Polaron versus Anderson Localization

Riccardo Fantoni*

Università di Trieste, Dipartimento di Fisica, strada Costiera 11, 34151 Grignano (Trieste), Italy
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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 $\omega(k) = \omega > 0$ independent of k and an acoustic branch $\omega(k) = vk$, with $v > 0$ the sound velocity, as $k \to 0$. For concreteness we will carry on our discussion assuming a three dimensional crystal.

The Hamiltonian $\mathscr{H} = \mathscr{H}_{\text{ele}} + \mathscr{H}_{\text{lat}} + \mathscr{H}_{\text{int}}$ 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 that $\hbar = m = v = 1$.

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 $a_{\boldsymbol{k}}' = -i a_{-\boldsymbol{k}}$ we find $q_{\boldsymbol{k}}' = p_{\boldsymbol{k}}$ and $p_{\boldsymbol{k}}' = -q_{\boldsymbol{k}}$ above and we can rewrite, dropping the primes,

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

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 $\beta = 1/k_B T$ 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 manipulate the polaron density matrix $\rho = e^{-\beta\mathscr{H}}$ and write the partition function

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

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

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

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]

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

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

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* riccardo.fantoni@scuola.istruzione.it

[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.

But one is free to choose even more exotic dispersion relations. For example for $\omega^3(k)/k^2 \propto k^{\gamma-d}$ as $k \to 0$ then $V_{\text{eff}} \propto \Delta r^{-\gamma}$ for $\Delta r = |\boldsymbol{r}(s) - \boldsymbol{r}(t)| \to \infty$ with $0 < \gamma < d, \gamma \neq d-2$ where d is the space dimension. Moreover V_{eff} will decay faster than any inverse power of Δr whenever $\omega^3(k)/k^2$ is analytic as $k \to 0$ [6].

The effective Hamiltonian for the polaron, after tracing out the phonons degrees of freedom, would then be

$$H = \frac{\hat{p}^2}{2} + V_{\text{eff}}(\Delta r, \Delta t). \tag{1.11}$$

with $\Delta r = |\boldsymbol{r} - \boldsymbol{r}'|$ and $\Delta t = |t - t'|$. And the density matrix satisfies the effective Bloch equation

$$-\frac{\partial \rho}{\partial \beta} = H\rho. \tag{1.12}$$

where the coordinate representation of the density matrix $\rho(\boldsymbol{r}, \boldsymbol{r}'; \beta)$ satisfies the initial condition $\rho(\boldsymbol{r}, \boldsymbol{r}'; 0) = \delta(\boldsymbol{r} - \boldsymbol{r}')$.

A. Anderson localization

We may think at the effective retarted interaction potential of the polaron problem as the Anderson site-site potential V^{And} [7] which determines the dynamics of his probability amplitude $a(\boldsymbol{r}, t)$. On the continuum, Anderson equation reads

$$i\frac{\partial a(\boldsymbol{r}, t)}{\partial t} = Ha(\boldsymbol{r}, t) = E(\boldsymbol{r})a(\boldsymbol{r}, t) + \int d\boldsymbol{r}' \, V^{\text{And}}(|\boldsymbol{r} - \boldsymbol{r}'|)a(\boldsymbol{r}', t), \tag{1.13}$$

where $E(\boldsymbol{r})$ is a stochastic variable with probability $p(E, \boldsymbol{r})dE$ that $E(\boldsymbol{r})$ assumes values in $[E(\boldsymbol{r}), E(\boldsymbol{r}) + dE]$. This probability distribution has a width $[-\zeta, \zeta]$. Anderson discretizes the d-dimensional space $\boldsymbol{r} = (x_1, x_2, \ldots, x_d)$ into a lattice.

When studied in imaginary time $t \to -i\beta$ Anderson equation (1.13) can be thought as the Bloch equation for a thermal density matrix a. Also, it is a Langevin equation where the first term on the right hand side is a noise term and the second term is a drift term

$$-\frac{\partial a_j(\beta)}{\partial \beta} = E_j a_j(\beta) + \sum_i V_{ji}^{\text{And}} a_i(\beta), \tag{1.14}$$

where V_{jj}^{And} in the sum may diverge to minus infinity.

We can then use Ito calculus [8] to write the corresponding Fokker-Planck equation to the stochastic differential equation (1.14), which describes the time evolution of the for the transition probability $p(\boldsymbol{a}, \boldsymbol{a}^0; \beta - \beta^0)$ that the stochastic process assumes the values $\boldsymbol{a} = (a_1, a_2, \ldots, a_N)$ at time β when it had assumed the values $\boldsymbol{a}^0$ at time β^0. Here we imagine a finite lattice made of N sites.

Assuming that the noise term is characterized by white noise $E_j = \xi_j$ (see Appendix A) one finds [8] [2]

$$\frac{\partial p(\boldsymbol{a}, \boldsymbol{a}^0; \beta - \beta^0)}{\partial \beta} = \left[\sum_i V_{ii}^{\text{And}} + \frac{N^2}{2}\right] p(\boldsymbol{a}, \boldsymbol{a}^0; \beta - \beta^0), \tag{1.15}$$

$$p(\boldsymbol{a}^0, \boldsymbol{a}^0; 0) = 1. \tag{1.16}$$

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[2] Note, that the Fokker-Planck equation (1.15) holds for the stochastic differential equation (1.14) only within the framework of Ito calculus. The relation between (1.14) and the Fokker-Planck equation is slightly different when Stratonovitch calculus is applied! Note also that the amplitude ζ of the stochastic kick does not enters in (1.15) only for our particular choice of the white noise, for more general stochastic variables E_j this will not be true anymore.

The solution for p can then be easily determined as

$$p(\boldsymbol{a}, \boldsymbol{a}^0; \Delta\beta) = \exp\left[\Lambda\Delta\beta\right], \tag{1.17}$$

$$\Lambda = \sum_i V_{ii}^{\text{And}} + \frac{N^2}{2}, \tag{1.18}$$

where $\Delta\beta = \beta - \beta^0$ and Λ is determined by a balance between two diverging terms. If $\Lambda > 0$, p diverges at large β whereas if $\Lambda < 0$ it decays to zero. So as Λ changes from positive to negative we have a phase transition from an extended state to a localized state around the initial position $\boldsymbol{a}^0$. The unconditional probability for the realization of $\boldsymbol{a}^1, \boldsymbol{a}^2, \dots$ at times $\beta^1, \beta^2, \dots$ will then be $p(\boldsymbol{a}^0, \boldsymbol{a}^1, \boldsymbol{a}^2, \dots) = p(\boldsymbol{a}^0)p(\boldsymbol{a}^1, \boldsymbol{a}^0; \Delta\beta)p(\boldsymbol{a}^2, \boldsymbol{a}^1; \Delta\beta) \dots$ with $p(\boldsymbol{a}^0)$ the unconditional probability at the initial time. Given the unconditional probability and the transition probability we can completely characterize the Markov process.

In Ref. [4, 5] we studied the low temperature properties of an acoustic polaron through Path Integral Monte Carlo (PIMC) and we found the existence of a phase transition from an extended state to a localized state as the phonons–electron coupling constant α is increased at constant temperature or as the temperature is decreased at constant α.

Comparing the polaron and the Anderson problems we see that the interaction terms in the stochastic differential Bloch equation (1.14) and in the partial differential Bloch equation (1.12) are similar and the kinetic term is deterministic in the polaron case and stochastic in the Anderson case. Therefore the probability amplitude in the Anderson problem, a, is a stochastic variable determined by the conditional probability $p(\boldsymbol{a}, \boldsymbol{a}'; \beta)$ and the coordinate representation of the density matrix in the polaron problem, $\rho(\boldsymbol{r}, \boldsymbol{r}'; \beta)$, is a determined function. At equilibrium we may assume that V_{eff} will not depend on the time interval so that $V_{\text{eff}}(\Delta r, \Delta t) \approx V_{\text{eff}}(\Delta r)$. We may then propose the following identification between the two problems

$$p \leftrightarrow \rho \qquad V^{\text{And}} \leftrightarrow V_{\text{eff}} \qquad \boldsymbol{a} \leftrightarrow \boldsymbol{r}, \tag{1.19}$$

where the site j in the Anderson problem plays the role of the polaron position. There is no exact analytic solution for the polaron problem so one must resort to an exact numerical solution like PIMC for example. In Ref. [4, 5] we performed some PIMC simulations showing that an acoustic polaron path $\boldsymbol{r}(t)$ becomes localized as one lowers the temperature, β large, or increases the coupling constant, α large, as predicted in 1933 by Landau [9–11]. The localization has not yet been observed in an optical polaron. It is believed that the existence of a localized or self-trapped path depends crucially on the dispersion relation. In the optical case $\omega^3(k)/k^2 \propto 1/k^2$ which is the special Coulombic case among the various long range cases which seem to prevent the self-trapped-state (TS) in favor of an extended-state (ES). On the other hand it is believed that a dispersion relation giving rise to a short range effective interaction, $V_{\text{eff}} \propto \Delta r^{-\gamma}$ with $\gamma > d$, would sustain the localization. This same relation that occurs between the existence of the translational symmetry breaking among the ES and the TS and the asymptotic behavior of the effective interaction holds also in the Anderson problem [7] where the path $j(t)$ is described by stochastic jumps amongst the different lattice sites.

Recent work has shown that a non interacting Anderson localized system can become many body localized. On the other hand theoretical treatments have been extended from one polaron to many polaron systems [12–14]. Already two polarons are expected to have counterintuitive properties like attraction between the two electrons due to the energy lowering as the two electrons come together therefore sharing their deformations of the underlying crystal. This could lead to a bound bipolaron. For strong attraction, bipolarons may be small. Small bipolarons have integer spin and thus share some of the properties of bosons. If many bipolarons form without coming too close, they might be able to form a Bose-Einstein condensate. This has led to a suggestion that bipolarons could be a possible mechanism for high-temperature superconductivity.

II. CONCLUSIONS

Appendix A: White noise

An important idealized stochastic process is the so-called "Gaussian white noise". This process, denoted by $\xi(t)$, is not characterized through transition probabilities, but through the following statistical moment and correlation function

$$\langle \xi_i \rangle = 0, \tag{A1}$$

$$\langle \xi_i \xi_j \rangle = \zeta \delta_{ij}, \tag{A2}$$

were $\langle\ldots\rangle = \int \ldots p(\xi_i)d\xi$ with $p(\xi_i)d\xi$ the probability that ξ_i assumes values in $[\xi_i, \xi_i + d\xi]$ on site i. The attribute Gaussian implies that all cumulants higher than of second order are 0.

The reason why this process is termed "white" is connected with its correlation function (A2), the Fourier transform of which is constant, i.e., entails all frequencies with equal amplitude just as white radiation. The importance of the process ξ_i comes from the fact that many other stochastic processes are described through stochastic differential equations with a (white) noise term ξ_i.

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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