Edwards Localization

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We study the localization problem in quantum stochastic mechanics. We start from the Edwards model for a particle in a bath of scattering centers and prove static localization of the ground state wavefunction of the particle in a one dimensional square well coupled to Dirac delta like scattering centers in arbitrary but fixed positions. We see how the localization increases for increasing coupling g. Then we choose the scattering centers positions as pseudo random numbers with a uniform probability distribution and observe an increase in the localization of the average of the ground state over the many positions realizations. We discuss how this averaging procedure is consistent with a picture of a particle in a Bose-Einstein condensate of of non interacting boson scattering centers interacting with the particle with Dirac delta functions pair potential. We then study the dynamics of the ground state wave function. We conclude with a discussion of the affine quantization version of the Lax model which reduces to a system of contiguous square wells with walls in arbitrary positions independently of the coupling constant g.

Keywords: Polaron localization; Anderson localization; Edwards localization

I. INTRODUCTION

In a recent work [1] we compared the localization property of a short range polaron and of the (Wick rotated) Anderson problems. In particular we showed how it is possible to study the thermal properties of the electron in a ionic crystal background, for the polaron problem, or of a particle with stochastic kinetic energy interacting with a background of scattering sites, for the Anderson problem, through a path integral description, after integrating out the degrees of freedom of the background.

Here we study a third kind of localization that occurs in the Edwards model of a particle with deterministic kinetic energy interacting with a background of scattering centers with stochastic positions after integrating out the degrees of freedom of the background. As the above two examples the washing out of the degrees of freedom of the background can be treated with Monte Carlo Path Integral methods in real or imaginary time. Here we will stick with real time.

While in the polaron problem both the particle and the background have a deterministic description, in the Anderson model the (kinetic energy of the) particle has a stochastic description, and in the Edwards model the (positions of the scattering centers forming the) background has a stochastic description. Nonetheless in all three cases we observe a localization phase transition of the particle interacting with the background. In particular here we will see how, in the Edwards model, the localization occurs on a circle independently of the strength g of the coupling between particle and background and of the switching on or off of the disorder. Increasing g or switching on aleatoricity of the background scattering centers positions simply increases (make more sharp) the localization of the particle ground state, static or dynamic, wavefunction.

In order to justify the Monte Carlo integration of the wavefunction of the particle and the background respect to the background degrees of freedom (the scattering centers positions) we will consider a background made of non interacting bosons scattering centers in their Bose-Einstein condensed phase [2].

II. EDWARDS MODEL

Consider [2] a d-dimensional system made of a particle of mass m in a periodic box of volume $\Omega = L^d$ interacting with N free spinless bosonic scattering centers of mass m_c at a density $\rho = N/\Omega$ and temperature $T < T_C$ with

$$T_C = \frac{2\pi\hbar^2}{m_c k_B}\sqrt{\frac{\rho}{\zeta(d/2)}}, \tag{2.1}$$

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the critical temperature for Bose-Einstein condensation, where $\hbar$ is Planck constant, k_B is Boltzmann constant, and ζ is Riemann zeta function. Moreover let $v(\boldsymbol{r})$ be the pairwise interaction potential between the particle and the centers according to *Edwards model* [3].

Then the wave function of the whole system will be $\Psi(\boldsymbol{x};\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)$ where $\boldsymbol{x}$ is the position of the particle and $\{\boldsymbol{r}_i\}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)$ are the positions of the N scattering centers. If we neglect the interaction between the N bosons and the particle we may write the normalized wave function of the centers as follows

$$\Phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)=\frac{1}{\sqrt{N!}}\mathrm{perm}||\phi_j(\boldsymbol{r}_i)||, \tag{2.2}$$

in terms of the permanent of the N normalized wave functions of each center

$$\phi_j(\boldsymbol{r}_i)=\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}_j\cdot\boldsymbol{r}_i}, \tag{2.3}$$

with $\boldsymbol{k}_j=2\pi\boldsymbol{n}_j/L$ and $\hbar\omega_j=(\hbar k_j)^2/2m_c$ his energy. Here $\boldsymbol{n}$ is a d-dimensional vector with integer components. Now below the critical temperature T_C the N centers will undergo condensation into the $\boldsymbol{n}_j=\boldsymbol{0}$ state. So that we will have

$$\Phi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\propto\int_\Omega\prod_{j=1}^{N}\delta^{(d)}(\boldsymbol{r}-\boldsymbol{r}_j)\,d\boldsymbol{r}_1d\boldsymbol{r}_2\cdots d\boldsymbol{r}_N, \tag{2.4}$$

where $\delta^{(d)}$ is the Dirac d-dimensional delta function. In general we may expand the wave function Ψ into a basis of product states $\psi(\boldsymbol{x})\Phi(\{\boldsymbol{r}_i\})$. We may also define

$$\begin{aligned}\widetilde{\Psi}(\boldsymbol{x})&=\langle\Psi(\boldsymbol{x};\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\rangle\\&=\frac{1}{\Omega^N}\int_\Omega\Psi(\boldsymbol{x};\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\,d\boldsymbol{r}_1d\boldsymbol{r}_2\ldots d\boldsymbol{r}_N.\end{aligned} \tag{2.5}$$

Clearly if we can neglect the interaction between the N bosons and the particle we will have $\widetilde{\Psi}\propto\psi$, but this is not true anymore in presence of a coupling between the particle and the scattering centers.

The Hamiltonian of the whole system

$$H=\frac{p^2}{2m}+\sum_j\hbar\omega_j+\sum_j v(\boldsymbol{x}-\boldsymbol{r}_j), \tag{2.6}$$

where $\boldsymbol{p}$ is the momentum of the particle, may also be rewritten, at $T<T_C$, as the following operator [1]

$$\begin{aligned}\hat{H}&=\frac{p^2}{2m}+\sum_j\hbar\omega_j\hat{b}_j^\dagger\hat{b}_j+\int_\Omega\sum_j v(\boldsymbol{x}-\boldsymbol{r}')\hat{b}_j^\dagger\hat{b}_j\,d\boldsymbol{r}'\\&=\frac{p^2}{2m}+\int_\Omega\sum_j v(\boldsymbol{x}-\boldsymbol{r}')\hat{b}_j^\dagger\hat{b}_j\,d\boldsymbol{r}',\end{aligned} \tag{2.7}$$

where $\hat{b}_j^\dagger$ is the creation operator of scattering center j such that the number operator $\hat{n}_j=\hat{b}_j^\dagger\hat{b}_j$, for example, in his position $\boldsymbol{r}$ representation acts as follows $\hat{n}_j|0\rangle=\delta^{(d)}(\boldsymbol{r}-\boldsymbol{r}_j)$, with $|0\rangle$ the vacuum defined as the state that is annihilated by the destruction operator $\hat{b}_j$. In the second equality of Eq. (2.7) we explicitly used the fact that below the Bose-Einstein critical temperature the N boson scattering centers are all in their condensed phase at $\omega_j=0$ for all j. Here we are thinking at the condensed N scattering centers as being independent one from the other and non interacting among themselves so that Eq. (2.4) may be rewritten as

$$\Phi(\{\boldsymbol{r}_j\})=\left(\prod_j\int_\Omega\hat{n}_j\,d\boldsymbol{r}_j\right)|0\rangle. \tag{2.8}$$

Then the Hamiltonian of Eq. (2.6) is the result of the action of the operator $\hat{H}$ of Eq. (2.7) on the vacuum. Written in the form of Eq. (2.7) the Edwards Hamiltonian resembles the polaron Hamiltonian [1, 4, 5]. In particular the recipe of Eq. (2.5) of washing out the degrees of freedom of the scattering centers by averaging on their positions finds its justification in the need of a polaron description [1].

In the next Section III we will choose a particular form for v and will see how the averaging recipe of Eq. (2.5) favors localization.

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[1] Here we use the hat only for the operators acting on the scattering centers vacuum and not on the operators of the particle.

III. THE LAX MODEL WITH CANONICAL QUANTIZATION

Lax and Phillips choose $d = 1$ and $v(x) = g\delta(x)$ [6] with g the coupling constant between the particle and the boson scattering centers in their condensed phase so that the kinetic energy of the bosons can be neglected in the Hamiltonian of Eq. (2.6) as in Eq. (2.7)

$$H = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} + g\sum_{j=1}^{N}\delta(x - r_j), \tag{3.1}$$

where we set $\hbar = 1$ and we may order $0 < r_1 < r_2 < \ldots < r_N < L$ the positions of the N scattering centers in the periodic segment $[0, L[$ (a circle). We will then define $r_0 = r_N$. In Appendix A of Ref. [2] it was shown that for an arbitrary choice of the N positions $\{r_i\}$, at large g, the eigenstates of the Hamiltonian (3.1), $\Psi_n(x; r_1, r_2, \ldots, r_N)$, become localized on the circle. Here $H\Psi_n(x; \{r_j\}) = E_n(\{r_j\})\Psi_n(x; \{r_j\})$ where their eigenvalues, $E_n(\{r_j\}) = k_n^2(\{r_j\})/2m$, are determined from the periodic boundary condition $\Psi_n(0; \{r_i\}) = \Psi_n(L; \{r_i\})$, where $n = 0$ corresponds to the ground state and integers $n > 0$ to the excited states (see Appendix A).

We here want to see whether the localization is *robust* against switching on of disorder, i.e. averaging over stochastic choices of the $\{r_i\}$. In a Monte Carlo spirit [7] we will then generate MN pseudo random numbers $\{r_i\}^k$, with $k = 1, 2, \ldots, M$, ordered within $[0, L[$ and according to Eq. (2.5) we will measure

$$\begin{aligned}\widetilde{\Psi}_n(x) &= \langle \Psi_n(x; r_1, r_2, \ldots, r_N)\rangle \\ &= \frac{1}{M}\sum_{k=1}^{M}\Psi_n(x; r_1^k, r_2^k, \ldots, r_N^k),\end{aligned} \tag{3.2}$$

at fixed n. Together with

$$\begin{aligned}\widetilde{E}_n &= \langle E_n(r_1, r_2, \ldots, r_N)\rangle \\ &= \frac{1}{M}\sum_{k=1}^{M}E_n(r_1^k, r_2^k, \ldots, r_N^k).\end{aligned} \tag{3.3}$$

In Fig. 1 we show the ground state for three choices of increasing M at low $g = 1$ and high $g = 100$ for $N = 3$. As we can see the randomness in the positions of the scattering centers produces localization. And moreover increasing the coupling g with the scattering centers increases the localization of the averaged ground state wavefunction. From the figure we also see how at small g the amplitude of the localized averaged ground state wavefunction is much smaller than the amplitude of the unaveraged ground state, but the opposite behavior is observed at high coupling g.

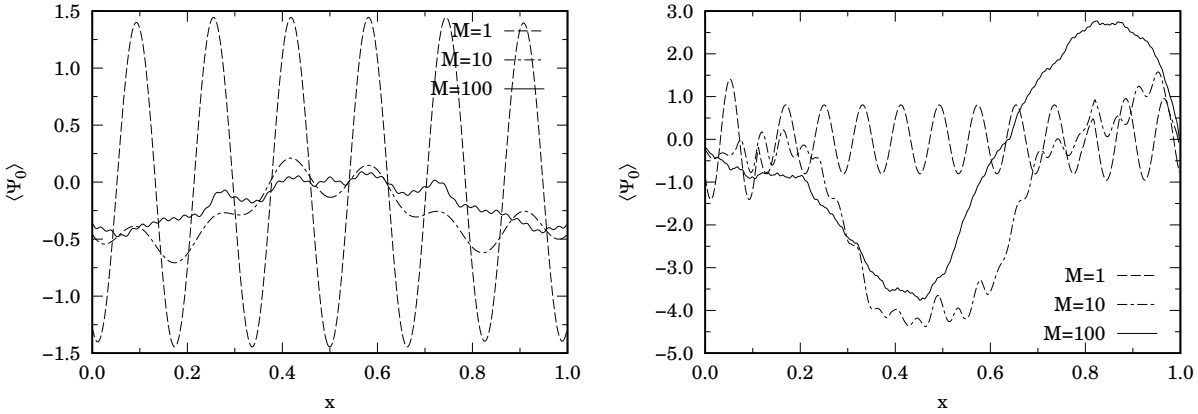

FIG. 1. We show the ground state from Eq. (3.2) for three choices of increasing M and $N = 3$. Low $g = 1$ in the left panel and high $g = 100$ in the right panel. From Eq. (3.3) the resulting ground state energy is as follows: for $g = 1 \longrightarrow$ ($\widetilde{E}_0 = 741.956$ for $M = 1$, $\widetilde{E}_0 = 148.428$ for $M = 10$, and $\widetilde{E}_0 = 613.504$ for $M = 100$) and for $g = 100 \longrightarrow$ ($\widetilde{E}_0 = 3027.62$ for $M = 1$, $\widetilde{E}_0 = 2343.16$ for $M = 10$, and $\widetilde{E}_0 = 3698.51$ for $M = 100$).

Dynamics

The dynamic evolution of the n-th eigenstate is as usual

$$\Psi_n(x;\{r_i\}|t) = e^{-iE_n(\{r_i\})t}\Psi_n(x;\{r_i\}), \tag{3.4}$$

according to the time, t, dependent Schrödinger equation $i\partial\Psi/\partial t = H\Psi$.

We may then initially think at the following severe short times Monte Carlo approximation

$$\begin{aligned}\widetilde{\Psi}_n(x|t) &= \langle\Psi_n(x;\{r_i\}|t)\rangle \\ &= \langle e^{-iE_n(\{r_i\})t}\Psi_n(x;\{r_i\})\rangle \\ &\approx \langle e^{-iE_n(\{r_i\})t}\rangle\langle\Psi_n(x;\{r_i\})\rangle \\ &\approx e^{-i\langle E_n(\{r_i\})\rangle t}\langle\Psi_n(x;\{r_i\})\rangle \\ &= e^{-i\widetilde{E}_n t}\widetilde{\Psi}_n(x),\end{aligned} \tag{3.5}$$

where the second approximation may be justified for a small times evolution. On the other hand, the first approximation is a rather severe one. Clearly it holds exactly only for $N = 0$. But from the approximation (3.5) follows that $|\widetilde{\Psi}_n(x|t)|^2 = |\widetilde{\Psi}_n(x)|^2$ independent of time.

We then see that in order to have a time dependent probability distribution it is essential to stick to the definition

$$|\widetilde{\Psi}_n(x|t)|^2 = |\langle\Psi_n(x;\{r_i\}|t)\rangle|^2. \tag{3.6}$$

In Fig. 2 we show the time evolution of the probability distribution for the ground state $n = 0$ for $N = 3, g = 100$ with $M = 100$. As we can see from the figure the probability density initially localized around $x \sim 0.4$ and 0.8 gets localized only at $x \sim 0.8$ at intermediate times and then finally faints out at large times.

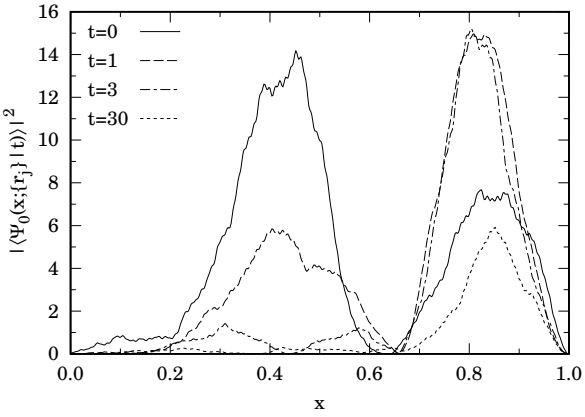

FIG. 2. We show the time evolution of the probability distribution of the ground state $|\widetilde{\Psi}_0(x|t)|^2$ from Eq. (3.6) for $N = 3, g = 100, M = 100$ at $t = 0, 1, 3, 30$.

We may be interested in solving Schrödinger equation with an initial condition

$$\Psi(x;\{r_j\}|0) = \delta(x - x_0). \tag{3.7}$$

with $x_0 \in [0, L[$. This is a much harder problem requiring a path integral according to

$$\Psi(x;\{r_j\}|\tau) = \overline{\int_{[0,\tau]\times[0,L[}} \int_{x(0)=x_0}^{x(\tau)=x} e^{iS(x,\dot{x};\{r_j\}|t)}\, Dx(t), \tag{3.8}$$

where we denote with a dot a time derivative and the action

$$S(x,\dot{x};\{r_j\}|\tau) = \int_0^\tau \left(\frac{1}{2}m\dot{x}^2 - g\sum_j \delta(x - r_j)\right) dt, \tag{3.9}$$

where the integrand is the Lagrangian.

IV. THE LAX MODEL WITH AFFINE QUANTIZATION

It would then be very interesting to repeat the calculation within *affine quantization* (see Appendix A in Ref. [8]) where

$$\mathscr{H} = \left[-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + v^{\rm aff}(x)\right] + g\sum_{j=1}^{N}\delta(x-r_j), \tag{4.1}$$

$$v^{\rm aff}(x) = \frac{3\left[\sum_j (x-a_j)\right]^2 + N\sum_j [b_j^2-(x-a_j)^2]}{2m\left\{\sum_j [b_j^2-(x-a_j)^2]\right\}^2}, \quad b_j = \frac{r_j - r_{j-1}}{2}, \quad a_j = \frac{r_j + r_{j-1}}{2}, \tag{4.2}$$

where the affine effective potential terms $v_j^{\rm aff}$ are the results of adopting the affine *dilation* operator $\mathscr{D}$, in place of the canonical momentum operator p,

$$\mathscr{D} = \sum_j \left\{p^\dagger [b_j^2-(x-a_j)^2] + [b_j^2-(x-a_j)^2]p\right\}/2, \tag{4.3}$$

in the affinely quantized Hamiltonian

$$\mathscr{H} = \mathscr{D}\left\{\sum_j [b_j^2-(x-a_j)^2]\right\}^{-2}\mathscr{D} + g\sum_{j=1}^{N}\delta(x-r_j), \tag{4.4}$$

where the effective affine potential insures that the particle will live in any of the segments $(x-a_j)^2 < b_j^2$, i.e. $x \in]r_{j-1}, r_j[$, tunneling from one to the other through the delta function. From Eq. (4.1) follows the eigenstate Schrödinger equation for an eigenvalue E

$$\left\{\sum_j [b_j^2-(x-a_j)^2]\right\}^2\left(\frac{\partial^2\Psi}{\partial x^2} + 2mE\Psi\right) = \left\{3\left[\sum_j (x-a_j)\right]^2 + N\sum_j [b_j^2-(x-a_j)^2]\right\}\Psi, \tag{4.5}$$

where the delta function terms vanished. This decouples the particle from the bosonic scattering centers. This would tell that in affine quantization the eigenstates must have a continuous first derivative, i.e. they are smooth functions, and that the localization holds independently from g! Again we expect that making the scattering centers stochastic will increase the localization of the particle ground state wave function averaged over the disorder. But this is a complicated computational problem that we will leave open for the future.

V. CONCLUSIONS

In this work we find numerically the ground state energy and wavefunction of a particle, in a one dimensional periodic square well, coupled through a pair Dirac delta function potential with N scattering centers situated at fixed random positions within the well as in the Edwards-Lax model. We show that the wavefunction becomes localized for $N > 1$ and for any value of the coupling constant g.

Averaging the ground state over the positions of the scattering centers chosen as pseudo random numbers uniformly distributed within the well we show that the localization increases.

We also show that the time dependent averaged ground state wavefunction becomes more localized at intermediate times and then faints out at large times.

We conclude studying the same system in affine quantization and show that the resulting problem is independent of the coupling constant g.

As a measure of the degree of localization in the wave function we may use the following estimator

$$\begin{aligned}
\xi &= \frac{1}{\int_0^L |\widetilde{\Psi}(x)|^2\,dx}\int_0^L |\widetilde{\Psi}(x)|^2 x\,dx,\\
\sigma^2 &= \frac{1}{\int_0^L |\widetilde{\Psi}(x)|^2\,dx}\int_0^L |\widetilde{\Psi}(x)|^2 (x-\xi)^2\,dx,\\
\zeta &= \sigma/L \geq 0,
\end{aligned} \tag{5.1}$$

where $\zeta = 1/12$ for a completely delocalized state and $\zeta = 0$ for a completely localized state. So that an increase of localization will be flagged by a diminution of ζ.

Even if we are still far from a unified theory of localization in quantum stochastic mechanics, we hope that the present study could represent a useful addition to the physics literature on the localization phenomenon.

Appendix A: Determination of the eigenstates and the eigenvalues of Lax model

Choose N ordered random real numbers $0 < r_1 < r_2 < \ldots < r_N < L$. Define $r_0 = 0$. Solve the Schrödinger equation for $\psi(x) = \Psi(x; \{r_j\})$

$$E\psi(x) = -\frac{1}{2m}\psi''(x) + g\sum_{j=1}^{N}\delta(x - r_j)\psi(x) \tag{A1}$$

with the *transfer matrix method*. As usual we denote with a prime a derivative respect to x. For $g > 0$ multiplying this equation by $\psi^\star$ and integrating over $x \in [0, L[$ follows immediately $E > 0$. On any subinterval $]r_j, r_{j+1}[$ the wavefunction takes the form

$$\psi(x) = A_j \sin(kx + \varphi_j), \tag{A2}$$

with A_i and φ_i an amplitude and a phase and $E = k^2/2m$. Integrating Eq. (A1) around r_j and using the continuity of $\psi(x)$ follows

$$\psi'(r_j^+) - \psi'(r_j^-) = 2mg\psi(r_j). \tag{A3}$$

Constructing the column vector $C(x) = (\psi'(x), k\psi(x))^T$, the conditions of Eqs. (A2) and (A3) can be rewritten as

$$C(r_{j+1}^-) = R[k(r_{j+1} - r_j)]C(x_j^+), \quad C(x_j^+) = TC(x_j^-), \tag{A4}$$

respectively, where

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 2mg/k \\ 0 & 1 \end{pmatrix}. \tag{A5}$$

Hence $C(L) = MC(0)$, with

$$M = R[k(L - r_N)]TR[k(r_N - r_{N-1})]T \cdots TR[k(r_1 - r_0)]T. \tag{A6}$$

The spectrum is fixed by the boundary condition $\psi(0) = \psi(L)$. For example for periodic boundary conditions $M = 1$ and $\mathrm{tr}M = 2$, which can be solved with the Newton-Raphson (NR) method. We found the ground state energy by choosing as seed for the NR algorithm $k = 0^+$.

Once the spectrum is determined one relates A_{j+1} and φ_{j+1} to A_j and φ_j using the continuity of $\psi(x)$ and the jump condition (A3). Thus, by recursion, any A_j and φ_j for $j = 0, 1, \ldots, N$ can be expressed in terms of A_0 and φ_0. We determine A_0 in terms of φ_0 requiring that $\psi(x)$ is normalized over the whole well $[0, L[$. Finally, we determine φ_0 numerically from the boundary condition $\psi(0) = \psi(L)$ with the NR method with any seed.

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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