1 Formulation of the polaron problem

Let us consider electron of momentum $\vec{p}$ interacting with the phonons

$$H = \frac{\vec{p}^{\,2}}{2m} + \hbar\omega \int \frac{d^3k}{(2\pi)^3} a^\dagger_{\vec{k}} a_{\vec{k}} + V(x). \tag{1}$$

Here $a_{\vec{k}}$ are Fourier components of the polarization vector $\vec{P}(\vec{x})$ induced by the displacements of the ions in the crystal due to the electron:

$$\vec{P}(\vec{x}) \sim \int \frac{d^3k}{(2\pi)^3} \sum_{s=1}^{3} \left[\vec{e}(\vec{k},s)\, a(\vec{k},s)\, e^{i\vec{k}\cdot\vec{x}} + \vec{e}(\vec{k},s)\, a^\dagger(\vec{k},s)\, e^{-i\vec{k}\cdot\vec{x}} \right], \tag{2}$$

where s is polarization, $\vec{e}(\vec{k},s)$ – polarization vector. Since in the polaron problem only *longitudinal* polarization enters

$$a_{\vec{k}} = a(\vec{k}, s = \text{long.}).$$

Interaction potential is then given as:

$$V(x) = i\left(\sqrt{2}\pi\alpha\right)^{1/2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} \left[a^\dagger_{\vec{k}}\, e^{-i\vec{k}\cdot\vec{x}} - a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} \right]. \tag{3}$$

Here α is a material constant. Setting $\hbar = \omega = m = 1$ and changing $\vec{k} \to -\vec{k}$ in the first term in (3) we arrive at

$$H = \frac{1}{2}\vec{p}^{\,2} + \int \frac{d^3k}{(2\pi)^3} a^\dagger_{\vec{k}} a_{\vec{k}} + i\left(\sqrt{2}\pi\alpha\right)^{1/2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k} \left[a^\dagger_{-\vec{k}} - a_{\vec{k}} \right] e^{i\vec{k}\cdot\vec{x}}. \tag{4}$$

It is convenient to introduce *coordinates* and *momenta*

$$\begin{aligned} q_{\vec{k}} &= \frac{i}{\sqrt{2}}\left(a^\dagger_{-\vec{k}} - a_{\vec{k}}\right),\ q^\dagger_{\vec{k}} = -\frac{i}{\sqrt{2}}\left(a_{-\vec{k}} - a^\dagger_{\vec{k}}\right) = q_{-\vec{k}}, \\ p_{\vec{k}} &= \frac{1}{\sqrt{2}}\left(a^\dagger_{\vec{k}} + a_{-\vec{k}}\right),\ p^\dagger_{\vec{k}} = \frac{1}{\sqrt{2}}\left(a_{\vec{k}} + a^\dagger_{-\vec{k}}\right) = p_{-\vec{k}}. \end{aligned} \tag{5}$$

In these variables Euclidean Lagrangian (remember $L_E(V) = L(-V) = H$) reads

$$L_E = \frac{1}{2}\vec{p}^{\,2} + \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{2}\left(\dot{q}^\dagger_{\vec{k}} \dot{q}_{\vec{k}} + q^\dagger_{\vec{k}} q_{\vec{k}} \right) + \left(2\sqrt{2}\pi\alpha\right)^{1/2} \frac{1}{k} e^{i\vec{k}\cdot\vec{x}} q_{\vec{k}} \right\}. \tag{6}$$

The application of path integral technique to the problem at hand consists in *undoing* the second quantization and replacing position operators $q_{\vec{k}}$ by classical variables.

We want to calculate the full partition function

$$\mathcal{Z} = \int dx(0) \int\limits_{x(0)=x(\beta)} \mathcal{D}[x(\tau)] \int dq(0) \int\limits_{q(0)=q(\beta)} \mathcal{D}[q(\tau)]\, e^{-\int_0^\beta dt\, L_E[\dot{x}(t), x(t), \dot{q}(t), q(t)]}. \tag{7}$$

Since for every $\vec{k}$ mode L_E looks like forced oscillator in variables $q_{\vec{k}}$ with

$$f_{\vec{k}}(t) = \left(2\sqrt{2}\pi\alpha\right)^{1/2} \frac{1}{k} e^{i\vec{k}\cdot\vec{x}(t)} \tag{8}$$

we can use the result for $\mathcal{Z}$ obtained previuously

$$\begin{aligned} \mathcal{Z} \;=\; & \int dx(0) \int\limits_{x(0)=x(\beta)} \mathcal{D}[x(\tau)] \qquad (9) \\ & \frac{1}{2\sinh\frac{\beta}{2}} \exp\left\{ -\frac{1}{2}\int\limits_0^\beta dt \frac{d\vec{x}}{dt}^2 + \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} \int\limits_0^\beta dt\, f_{\vec{k}}(t) \int\limits_0^t ds\, f_{\vec{k}}^*(s) \frac{e^{(t-s)-\beta} + e^{-(t-s)}}{1-e^{-\beta}} \right\}. \end{aligned}$$

Note that factor 1/2 in front of the d^3k integral is due to the fact that we integrate over ds up to t rather than to β.

2 Variational approach to the polaron

We shall apply to (9) variational approach based on the equality

$$E - E_0 \leq \frac{1}{\beta} \left\langle S - S_0 \right\rangle_{S_0}. \tag{10}$$

Here S is the effective action derived in the previous section

$$S = \frac{1}{2}\int\limits_0^\beta dt \frac{d\vec{x}}{dt}^2 - \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} \int\limits_0^\beta dt\, f_{\vec{k}}(t) \int\limits_0^t ds\, f_{\vec{k}}^*(s) \frac{e^{(t-s)-\beta} + e^{-(t-s)}}{1-e^{-\beta}} \tag{11}$$

Variation refers to the choice of S_0. Choosing

$$S_0 = \frac{1}{2}\int\limits_0^\beta dt \frac{d\vec{x}}{dt}^2 \tag{12}$$

we have

$$\begin{aligned} S - S_0 &= -2\sqrt{2}\pi\alpha \int \frac{d^3k}{(2\pi)^3} \frac{1}{k^2} \frac{1}{2} \int\limits_0^\beta dt \int\limits_0^t ds\, e^{-i\vec{k}\cdot(\vec{x}(s)-\vec{x}(t))} \frac{e^{(t-s)-\beta} + e^{-(t-s)}}{1-e^{-\beta}} && (13) \\ &= -\frac{\sqrt{2}\alpha}{2} \frac{1}{(2\pi)^2} \int \frac{d^3k}{k^2} \int\limits_0^\beta dt \int\limits_0^t ds\, e^{-i\vec{k}\cdot(\vec{x}(s)-\vec{x}(t))} \frac{e^{(t-s)-\beta} + e^{-(t-s)}}{1-e^{-\beta}}. && (14) \end{aligned}$$

Therefore

$$\frac{1}{\beta} \left\langle S - S_0 \right\rangle_{S_0} = -\frac{\sqrt{2}\alpha}{2\beta} I(\beta) \tag{15}$$

where $I(\beta)$ is given by

$$I(\beta) = \int\limits_{\vec{r}(0)=\vec{x}}^{\vec{r}(\beta)=\vec{x}} \mathcal{D}\left[\vec{r}(\tau)\right] \, e^{-\frac{1}{2}\int\limits_0^\beta d\tau \, \frac{d\vec{r}}{d\tau}^2} \int\limits_0^\beta dt \int\limits_0^t ds \frac{e^{(t-s)-\beta} + e^{-(t-s)}}{1-e^{-\beta}} \frac{1}{(2\pi)^2} \int\limits_0^\infty \frac{d^3k}{k^2} e^{-i\vec{k}\cdot(\vec{r}(s)-\vec{r}(t))} \tag{16}$$

where we have expressed $\langle \ldots \rangle_{S_0}$ explicitly by the path integral. Note that symbol $\langle \ldots \rangle_{S_0}$ includes normalization to the free case, which has not been explicitly included in (16). This will be taken care of later.