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CHARACTERISTICS OF BOGOLUBOV'S POLARON AT FINITE TEMPERATURES

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1. As is well known[1,2] the behaviour of a conduction electron in a polar crystal is described, after some idealizations, by the Pekar-Frohlich hamiltonian:

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + \sum_{\vec{k}} \omega \left(\hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}} + \frac{1}{2}\right) + \sum_{\vec{k}} \frac{\mathcal{L}(k)}{\sqrt{2\omega\Omega}} \left(\hat{a}_{\vec{k}} + \hat{a}^+_{-\vec{k}}\right) e^{i\vec{k}\cdot\vec{r}}$$

$$\mathcal{L}(k) = \frac{2e\omega\pi^{1/2}C_0^{1/2}}{k} \qquad C_0 = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)^{-1}, \tag{1}$$

where we use the units corresponding to $\hbar = 1$, $\hat{\vec{p}}$ and $\vec{r}$ are the momentum and coordinate operators of the electron, m is its conduction effective mass in a rigid lattice, $\hat{a}^+_{\vec{k}}$ and $a_{\vec{k}}$ are the creation and annihilation operators of phonons with quasimomentum $\vec{k}$ and frequency ω, $\vec{k}$ takes values in the first Brillouin zone, Ω is the volume of the system, ε_∞ and ε_0 stand for the high frequency and low frequency dielectric constants, $-e$ is the electron charge. The constant of coupling strength is defined by $\alpha = e^2 C_0 \left(\frac{m}{2\omega}\right)^{1/2}$.

The problem formally corresponds to that of a particle (the electron) with mass m interacting with a quantum Bose field which carries momentum $\sum_{\vec{k}} \vec{k}\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$. The total momentum $\vec{\mathcal{P}} = \hat{\vec{p}} + \sum_{\vec{k}} \vec{k}\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$ is conserved and forms together with all other quantum numbers ν a complete set to determine the eigenvalues $\mathcal{E}(\nu, \vec{\mathcal{P}})$ and eigenvectors $|\nu, \vec{\mathcal{P}}\rangle$ of the hamiltonian. In paper[3] it was shown that in the state $|\nu, \vec{\mathcal{P}}\rangle$ the mean velocity of the electron is given by $\vec{v}(\nu,\vec{\mathcal{P}}) \equiv \langle \nu, \vec{\mathcal{P}} | \hat{\vec{p}}/m | \nu, \vec{\mathcal{P}}\rangle = \frac{\partial \mathcal{E}(\nu,\vec{\mathcal{P}})}{\partial \vec{\mathcal{P}}}$.

If it is possible to describe the system in terms of a free phonon field and a quasiparticle with renormalized mass and self energy, then, such a quasiparticle is called polaron. Of course, as it was noted in[3], in the general case the effective mass and the self energy will be temperature dependent quantities ($E(\alpha,\beta)$; $m^*(\alpha,\beta)$; $\beta = (k_B T)^{-1}$).

In paper[3] this idea is performed in the following way, for $T = 0°K$. Let $|\nu_0, \vec{\mathcal{P}}\rangle$ be the state with lower energy $\mathcal{E}(\nu_0, \vec{\mathcal{P}})$ for fixed $\vec{\mathcal{P}}$. The electron mean velocity in this state is $\vec{v}(\nu_0,\vec{\mathcal{P}}) = \frac{\partial \mathcal{E}(\nu_0,\vec{\mathcal{P}})}{\partial \vec{\mathcal{P}}}$ which determines $\vec{\mathcal{P}}$ as a function of

$\vec{v}$, $\vec{\mathcal{P}} = \vec{\mathcal{P}}(\nu_0, \vec{v})$. The energy of the free phonon field at $T = 0^\circ K$ is $\sum_{\vec{k}} \frac{\omega}{2}$. Then, the polaron ground state energy E_0 and the effective mass m^* are defined through

$$E(\vec{v}) \equiv \mathcal{E}[\nu_0, \vec{\mathcal{P}}(\nu_0, \vec{v})] - \sum_{\vec{k}} \frac{\omega}{2} = E_0 + \frac{1}{2} m^* \vec{v}^2 + \dots$$

At zero temperature the free field momentum is zero and the polaron momentum coincides with the total momentum $\vec{\mathcal{P}}$, then we have for small $\vec{v}$

$$\vec{v} = \frac{\partial \mathcal{E}(\nu_0, \vec{\mathcal{P}})}{\partial \vec{\mathcal{P}}} \simeq \frac{\vec{\mathcal{P}}}{m^*} .$$

An extensive literature exists /1-5/ devoted to the calculation of $E_0(\alpha)$ and $m^*(\alpha)$ using a great variety of methods. In the framework of the Feynman approach /6/ to the problem the expression for $E(\alpha, \beta)$ has been given in /7,8/. However, to our knowledge, expressions for $m^*(\alpha, \beta)$ generalizing the definition given in /3/ have not been obtained. As will be shown, Bogolubov's approach is adequate and very useful to treat this problem.

2. To obtain the polaron characteristics at finite temperatures we start from the notion that, in the state of thermodynamical equilibrium at temperature T $\left(\beta = \frac{1}{k_B T}\right)$ we have a free phonon field with free energy $F_\Phi(\beta)$ and a noninteracting (with the field) quasiparticle with mass $m^*(\alpha, \beta)$ and self energy $E(\alpha, \beta)$. The last may be obtained from the corresponding "polaron free energy" (see below). To obtain the effective mass it is necessary to determine the additional energy acquired by the quasiparticle when it moves with small, but finite, average velocity $\vec{v}$. This is precisely the picture observed in a frame of reference S' moving with velocity $-\vec{v}$ with respect to the laboratory. In S' the hamiltonian of our system is /9/:

$$\hat{H}' = \hat{H} - \vec{v} \cdot \hat{\vec{\mathcal{P}}} \qquad (2)$$

and the statistical operator, according to the general principles of statistical mechanics, must have the form

$$\hat{\rho}(\vec{v}) = e^{-\beta(\hat{H}' - \vec{\lambda} \cdot \hat{\vec{\mathcal{P}}})} . \qquad (3)$$

The parameter $\vec{\lambda}$ may be determined from the condition that the electron mean velocity in this system is $\vec{v}$. It is not difficult

to show that $\vec{\lambda} = \vec{0}$. For the free energy of the whole system in the frame of reference S' we have

$$\Phi(\alpha, \beta, \vec{v}) = -\frac{1}{\beta} \ln \mathrm{Sp} \exp\left[-\beta(\hat{H} - \vec{v} \cdot \hat{\vec{\mathcal{P}}})\right] \qquad (4)$$

and the free phonon field free energy is given by

$$F_\Phi(\beta, \vec{v}) = \sum_{\vec{k}} \left\{ \frac{\omega}{2} + \frac{1}{\beta} \ln\left[1 - e^{-\beta(\omega - \vec{k} \cdot \vec{v})}\right] \right\} . \qquad (5)$$

Then the "polaron free energy" in S' is

$$F(\alpha, \beta, \vec{v}) = \Phi(\alpha, \beta, \vec{v}) - F_\Phi(\beta, \vec{v}) . \qquad (6)$$

Taking into account (4) and (5), $F(\alpha, \beta, \vec{v})$ may be rewritten in the form

$$F(\alpha, \beta, \vec{v}) = -\frac{1}{\beta} \ln \frac{\mathrm{Sp}\, e^{-\beta(\hat{H} - \vec{v} \cdot \hat{\vec{\mathcal{P}}})}}{\prod_{\vec{k}} \frac{e^{-\beta \frac{\omega}{2}}}{1 - e^{-\beta(\omega - \vec{k} \cdot \vec{v})}}} . \qquad (7)$$

For small $\vec{v}$ we have

$$F(\alpha, \beta, \vec{v}) = F(\alpha, \beta) - \frac{1}{2} m^*(\alpha, \beta) \vec{v}^2 + \dots \qquad (8)$$

where $F(\alpha, \beta)$ is the polaron free energy in the frame of reference where the electron mean velocity is zero and $m^*(\alpha, \beta)$ is the polaron effective mass. The self energy is obtained from $F(\alpha, \beta)$ by the formula $E(\alpha, \beta) = \frac{\partial}{\partial \beta} \beta F(\alpha, \beta) - \frac{3}{2\beta}$. Then, to obtain the polaron characteristics we have to calculate the quantity $F(\alpha, \beta, \vec{v})$ for small $\vec{v}$. Of course, we suppose that $\omega - \vec{k} \cdot \vec{v} > 0$ for all $\vec{k}$ in the first Brillouin zone. When $\beta \to \infty$ the free energy $F(\alpha, \beta)$ and the mass $m^*(\alpha, \beta)$ tend to $E_0(\alpha)$ and $m^*(\alpha)$ respectively. To show this note that from (7) it follows that

$$\lim_{\beta \to \infty} F(\alpha, \beta, \vec{v}) = \min_{\{\nu, \vec{\mathcal{P}}\}} \left[\mathcal{E}(\nu, \vec{\mathcal{P}}) - \vec{v} \cdot \vec{\mathcal{P}}\right] - \sum_{\vec{k}} \frac{\omega}{2}$$

for small enough $\vec{v}$

$$\lim_{\beta \to \infty} F(\alpha, \beta, \vec{v}) = \mathcal{E}(\nu_0, \vec{\mathcal{P}}_0) - \vec{v} \cdot \vec{\mathcal{P}}_0 - \sum_{\vec{k}} \frac{\omega}{2}$$

and from the condition of minimum $\vec{V} = \dfrac{\partial E(\nu_0, \vec{\mathcal{P}}_0)}{\partial \vec{\mathcal{P}}_0}$. Now, taking into account the expressions for $E(\vec{V})$ and $\vec{V}(\nu_0, \vec{\mathcal{P}})$, we have

$$\lim_{\beta \to \infty} F(\alpha, \beta, \vec{V}) = E_0 - \frac{1}{2} m^* V^2$$

so that

$$\lim_{\beta \to \infty} F(\alpha, \beta) = E_0(\alpha) \quad ; \quad \lim_{\beta \to \infty} m^*(\alpha, \beta) = m^*(\alpha) .$$

3. Now we pass to obtain an exact path integral representation for $F(\alpha, \beta, \vec{V})$. The path integral method has been shown to be very useful in polaron theory/4-8/ since it allows one to deal in an unique approach with the weak coupling ($\alpha < 1$), strong coupling ($\alpha \gg 1$) and intermediate coupling cases. To obtain the path integral representation for $F(\alpha, \beta, \vec{V})$ we will make use of the method described in/10/.

Using the Bogolubov canonical transformation/3/:

$$\hat{b}_{\vec{K}} = \hat{a}_{\vec{K}} e^{i\vec{K}\cdot\vec{r}} \; ; \; \hat{b}^+_{\vec{K}} = \hat{a}^+_{\vec{K}} e^{-i\vec{K}\cdot\vec{r}} \; ; \; \hat{\vec{\mathcal{P}}} = \hat{\vec{p}} + \sum_{\vec{K}} \vec{K}\, \hat{b}^+_{\vec{K}} \hat{b}_{\vec{K}} .$$

The hamiltonian is written in the following way

$$\hat{H} = \frac{\hat{\vec{\mathcal{P}}}^2}{2m} + \sum_{\vec{K}} \left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)\left(\hat{b}^+_{\vec{K}} \hat{b}_{\vec{K}} + \frac{1}{2}\right) + \sum_{\vec{K}} \frac{\mathcal{L}(K)}{\sqrt{2\omega\Omega}} \left(\hat{b}^+_{\vec{K}} + \hat{b}_{\vec{K}}\right) + \sum_{\vec{K},\vec{K}'} \frac{\vec{K}\cdot\vec{K}'}{2m} \hat{b}^+_{\vec{K}} \hat{b}_{\vec{K}} \hat{b}^+_{\vec{K}'} \hat{b}_{\vec{K}'} \tag{9}$$

The trace in expression (7) can be calculated using the complete set of states of (9) for $\mathcal{L}(K) = 0$. We have

$$\mathop{Sp} e^{-\beta(\hat{H} - \vec{V}\cdot\hat{\vec{\mathcal{P}}})} = \int \frac{d^3\vec{\mathcal{P}}}{(2\pi)^3} e^{-\beta\left(\frac{\vec{\mathcal{P}}^2}{2m} - \vec{V}\cdot\vec{\mathcal{P}}\right)} W(\vec{\mathcal{P}}) , \tag{10}$$

where $W(\vec{\mathcal{P}}) = \mathop{Sp}_{\Phi} \exp\left[-\beta\left(\hat{H}_1 + \hat{H}_2 + \hat{H}_3\right)\right]$

$$\hat{H}_1 = \sum_{\vec{K}} \left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)\left(\hat{b}^+_{K} \hat{b}_{K} + \frac{1}{2}\right) ; \; \hat{H}_2 = \sum_{\vec{K}} \frac{\mathcal{L}(K)}{\sqrt{2\omega\Omega}} \left(\hat{b}_{\vec{K}} + \hat{b}^+_{\vec{K}}\right) ; \; \hat{H}_3 = \sum_{\vec{K},\vec{K}'} \frac{\vec{K}\cdot\vec{K}'}{2m} \hat{b}^+_{\vec{K}} \hat{b}_{\vec{K}} \hat{b}^+_{\vec{K}'} \hat{b}_{\vec{K}'} . \tag{11}$$

As in/10/ we define the generating functional

$$W_g(\vec{\mathcal{P}}, \vec{\xi}) = \mathop{Sp}_{\Phi} e^{-\beta \hat{H}_1} T\exp\left\{-\int_0^\beta d\tau \left[\hat{H}_2(\tau) + g\, \hat{H}_3(\tau) + i\sqrt{\frac{2}{m}}\, \vec{\xi}(\tau)\cdot \sum_{\vec{K}} \vec{K}\, \hat{b}^+_{K}(\tau) \hat{b}_{K}(\tau)\right]\right\},$$

where

$$\hat{A}(\tau) = e^{\hat{H}_1 \tau} \hat{A} e^{-\hat{H}_1 \tau} \; ; \; \hat{b}_{\vec{K}}(\tau) = \hat{b}_{\vec{K}} e^{-\left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)\tau} \; ; \; \hat{b}^+_{\vec{K}}(\tau) = \hat{b}^+_{\vec{K}} e^{\left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)\tau} .$$

As was shown in/10/ the functional $W_g(\vec{\mathcal{P}}, \vec{\xi})$ satisfies the equation

$$\frac{\partial W_g(\vec{\mathcal{P}}, \vec{\xi})}{\partial g} = \frac{1}{4} \int_0^\beta d\tau \; \frac{\delta^2 W_g(\vec{\mathcal{P}}, \vec{\xi})}{\delta \vec{\xi}(\tau)\, \delta \vec{\xi}(\tau)} \tag{12}$$

with the initial condition

$$W_0(\vec{\mathcal{P}}, \vec{\xi}) = \mathop{Sp}_{\Phi} e^{-\beta \hat{H}_1} T\exp\left\{-\int_0^\beta d\tau \left[\hat{H}_2(\tau) + i\sqrt{\frac{2}{m}}\, \vec{\xi}(\tau)\cdot \sum_{\vec{K}} \vec{K}\, \hat{b}^+_{\vec{K}}(\tau) \hat{b}_{\vec{K}}(\tau)\right]\right\}. \tag{13}$$

The solution of (12),(13) may be written as a functional integral (see/10/) and for $W(\vec{\mathcal{P}}) \equiv W_1(\vec{\mathcal{P}}, \vec{0})$ we have

$$W(\vec{\mathcal{P}}) = \frac{\int \mathcal{D}\vec{\xi} \exp\left[-\int_0^\beta d\tau\, \xi^2(\tau)\right] W_0(\vec{\mathcal{P}}, \vec{\xi})}{\int \mathcal{D}\vec{\xi} \exp\left[-\int_0^\beta d\tau\, \vec{\xi}^2(\tau)\right]} \tag{14}$$

now, using the results of paper/11/ the expression (22) may be rewritten in the following way

$$W_0(\vec{\mathcal{P}}, \vec{\xi}) = \prod_{\vec{K}} R_{\vec{K}} \mathop{Sp}_{\Phi} \left\{ e^{-\beta \lambda_{\vec{K}} \left(\hat{b}^+_{\vec{K}} \hat{b}_{\vec{K}} + \frac{1}{2}\right)} e^{-A_{\vec{K}} \hat{b}^+_{\vec{K}}} e^{-B_{\vec{K}} \hat{b}_{\vec{K}}} \right\} , \tag{15}$$

where

$$\lambda_{\vec{K}} = \omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m} + \frac{i}{\beta}\sqrt{\frac{2}{m}}\, \vec{K}\cdot \int_0^\beta d\tau\, \vec{\xi}(\tau)$$

$$R_{\vec{K}} = \exp\left\{ \frac{\mathcal{L}^2(K)}{2\omega\Omega} \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2\, e^{-\left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)(\tau_1 - \tau_2) - i\sqrt{\frac{2}{m}}\, \vec{K}\cdot \int_{\tau_1}^{\tau_2} \vec{\xi}(\tau)\, d\tau} \right\}$$

$$\left\{ \begin{matrix} A_{\vec{K}} \\ B_{\vec{K}} \end{matrix} \right\} = \frac{\mathcal{L}(K)}{\sqrt{2\omega\Omega}} \int_0^\beta d\tau\, e^{\pm\left(\omega - \frac{\vec{K}\cdot\vec{\mathcal{P}}}{m}\right)\tau \pm i\sqrt{\frac{2}{m}}\, \vec{K}\cdot \int_0^\tau \vec{\xi}(\tau)\, d\tau}$$

making the change of functional variables

$$\dot{\vec{r}}(\tau) = \sqrt{\frac{2}{m}}\, \vec{\xi}(\tau) + i\left(\frac{\vec{\mathcal{P}}}{m} - \vec{V}\right) . \tag{16}$$

We have $\lambda_{\vec{K}} = \omega - \vec{K}\cdot\vec{V} + i\,\frac{\vec{K}}{\beta}\left[\vec{r}(\beta) - \vec{r}(0)\right]$. If $\mathrm{Re}\, \lambda_{\vec{K}} > 0$ the trace in (15) is easily calculated and we obtain

$$W_0(\vec{\mathcal{P}}, \vec{\xi}) = \prod_{\vec{K}} R_{\vec{K}} \frac{e^{-\beta \lambda_{\vec{K}}/2}}{1 - e^{-\beta \lambda_{\vec{K}}}} \exp \frac{A_{\vec{K}} B_{\vec{K}}}{e^{\beta \lambda_{\vec{K}}} - 1} . \tag{17}$$

Now putting (14) into (10), taking into account (16),(17) and performing the integration over $\vec{\mathcal{P}}$ we achieve the result

$$S_p e^{-\beta(\hat{H}-\vec{v}\cdot\hat{\vec{\mathcal{P}}})} = e^{\beta\frac{mv^2}{2}} \prod_{\vec{K}} \left[\frac{e^{-\frac{\beta\omega}{2}}}{1-e^{-\beta(\omega-\vec{K}\cdot\vec{v})}} \right] \int_{\vec{r}(0)=0}^{\vec{r}(\beta)=0} \mathcal{D}\vec{r}\, e^{-\frac{m}{2}\int_0^\beta d\tau\, \dot{\vec{r}}^2(\tau)} \prod_{\vec{K}} R_{\vec{K}} \exp\frac{A_{\vec{K}} B_{\vec{K}}}{e^{\beta\lambda_{\vec{K}}}-1} . \quad (18)$$

Making now the change of functional variables $\vec{r}(\tau) = \vec{X}(\tau) - \vec{u}\tau$, where $\vec{u} = i\vec{v}$ and taking into account expression (7) we get the final result.

$$F(\alpha,\beta,\vec{v}) = -\frac{1}{\beta} \ln \int_{\vec{X}(0)=0}^{\vec{X}(\beta)=\vec{u}\beta} \mathcal{D}\vec{X}\, e^{-S[\vec{X},\vec{u}]} , \quad (19)$$

where

$$S[\vec{x},\vec{u}] = \frac{m}{2}\int_0^\beta d\tau\, \dot{\vec{X}}^2(\tau) - \sum_{\vec{K}} \frac{\mathcal{L}^2(K)}{2\omega\Omega} \iint_0^\beta d\tau_1 d\tau_2 \left\{ \frac{e^{-\omega|\tau_1-\tau_2|}}{2} + \frac{e^{\omega(\tau_1-\tau_2)}}{e^{\beta(\omega+i\vec{K}\cdot\vec{u})}-1} \right\} e^{i\vec{K}\cdot[\vec{X}(\tau_1)-\vec{X}(\tau_2)]} . \quad (20)$$

Formulae (19) and (20) solve in principle the problem of obtaining the polaron self energy and effective mass at finite temperatures. Starting from (19) and (20) different approximation schemes may be developed (perturbation theory, variational calculations, etc.) to calculate $F(\alpha,\beta,\vec{v})$ and from it using (8), obtain the energy and the effective mass. Concrete results will be published in our next paper.

4. Let us pass now to discuss the problem of the validity of the Pekar-Frolich model to describe the electron-phonon interaction in polar crystals. As is well known /1/ this description is valid if the main contribution to the electron phonon interaction is given by those regions of the crystal located at a distance from the electron much larger than the lattice constant. In the opposite case it is necessary to consider the discrete structure of the crystal which is neglected in Pekar-Frohlich's model. The parameter giving a quantitative criterium of the validity of this description is the polaron radius which is defined as some effective radius of the polarization charge distribution formed around the electron. Knowledge of the polaron radius as a function of α and β allows us to determine until which temperatures the large polaron picture is correct.

Let $\rho(\vec{x})$ be the average polarization charge density in the point $\vec{x}$ if the electron is located at the origin. The total charge of this distribution is $q = \int_\Omega \rho(\vec{x})\, d^3\vec{x}$ and the mean interaction potential energy between the electron and the polarization charge distribution is

$$U = -e \int_\Omega d^3\vec{x}\, \frac{\rho(\vec{x})}{|\vec{x}|} .$$

We define the polaron radius R as the distance from the electron at which must be located the point charge q in order that its interaction potential energy with the electron be equal to U. Then R is given by

$$\frac{1}{R} = \frac{\int_\Omega d^3\vec{x}\, \frac{\rho(\vec{x})}{|\vec{x}|}}{\int_\Omega d^3\vec{x}\, \rho(\vec{x})} . \quad (21)$$

Note that the definition of radius given in /1/ has essentially the same physical sense. The operator of polarization charge density is defined by $\hat{\rho}(\vec{x}) = -\nabla\cdot\hat{\vec{P}}(\vec{x})$, where $\hat{\vec{P}}(\vec{x})$ is the polarization operator and is given by

$$\hat{\rho}(\vec{x}) = -\sum_{\vec{K}} \frac{\omega}{2}\left(\frac{C_0}{\pi\Omega}\right)^{1/2} K \hat{q}_{\vec{K}}\, e^{i\vec{K}\cdot\vec{x}} \;;\; \hat{q}_{\vec{K}} = \sqrt{\frac{1}{2\omega}}\,(\hat{a}_{\vec{K}} + \hat{a}^{+}_{-\vec{K}}) \quad (22)$$

The average polarization charge density $\rho(\vec{x})$ is, by definition

$$\rho(\vec{x}) = \frac{\int dQ\, \langle Q|\hat{\rho}(\vec{x})|Q\rangle \langle 0,Q|e^{-\beta\hat{H}}|0,Q\rangle}{\int dQ\, \langle 0,Q|e^{-\beta\hat{H}}|0,Q\rangle} . \quad (23)$$

where $Q = \{q_{\vec{K}}\}$ is the set of oscillator coordinates and

$$\langle Q|\hat{\rho}(\vec{x})|Q\rangle = -\sum_{\vec{K}} \frac{\omega}{2}\left(\frac{C_0}{\pi\Omega}\right)^{1/2} q_{\vec{K}}\, K\, e^{i\vec{K}\cdot\vec{x}} .$$

For the statistical operator in the coordinate representation $\langle \vec{r}',Q'|e^{-\beta\hat{H}}|\vec{r},Q\rangle$ according to /12/ we have

$$\langle \vec{r}',Q'|e^{-\beta\hat{H}}|\vec{r},Q\rangle = \frac{1}{\Omega} \int_{\vec{r}(0)=\vec{r}}^{\vec{r}(\beta)=\vec{r}'} \mathcal{D}\vec{r} \int_{Q(0)=Q}^{Q(\beta)=Q'} \mathcal{D}Q\, \exp\left\{-\int_0^\beta du\, H[\vec{r}(u),Q(u)]\right\} , \quad (24)$$

where

$$H[r,Q] = \frac{1}{2}m\dot{\vec{r}}^2 + \frac{1}{2}\sum_{\vec{K}} \dot{q}_{\vec{K}}^2 + \omega^2 q_{\vec{K}}^2 + \sum_{\vec{K}} \frac{\mathcal{L}(K)}{\Omega^{1/2}} q_{\vec{K}}\, e^{i\vec{K}\cdot\vec{r}} \;;\; \int_{Q(0)=Q}^{Q(\beta)=Q'} \mathcal{D}Q \cdots = \prod_{\vec{K}} \int_{q_{\vec{K}}(0)=q_{\vec{K}}}^{q_{\vec{K}}(\beta)=q'_{\vec{K}}} \mathcal{D}q_{\vec{K}} \cdots$$

The path integral over oscillator paths $q_{\vec k}(u)$ is obtained using the general formulae of [12]. Using the notation

$$A_{\vec k}(\vec r) = \frac{f(k)}{2\omega}\int_0^\beta d\tau\, e^{-i\vec k\cdot\vec r(\tau)}\left[\frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}+\frac{e^{\omega\tau}}{e^{\beta\omega}-1}\right] \qquad (25)$$

we obtain

$$\langle 0,Q|\, e^{-\beta\hat H}\,|0,Q\rangle = \frac{1}{\Omega}\int_{\vec r(0)=0}^{\vec r(\beta)=0}\mathcal{D}\vec r\, e^{-S[\vec r,0]}\prod_{\vec k}\sqrt{\frac{\omega}{2\pi\,\mathrm{sh}\,\beta\omega}}\exp\left\{-\beta\,\mathrm{th}\frac{\beta\omega}{2}\left[q_k+A_{\vec k}\right]^2\right\}$$

Now, taking into account (22) and (25) we have for $\rho(\vec x)$

$$\rho(\vec x)=\left(\frac{C_0}{\pi\Omega}\right)^{1/2}\sum_{\vec k}\frac{k f(k)}{4}e^{i\vec k\cdot\vec x}\int_0^\beta d\tau\left[\frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}+\frac{e^{\omega\tau}}{e^{\beta\omega}-1}\right]\langle e^{-i\vec k\cdot\vec r(\tau)}\rangle_S^0\,, \qquad (26)$$

where

$$\langle e^{-i\vec k\cdot\vec r(\tau)}\rangle=\frac{\int_{\vec r(0)=0}^{\vec r(\beta)=0}\mathcal{D}\vec r\; e^{-S[\vec r,0]-i\vec k\cdot\vec r(\tau)}}{\int_{\vec r(0)=0}^{\vec r(\beta)=0}\mathcal{D}\vec r\; e^{-S[\vec r,0]}}\,.$$

It is not difficult to note that $\langle e^{-i\vec k\cdot\vec r(\tau)}\rangle_S^0=\langle e^{-i\vec k\cdot\vec r(\beta-\tau)}\rangle_S^0$ because the paths satisfying the conditions $\vec r(0)=\vec r(\beta)=0$ can be extended as even periodic functions outside the interval $[0,\beta]$ so that $\vec r(0)=\vec r(\beta)=0$. Then, taking into account the definition of $f(k)$, we obtain for $\rho(\vec x)$

$$\rho(\vec x)=\frac{e\omega C_0}{\Omega}\sum_{\vec k}e^{i\vec k\cdot\vec x}\int_0^\beta d\tau\,\frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}\,\langle e^{-i\vec k\cdot\vec r(\tau)}\rangle_S^0 \qquad (27)$$

and the polaron radius, according to (21), is given by

$$\frac{1}{R}=\frac{4\pi\omega}{\Omega}\sum_{\vec k}\frac{1}{k^2}\int_0^\beta d\tau\,\frac{e^{-\omega\tau}}{1-e^{-\beta\omega}}\,\langle e^{-i\vec k\cdot\vec r(\tau)}\rangle_S^0\,. \qquad (28)$$

From (27), it follows that the total charge q of the polarization charge distribution around the electron is $q=eC_0$. As in Pekar-Frolich's model C_0 is considered to be a constant we see that the charge q is temperature independent. The effective charge of the polaron is $e(C_0-1)$.

Expression (28) will be used by us to evaluate the polaron radius in the framework of different approximations used to calculate the polaron characteristics.

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