\phi(\mathbf{x}_1-\mathbf{x}_4\,|\,i\Omega_4)\delta_{\Omega_1,\Omega_4}\end{aligned}$$

These results correspond to our preliminary estimates that the irreducible parts in Eqs. (3) and (4) can be omitted because they are not important in the strong-coupling limit. Hence, without the irreducible parts the equations assume a form corresponding to Wick's theorem applied to two-cloud propagators. This can easily be generalized to the case of a larger number of clouds. Thus, there is an analogy of having a generalized Wicks's theorem for the case of correlated electrons [1] and a corresponding theorem for correlated phonon clouds. This allows us now to develop a thermodynamical perturbation theory for correlated electrons interacting strongly with phonons.

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