Polaron versus Anderson Localization

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I. INTRODUCTION

A *polaron* is an electron in a ionic crystal of volume Ω. The electron polarizes the lattice in its neighborhood. The dispersion in a crystal has two branches: an optical branch $\omega(k)=\omega$ independent of k and an acoustic branch $\omega(k)=vk$, with v the sound velocity, as $k\to 0$. For concreteness we will carry on our discussion assuming a three dimensional crystal.

The Hamiltonian $\mathscr{H}=\mathscr{H}_{\rm ele}+\mathscr{H}_{\rm lat}+\mathscr{H}_{\rm int}$ for the electron of mass m and the lattice is due to Fröhlich [1–3]

$$\mathscr{H}=\frac{\hat{\boldsymbol{p}}^2}{2m}+\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\hbar\omega(k)a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}+i\alpha\sqrt{\frac{\hbar}{mv^4}}\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{\omega^{3/2}(k)}{k}\left[a_{\boldsymbol{k}}^\dagger e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}-a_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right], \tag{1.1}$$

where $\boldsymbol{r}$ is the electron position, $\hat{\boldsymbol{p}}=-i\hbar\boldsymbol{\nabla}$ its conjugate momentum, $a_{\boldsymbol{k}}^\dagger, a_{\boldsymbol{k}}$ are the creation and annihilation operators for a *phonon* of dispersion relation $\omega(k)$ and momentum $\hbar\boldsymbol{k}$, and α is the adimensional coupling constant. We will adopt units such as $\hbar=m=v=1$.

Next we recall that the positions and momenta of the phonons are given by

$$q_{\boldsymbol{k}}=\sqrt{\frac{1}{2\omega(k)}}(a_{\boldsymbol{k}}^\dagger+a_{-\boldsymbol{k}}), \tag{1.2}$$

$$p_{\boldsymbol{k}}=i\sqrt{\frac{\omega(k)}{2}}(a_{-\boldsymbol{k}}^\dagger-a_{\boldsymbol{k}}), \tag{1.3}$$

defining $a'_{\boldsymbol{k}}=-ia_{-\boldsymbol{k}}$ we find $q'_{\boldsymbol{k}}=p_{\boldsymbol{k}}$ and $p'_{\boldsymbol{k}}=-q_{\boldsymbol{k}}$ above and we can rewrite, dropping the primes,

$$\mathscr{H}=\frac{\hat{\boldsymbol{p}}^2}{2}+\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{1}{2}\left[p_{\boldsymbol{k}}^2+\omega(k)^2q_{\boldsymbol{k}}^2\right]+\sqrt{2}\alpha\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{\omega^2(k)}{k}q_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{1.4}$$

where we accomplished the task of rewriting the interaction term as a function of the electron and phonons positions only.

Assume now that the ssystem is in thermal equilibrium at an inverse temperature $\beta=1/k_BT$ with k_B the Boltzmann constant and T the absolute temperature. We will also assume to be at very low temperature. We can then use a path integral [3] to write the polaron partition function

$$\mathscr{Z}=\mathrm{Tr}\left(e^{-\beta\mathscr{H}}\right)=\int_{\substack{\boldsymbol{r}(0)=\boldsymbol{r}(\beta)\\ q_i(0)=q_i(\beta)}}e^{-\mathscr{S}}\,\mathscr{D}\boldsymbol{r}(u)\mathscr{D}q_1(u)\mathscr{D}q_2(u)\cdots, \tag{1.5}$$

where the action integral $\mathscr{S}$ is

$$\mathscr{S}=\int_0^\beta\left\{\frac{\dot{\boldsymbol{r}}^2(u)}{2}+\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{1}{2}\left[\dot{q}_{\boldsymbol{k}}^2+\omega(k)^2q_{\boldsymbol{k}}^2\right]+\sqrt{2}\alpha\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{\omega^2(k)}{k}q_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right\}du. \tag{1.6}$$

The path integral over the phonons in (1.5) can easily be performed [3] because $\dot{q}_{\boldsymbol{k}}$ and $q_{\boldsymbol{k}}$ both appear quadratically and linearly in the action (1.6). The result is [1]

$$\mathscr{Z}=\mathrm{Tr}\left(e^{-\beta\mathscr{H}}\right)=\int_{\boldsymbol{r}(0)=\boldsymbol{r}(\beta)}e^{-S}\,\mathscr{D}\boldsymbol{r}(u), \tag{1.7}$$

$$S=\frac{1}{2}\int_0^\beta\dot{\boldsymbol{r}}^2(u)\,du-\frac{\alpha^2}{2}\int_0^\beta\int_0^\beta\Omega\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{\omega^3(k)}{k^2}e^{i\boldsymbol{k}\cdot[\boldsymbol{r}(t)-\boldsymbol{r}(s)]}e^{-\omega(k)|t-s|}\,dtds. \tag{1.8}$$

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[1] Here we are assuming to be working at low temperature when β is large. The exact result would require to substitute the term $e^{-\omega(k)|t-s|}$ with $e^{-\omega(k)|t-s|}/[1-e^{-\omega(k)\beta}]+e^{\omega(k)|t-s|}e^{-\omega(k)\beta}/[1-e^{-\omega(k)\beta}]$.

For example for an optical polaron one finds [3] for the effective *retarded* interaction potential,

$$V_{\text{eff}}^{\text{opt}} = -\frac{\Omega\alpha^2\omega^3}{8\pi}\frac{e^{-\omega|t-s|}}{|\boldsymbol{r}(s)-\boldsymbol{r}(t)|}, \tag{1.9}$$

whereas for an acoustic polaron one would get [4, 5],

$$V_{\text{eff}}^{\text{aco}} = -\frac{\Omega\alpha^2}{(2\pi)^2}\frac{1}{|\boldsymbol{r}(s)-\boldsymbol{r}(t)|}\int_0^{k_0} dk\, k^2\sin(k|\boldsymbol{r}(s)-\boldsymbol{r}(t)|)e^{-k|t-s|}, \tag{1.10}$$

where k_0 is the Debye cutoff. The effective Hamiltonian for the polaron, after tracing out the phonons degrees of freedom, would then be

$$H = \frac{\hat{p}^2}{2} + V_{\text{eff}}(|\boldsymbol{r}-\boldsymbol{r}'|, |t-t'|). \tag{1.11}$$

But one is free to choose even more exotic dispersion relations....

A. Anderson localization

We may think at the effective retarted interaction potential of the polaron problem as the Anderson site-site potential V_{And} [6] which determines the dynamics of his probability amplitude $a(\boldsymbol{r}, t)$. On the continuum, Anderson equation reads

$$i\frac{\partial a(\boldsymbol{r},t)}{\partial t} = Ha(\boldsymbol{r},t) = E(\boldsymbol{r})a(\boldsymbol{r},t) + \int d\boldsymbol{r}'\, V_{\text{And}}(|\boldsymbol{r}-\boldsymbol{r}'|)a(\boldsymbol{r}',t), \tag{1.12}$$

where $E(\boldsymbol{r})$ is a stochastic variable with probability distribution $P(E)dE$ with a width $[-W, W]$. Anderson discretizes the d-dimensional space $\boldsymbol{r} = (x_1, x_2, \ldots, x_d)$ into a lattice.

At equilibrium we may assume that V_{eff} will not depend on the time interval so that $V_{\text{eff}}(\Delta r, \Delta t) \approx V_{\text{eff}}(\Delta r)$ with $\Delta r = |\boldsymbol{r}-\boldsymbol{r}'|$ and $\Delta t = |t-t'|$.

When studied in imaginary time $t \to -i\beta$ Anderson equation (1.12) can be thought as the Bloch equation for a thermal density matrix a.

In Ref. [4, 5] we studied the low temperature properties of an acoustic polaron through a path integral Monte Carlo study and we ...

II. CONCLUSIONS

AUTHOR DECLARATIONS

Conflicts of interest

None declared.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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