Polaron versus Anderson Localization

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We compare two kinds of affine localizations in physics: the localization in a short range polaron and the one in the Anderson stochastic model. The conditions on the interaction potential necessary to see the transnational symmetry breaking localization phase transition is identical in the two problems. We therefore suggest that they should belong to the same universality class of the renormalization group for the localization phase transition.

Keywords: Polaron localization; Anderson localization; renormalization group

I. INTRODUCTION

In physics, *phase transitions* occur in a many body system only in the mathematical thermodynamic limit. In a one body system it is necessary, on the other hand, to imagine a *background* that drives the body change of behavior in correspondence of the phase transition. In this short work we will consider two examples of backgrounds. A deterministic one made of a ionic crystal in the thermodynamic limit and a stochastic one made of a disordered medium with probability amplitudes of sites occupation. The former is the problem of a polaron [1] and the latter is Anderson problem [2] where the thermodynamic limit is substituted with a probabilistic description of the sites occupation. The change in behavior for the body observed in both systems is that from an *extended state* to a *localized state* where we have a transnational symmetry breaking. The existence of the phase transition requires a short range interaction potential in both cases: the retarded potential for the polaron and the site-site potential for the Anderson problem. The transition from one state to the other depends on the coupling constant with the background in the deterministic case and on the width of the probability distribution of the stochastic noise giving rise to the "kinetic" energy contributing for the jumps between Anderson sites.

We will then describe first the polaron localization problem and then the Anderson localization problem and suggest that the two should belong to the same universality class of the renormalization group describing the physical localization phase transition.

It is no surprise that the Anderson problem has played a relevant role in the modellization of the Metal-to-Insulator-Transition (MIT) [3, 4].

II. TWO KINDS OF LOCALIZATIONS

In this section we compare two kinds of affine localizations in physics: the localization in a short range (deterministic) polaron and the one in the Anderson stochastic model.

A. Polaron localization

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, 5, 6]

$$\mathscr{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \hbar\omega(k) a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + i\alpha\sqrt{\frac{\hbar}{mv^4}}\Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\omega^{3/2}(k)}{k} \left[a_{\boldsymbol{k}}^\dagger e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} - a_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \right], \qquad (2.1)$$

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 $\hbar = m = v = 1$.

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

$$q_{\boldsymbol{k}} = \sqrt{\frac{1}{2\omega(k)}}(a_{\boldsymbol{k}}^\dagger + a_{-\boldsymbol{k}}), \tag{2.2}$$

$$p_{\boldsymbol{k}} = i\sqrt{\frac{\omega(k)}{2}}(a_{-\boldsymbol{k}}^\dagger - a_{\boldsymbol{k}}), \tag{2.3}$$

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,

$$\mathscr{H} = \frac{\hat{\boldsymbol{p}}^2}{2} + \Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{1}{2} \left[p_{\boldsymbol{k}}^2 + \omega(k)^2 q_{\boldsymbol{k}}^2 \right] + \sqrt{2}\alpha\Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\omega^2(k)}{k} q_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{2.4}$$

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 [6] to manipulate the polaron density matrix $\rho = e^{-\beta\mathscr{H}}$ and write the partition function

$$\mathscr{Z} = \mathrm{Tr}\left(e^{-\beta\mathscr{H}}\right) = \int_{\substack{\boldsymbol{r}(0)=\boldsymbol{r}(\beta) \\ q_i(0)=q_i(\beta)}} e^{-\mathscr{S}} \mathscr{D}\boldsymbol{r}(u)\mathscr{D}q_1(u)\mathscr{D}q_2(u)\cdots, \tag{2.5}$$

where $\mathrm{Tr}(\cdot)$ is the operator trace and the action integral $\mathscr{S}$ is

$$\mathscr{S} = \int_0^\beta \left\{ \frac{\dot{\boldsymbol{r}}^2(u)}{2} + \Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{1}{2} \left[\dot{q}_{\boldsymbol{k}}^2 + \omega(k)^2 q_{\boldsymbol{k}}^2 \right] + \sqrt{2}\alpha\Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\omega^2(k)}{k} q_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \right\} du. \tag{2.6}$$

The path integral over the phonons in (2.5) can easily be performed [6] because $\dot{q}_{\boldsymbol{k}}$ and $q_{\boldsymbol{k}}$ both appear quadratically and linearly in the action (2.6). The result is [1]

$$\mathscr{Z} = \mathrm{Tr}\left(e^{-\beta\mathscr{H}}\right) = \int_{\boldsymbol{r}(0)=\boldsymbol{r}(\beta)} e^{-S_H} \mathscr{D}\boldsymbol{r}(u), \tag{2.7}$$

$$S_H = \frac{1}{2}\int_0^\beta \dot{\boldsymbol{r}}^2(u)\,du - \frac{\alpha^2}{2}\int_0^\beta \int_0^\beta \Omega \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{\omega^3(k)}{k^2} e^{i\boldsymbol{k}\cdot[\boldsymbol{r}(t)-\boldsymbol{r}(s)]} e^{-\omega(k)|t-s|}\,dtds. \tag{2.8}$$

For example for an optical polaron one finds [6] for the effective *retarded* interaction potential,

$$V_{\mathrm{eff}}^{\mathrm{opt}} = -\frac{\Omega\alpha^2\omega^3}{8\pi} \frac{e^{-\omega|t-s|}}{|\boldsymbol{r}(s)-\boldsymbol{r}(t)|}, \tag{2.9}$$

whereas for an acoustic polaron one would get [7, 8],

$$V_{\mathrm{eff}}^{\mathrm{aco}} = -\frac{\Omega\alpha^2}{(2\pi)^2} \frac{1}{|\boldsymbol{r}(s)-\boldsymbol{r}(t)|} \int_0^{k_0} dk\, k^2 \sin(k|\boldsymbol{r}(s)-\boldsymbol{r}(t)|)e^{-k|t-s|}, \tag{2.10}$$

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 $V_{\mathrm{eff}} \propto \Delta r^{-\gamma}$ 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 $k \to 0$ [9].

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

$$H = \frac{\hat{p}^2}{2} + V_{\mathrm{eff}}(\Delta r, \Delta t). \tag{2.11}$$

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

$$-\frac{\partial\rho}{\partial\beta} = H\rho. \tag{2.12}$$

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

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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 $e^{-\omega(k)|t-s|}/[1-e^{-\omega(k)\beta}] + e^{\omega(k)|t-s|}e^{-\omega(k)\beta}/[1-e^{-\omega(k)\beta}]$.

B. Anderson localization

We may think at the effective retarted interaction potential of the polaron problem as the Anderson site-site potential V^{And} [2] which determines the dynamics of his *probability amplitude* $a(\boldsymbol{r}, t)$. On the continuum, Anderson equation reads

$$i\frac{\partial a(\boldsymbol{r}, t)}{\partial t} = Ha(\boldsymbol{r}, t) = E(\boldsymbol{r})a(\boldsymbol{r}, t) + \int d\boldsymbol{r}' \, V^{\text{And}}(|\boldsymbol{r} - \boldsymbol{r}'|)a(\boldsymbol{r}', t), \tag{2.13}$$

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 (2.13) can be thought as the Bloch equation for a thermal density matrix a_j at each lattice site. 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

$$-\frac{\partial a_j(\beta)}{\partial \beta} = E_j a_j(\beta) + \sum_{i \neq j} V_{ji}^{\text{And}} a_i(\beta). \tag{2.14}$$

We can then use Ito calculus [10] to write the Fokker-Planck equation corresponding to the stochastic differential equation (2.14), which describes the time evolution of 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 Gaussian white noise $E_j = \xi_j$ (see Appendix A) one finds [10] [2]

$$\frac{\partial p(\boldsymbol{a}, \boldsymbol{a}^0; \beta - \beta^0)}{\partial \beta} = \Lambda p(\boldsymbol{a}, \boldsymbol{a}^0; \beta - \beta^0), \tag{2.15}$$

$$\Lambda = \sum_{i \neq j} V_{ji}^{\text{And}} a_i \frac{\partial}{\partial a_j} + \sum_i \frac{\partial^2}{\partial a_i^2} a_i^2, \tag{2.16}$$

$$p(\boldsymbol{a}^0, \boldsymbol{a}^0; 0) = 1, \tag{2.17}$$

Where Λ is made up of two differential operators acting on p. The unconditional probability for the realization of $\boldsymbol{a}^1, \boldsymbol{a}^2, \ldots$ at times $\beta^1, \beta^2, \ldots$ will then be $p(\boldsymbol{a}^0, \boldsymbol{a}^1, \boldsymbol{a}^2, \ldots) = p(\boldsymbol{a}^0; \beta^0)p(\boldsymbol{a}^1, \boldsymbol{a}^0; \Delta\beta)p(\boldsymbol{a}^2, \boldsymbol{a}^1; \Delta\beta) \ldots$ with $p(\boldsymbol{a}^0; \beta^0)$ the unconditional probability at the initial time. Given the unconditional probability and the transition probability we can completely characterize the Markov process.

In Ref. [7, 8] 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" (2.14) and in the partial differential Bloch equation (2.12) 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, $\boldsymbol{a}$, is a stochastic vector determined by the conditional probability $p(\boldsymbol{a}, \boldsymbol{a}'; \beta)$ and the coordinate representation of the density matrix in the polaron problem $\rho(\boldsymbol{r}, \boldsymbol{r}'; \beta)$ play parallel roles. We may then propose the following identification between the two problems

$$p \leftrightarrow \rho \qquad \Lambda \leftrightarrow H \qquad \boldsymbol{a} \leftrightarrow \boldsymbol{r}, \tag{2.18}$$

where the probability amplitude vector $\boldsymbol{a}$ in the Anderson problem plays the role of the polaron position $\boldsymbol{r}$. In the two problems the solution of the Bloch equation for the density matrix of the polaron problem and the solution of the Fokker-Planck equation for the conditional probability of the amplitude vector $\boldsymbol{a}$ require a path integral. In fact if one is only interested in the probability distribution of the ending value of the probability amplitude vector at a

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[2] Note, that the Fokker-Planck equation (2.15) holds for the stochastic differential equation (2.14) only within the framework of Ito calculus. The relation between (2.14) 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 enter in (2.15) for our particular choice of the Gaussian white noise, but for more general asymmetric stochastic variables E_j this will not be the case anymore.

large β one has to compute

$$p(\boldsymbol{a};\beta) = \int d\boldsymbol{a}^0 d\boldsymbol{a}^1 d\boldsymbol{a}^2 \ldots p(\boldsymbol{a}^0;\beta^0)p(\boldsymbol{a}^1,\boldsymbol{a}^0;\Delta\beta)p(\boldsymbol{a}^2,\boldsymbol{a}^1;\Delta\beta)\ldots p(\boldsymbol{a},\boldsymbol{a}^{M-1};\Delta\beta) \qquad (2.19)$$

$$= \int d\boldsymbol{a}^0 p(\boldsymbol{a}^0;\beta^0) \int_{\substack{\boldsymbol{a}(\beta^0)=\boldsymbol{a}^0 \\ \boldsymbol{a}(\beta)=\boldsymbol{a}}} e^{-S_\Lambda} \mathscr{D}\boldsymbol{a}(t), \qquad (2.20)$$

where in Eq. (2.19) we discretized also the imaginary time so that $\Delta\beta = (\beta - \beta^0)/M = \tau$. In the limit of M very large we can rewrite this equation in terms of a path integral as in Eq. (2.20) where we indicated with S_Λ the "action" which determines the dynamics (2.15) of the stochastic probability amplitude vector $\boldsymbol{a}$ [3]. As is shown in Appendix B the short time propagator $p(\boldsymbol{a},\boldsymbol{a}';\tau)$ is made up of three terms, two delta functions and a Gaussian. In reconstructing the path integral, the product of all the first delta functions in Eq. (B1) will simply contribute to the probability for the path to remain fixed at $\boldsymbol{a}_0$. All the other product terms will be responsible for the probability of a jump between one site and another.

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. [7, 8] 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 [12–14]. 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 connection that occurs between the existence of the translational symmetry breaking between the ES and the TS and the asymptotic behavior of the effective interaction *surprisingly* holds also in the Anderson problem [2] where the path $\boldsymbol{a}(t)$ 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 [15–17]. 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.

III. RENORMALIZATION GROUP

The findings of the previous section should not be so surprising after all and certainly suggest that the polaron localization problem and the Anderson localization problem belong to the same *universality class* of the Renormalization Group (RG) [18] with a *fixed point* corresponding to the localization phase transition. We can then think of a *reduced Hamiltonians* very large space $\mathscr{H}[\boldsymbol{Q};\boldsymbol{K}]$ to which the two *physical Hamiltonians* H and Λ belong. Where $\boldsymbol{Q}$ stands for the "coordinate variables" ($\boldsymbol{r}$ for the polaron problem and $\boldsymbol{a}$ for the Anderson problem) and $\boldsymbol{K}$ are the various *thermodynamic fields* like the temperature that can be controlled directly by the experimenter and others that embody details of the physical system that are "fixed by nature". At the heart of RG theory there is the renormalization of the "coordinates" via $\boldsymbol{Q} \to \boldsymbol{Q}' = b\boldsymbol{Q}$ with $b > 0$ [4]. Iterating this scaling transformation l times we can introduce the *flow parameter* $l = \log_b(Q'/Q)$ from which we can derive a *differential* or continuous RG flow as $d\mathscr{H}/dl = \mathcal{B}\mathscr{H}$. So that starting from the physical critical point on the *physical manifold* $\mathscr{H}$, after the first iteration we reach the first renormalized critical point for $\mathscr{H}'[\boldsymbol{Q}';\boldsymbol{K}']$ on the first renormalized manifold $\mathscr{H}'$. Repeating many times the scaling transformation we can then follow the critical trajectories of the various subsequent renormalized critical points and eventually reach a *nontrivial* fixed point $\mathscr{H}^*$ such that $\mathcal{B}\mathscr{H}^* = 0$. All physical Hamiltonians whose critical trajectories converge to the same fixed point belong to the same universality class. We can then choose an expansion [19–25] on the *tangent space* to the smooth Hamiltonian space at the fixed point $\mathscr{H}^*$ to determine the various *critical exponents*. In fact we expect that something similar to what happens for the (short range) Ising model, which share the same critical exponents [26], should also happen here where one expects a strong dependence on dimensionality (2 is expected to be the lower critical dimension of the localization problem).

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[3] Note that the use of Trotter formula [11] requires that the two addend operators in Λ of Eq. (2.16) be bounded from below.

[4] Note that for the polaron localization problem iteration of such scaling would simply bring the TS into an ES and in the Anderson localization problem it will affect the site probability amplitudes again producing delocalization.

IV. CONCLUSIONS

We compared the localization that occurs in a short range polaron and the Anderson localization that occurs for a short range site-site interaction. We put the two systems side by side on the "mirror" of the renormalization group suggesting that they should belong to the same universality class. It would be interesting to find other physical Hamiltonians whose critical flows for the translational symmetry breaking of the localization phase transition fall on the same fixed point. It would also be interesting to study the dependence on dimensionality of the fixed point.

Appendix A: Gaussian noise

An important idealized stochastic process is the so-called Gaussian white noise. This process, denoted by ξ_i, is not characterized through transition probabilities, but through the following statistical moment and correlation function

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

$$\langle \xi_i \xi_j \rangle = \zeta^2 \delta_{ij}, \tag{A2}$$

were $\langle \ldots \rangle = \int \ldots p_{\mathrm{wn}}(\xi) d\xi$ with $p_{\mathrm{wn}}(\xi) d\xi$ the Gaussian probability that ξ assumes values in $[\xi, \xi + d\xi]$ on a given site. All cumulants higher than of second order are 0. The integral of white noise over imaginary time is a Wiener process $\omega(\beta)$ with $d\omega = \xi d\beta$ and unconditional and conditional probabilities distributions

$$p_{\mathrm{W}}(\omega; \beta) = \frac{1}{\sqrt{2\pi\zeta^2\beta}} e^{-\omega^2/2\zeta^2\beta}, \tag{A3}$$

$$p_{\mathrm{W}}(\omega, \omega'; \beta - \beta') = \frac{1}{\sqrt{2\pi\zeta^2\Delta\beta}} e^{-(\Delta\omega)^2/2\zeta^2\Delta\beta}, \tag{A4}$$

with $\Delta\omega = \omega - \omega'$ and $\Delta\beta = \beta - \beta'$. It is this last process that enters in Ito calculus [10].

Appendix B: Anderson "action"

Using, as usual, the set of orthonormal plane waves we find for the Anderson short time conditional probability in Eq. (2.19) the following expression

$$p(\boldsymbol{a}, \boldsymbol{a}'; \tau) \propto \prod_{i=1}^{N} \left\{ e^{\tau 2N} \delta(a_i - a_i') + \delta \left[(1 + 4\tau)a_i + \tau \sum_{i \neq j} V_{ij}^{\mathrm{And}} a_j - a_i' \right] + \sqrt{\frac{2\pi}{\tau a_i^2}} e^{-(1 - a_i'/a_i)^2/\tau} \right\}, \tag{B1}$$

where δ is a one dimensional Dirac delta.

The unconditional probability of Eq. (2.20) and the averages stemming from it can then be numerically computed exactly through the Path Integral Monte Carlo (PIMC) method [27], for example.

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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