Realism in energy transition processes: an example from Bohmian Quantum Mechanics

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1 Introduction

To study the exchange of energy between two systems, we may start by analyzing a well known physical effect: the absorption of a photon by a photo-detector. In doing so, we have to choose between two different and simple models of a photo-detector: a photo-detector with discrete or continuous band. For the purposes of simplicity, we will choose the former. However, since we are only interested in the aspects of energy transfer between the two systems, we will make an even further simplification and consider that the photon and the detector will both be described by a single harmonic oscillator. Furthermore, during some time ΔT_{int}, we will assume that a linear interaction exists between the two oscillators, and that this interaction is weak. As we will see, this "toy model" will allow us to capture some important features of the entanglement between the two systems.

This paper is organized in the following way. In Section 2 we will quickly review the interaction between two harmonic oscillators for the classical case. This will allow us to understand how the transfer of energy happens in the classical case. We then compute the exact solutions for the quantum mechanical system with interaction (Section 3). In Section 4 we use Bohm's theory to interpret the results obtained.

2 The Classical Case

Before we go into the details of the quantum mechanical examples, let us begin by analyzing the classical system of two one-dimensional coupled harmonic oscillators with the same mass m, elastic constant k, and coupling constant λ. The Hamiltonian for this system is given by

$$H = \frac{1}{2m}\left(P_1^2 + P_2^2\right) + \frac{1}{2}k\left((X_1+d)^2 + (X_2-d)^2\right) + \frac{1}{2}\lambda\left(X_1 - X_2 + 2d\right)^2. \quad (1)$$

To simplify the equations of motion and eliminate the undesirable constant d we can make the canonical transformation $x_1 = X_1 + d, x_2 = X_2 - d, p_1 = P_1, p_2 = P_2$. We will assume that the two oscillators are initially at rest the first one in its equilibrium position (null initial energy, $E_1^i = 0$), while the second one is dislocated from its equilibrium position by a distance D, yielding as solutions to the equations of motion

$$x_1(t) = \frac{D}{2}\left[\cos(\omega t) - \cos\left(\omega' t\right)\right] \quad (2)$$

$$x_2(t) = \frac{D}{2}\left[\cos(\omega t) + \cos(\omega' t)\right]. \tag{3}$$

where we defined $\omega \equiv \sqrt{k/m}$ and $\omega' \equiv \omega\sqrt{1+\varepsilon}$, with $\varepsilon = 2\lambda/k$.

We will now assume that the interaction constant λ is weak when compared to the elastic constant k, $\varepsilon \ll 1$. Then, we can expand ω' around $\varepsilon = 0$, yielding$\omega' = \sqrt{\frac{k+2\lambda}{m}} = \omega\sqrt{1+\varepsilon} \approx \omega + \delta\omega$, with $\delta\omega \equiv \frac{\omega'-\omega}{2}$. Defining $\bar{\omega} \equiv \frac{\omega'+\omega}{2}$, the solutions can now be written as

$$\begin{aligned} x_1(t) &= D\sin(\delta\omega\, t)\sin[\bar{\omega}\, t], \qquad (4)\\ x_2(t) &= D\cos(\delta\omega\, t)\cos[\bar{\omega}\, t]. \qquad (5)\end{aligned}$$

One should note that even though (4) and (5) do not contain explicitly the coupling constant λ, the coupling is still present as $\delta\omega$ does depend on the coupling. It is easy to check that the total energy of the system is

$$E_T = \frac{kD^2}{2}\left(1 + 2\frac{\delta\omega}{\bar{\omega}}\right) + O(\delta\omega^2), \tag{6}$$

a value that is constant for the whole movement, as we should expect.

3 Quantum Evolution: Exact Solutions

Now we want to study the quantized version of the resonant spinless one-dimensional coupled harmonic oscillator presented in the previous Section. First, we note that the total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is spanned by $\mathcal{H}_1$ and $\mathcal{H}_2$, the Hilbert spaces for particles 1 and 2, respectively. For example, the two canonical variables describing particle 1 are $\hat{X}_1, \hat{P}_1 \in \mathcal{H}_1$, with $[\hat{X}_1, \hat{P}_1] = i\hbar\hat{1}$, and are therefore represented as $\hat{X}_1 \otimes \hat{1}_2, \hat{P}_1 \otimes \hat{1}_2 \in \mathcal{H}$, where $\hat{1}_2 \in \mathcal{H}_2$ is the identity operator. In this way, the Hamiltonian operator for particle 1, is written as

$$\hat{H}_1 = \frac{1}{2m}\left(\hat{P}_1 \otimes \hat{1}\right)^2 + \frac{1}{2}k\left(\hat{X}_1 \otimes \hat{1} + d\hat{1} \otimes \hat{1}\right)^2.$$

For shortness of notation, we will drop the tensor product and keep in mind that operators regarding particle 1 act on $\mathcal{H}_1$ whereas operators regarding particle 2 act on $\mathcal{H}_2$.

With the simplified notation, the total quantum Hamiltonian operator for the two oscillators plus the interaction term is

$$\hat{H} = \frac{1}{2m}\hat{P}_1^2 + \frac{1}{2}k\left(\hat{X}_1 + \hat{d}\right)^2 + \frac{1}{2m}\hat{P}_2^2 + \frac{1}{2}k\left(\hat{X}_2 - \hat{d}\right)^2 + \frac{1}{2}\lambda\left(\hat{X}_1 - \hat{X}_2 + 2\hat{d}\right)^2.$$

In the coordinate representation we have the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{1}{2}k\left(x_1^2 + x_2^2\right) + \frac{1}{2}\lambda\left(x_1 - x_2\right)^2. \tag{7}$$

With the normal coordinates, the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \xi_+^2} + \frac{\partial^2}{\partial \xi_-^2}\right) + \frac{1}{2}k\xi_+^2 + \frac{1}{2}\left(k + 2\lambda\right)\xi_-^2, \tag{8}$$

The Schroedinger equation for the system is

$$\hat{H}\psi(\xi_+, \xi_-, t) = i\hbar\frac{\partial}{\partial t}\psi(\xi_+, \xi_-, t). \tag{9}$$

To solve (9) we need to find the solutions to the time independent Schroedinger equation

$$\hat{H}\psi^{(l)}(\xi_+, \xi_-) = \mathcal{E}_l\psi^{(l)}(\xi_+, \xi_-), \tag{10}$$

where l is an index (perhaps a collective index for both oscillators) for the energy to be determined. Since $\hat{H}$ is separable, we can write (10) as two independent eigenvalue equations

$$\hat{H}_+\phi_+^{(n)}(\xi_+) = E_n\phi_+^{(n)}(\xi_+) \tag{11}$$

and

$$\hat{H}_-\phi_-^{(n')}(\xi_-) = E'_{n'}\phi_-^{(n')}(\xi_-), \tag{12}$$

where we define

$$\psi^{(l)}(\xi_+,\xi_-) = \phi_+^{(n)}(\xi_+)\phi_-^{(n')}(\xi_-), \tag{13}$$

and

$$\mathcal{E}_l = E_n + E'_{n'}.$$

Clearly, l is an index that depends on both n and n', and for that reason we will write $\psi^{(n,n')}(\xi_+,\xi_-)$ instead of $\psi^{(l)}(\xi_+,\xi_-)$.

The solution to the time dependent Schroedinger equation (9) is obtained applying the time evolution operator $\hat{U}(t,t_0) = \exp\left(-i\hat{H}(t-t_0)/\hbar\right)$ and is, keeping terms up to $\delta\omega/\bar{\omega}$,

$$\begin{aligned}\psi(x_1,x_2,t) \quad = \quad & \sqrt{\frac{1}{2\pi}\frac{m\bar{\omega}}{\hbar}}\exp\left\{-\frac{m\bar{\omega}}{2\hbar}\left[x_1^2+x_2^2-2x_1x_2\frac{\delta\omega}{\bar{\omega}}\right]\right\}\exp\left\{-i2\bar{\omega}t\right\}\times \\ & \Bigg\{2ix_1\sin\left(\delta\omega t\right)+2x_2\cos\left(\delta\omega t\right)-\frac{\delta\omega}{\bar{\omega}}\left[x_1\cos\left(\delta\omega t\right)+ix_2\sin\left(\delta\omega t\right)\right]+ \\ & \frac{1}{2}\frac{\delta\omega}{\bar{\omega}}\left(x_1+x_2\right)\left[\frac{m\bar{\omega}}{\hbar}\left(x_1-x_2\right)^2-1\right]\exp\left\{-i\left(2\bar{\omega}+\delta\omega\right)t\right\}- \\ & \frac{1}{2}\frac{\delta\omega}{\bar{\omega}}\left(x_1-x_2\right)\left[\frac{m\bar{\omega}}{\hbar}\left(x_1-x_2\right)^2-3\right]\exp\left\{-i\left(2\bar{\omega}+3\delta\omega\right)t\right\}\Bigg\}+O(\delta\omega^2).\end{aligned} \tag{14}$$

The wavefunction (14) determines the evolution of the system. We will now proceed to analyze the system using (14).

4 The Bohmian Interpretation

For our case of two coupled-HO the configuration space has two variables, x_1 and x_2, the positions of particles 1 and 2, respectively. For two particles, the nonlocality of Bohm's interpretation becomes evident as the Schrödinger equation becomes

$$i\hbar\frac{\partial\Psi(x_1,x_2,t)}{\partial t} = \left[-\frac{\hbar^2}{2m_1}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2+V(x_1,x_2)\right]\Psi(x_1,x_2,t), \tag{15}$$

where ∇_i^2 is the laplacian operator with respect to the coordinates of particle i. If we follow the same transformation as before, we can obtain the following equations.

$$\frac{\partial S}{\partial t}+\frac{(\nabla_1 S)^2}{2m_1}+\frac{(\nabla_2 S)^2}{2m_2}+V-\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = 0, \tag{16}$$

$$\frac{\partial R^2}{\partial t}+\nabla_1\cdot\left(R^2\frac{\nabla_1 S}{m_1}\right)+\nabla_2\cdot\left(R^2\frac{\nabla_2 S}{m_2}\right) = 0. \tag{17}$$

The nonlocality comes from the fact that, even if the potential $V(x_1,x_2)$ is local, it is possible that the quantum potential given by

$$Q = -\frac{\hbar^2}{2m_1}\frac{\nabla_1^2 R}{R}-\frac{\hbar^2}{2m_2}\frac{\nabla_2^2 R}{R}$$

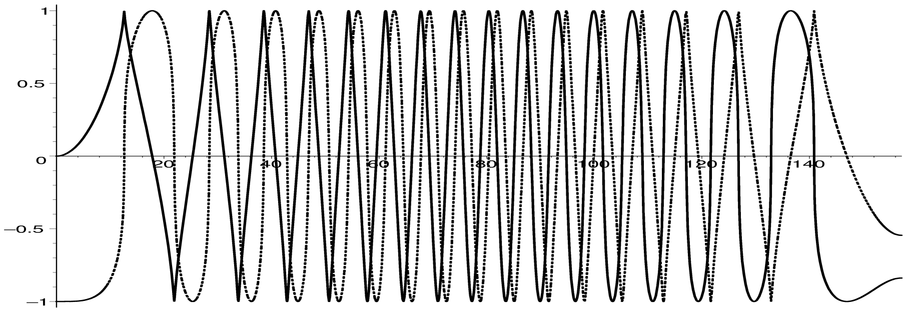

Figure 1: Bohmian trajectories for two CHO. The trajectories correspond to $\bar{\omega} = 1\,\text{fs}^{-1}$, $\delta\omega/\bar{\omega} = 0.01, x_1(0) = 0$, and $x_2(0) = -1$. The solid line represents the trajectory of $x_1(t)$ whereas the dashed line represents that of $x_2(t)$. The scale for the ordinates is in Å and the time scale is in fs.

is nonlocal, depending on the form of R. This characteristic is necessary, as proved by Bell, if Bohm's theory is to recover all quantum mechanical predictions.

Using (14) it is straightforward to compute the phase $S(x_1, x_2, t)$. After some long and tedious algebra we obtain that the differential equation that describes the trajectories of particles x_1 and x_2 as

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = \frac{1}{m}\frac{\partial S(x_1, x_2 t)}{\partial x_1} = -\frac{\cos(\delta\omega t)\sin(\delta\omega t)\,x_2}{m\left[(\sin(\delta\omega t)\,x_1)^2 + (\cos(\delta\omega t)\,x_2)^2\right]} \tag{18}$$

and

$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = \frac{1}{m}\frac{\partial S(x_1, x_2 t)}{\partial x_2} = \frac{\cos(\delta\omega t)\sin(\delta\omega t)\,x_1}{m\left[(\sin(\delta\omega t)\,x_1)^2 + (\cos(\delta\omega t)\,x_2)^2\right]}. \tag{19}$$

We can see that the differential equations for the trajectories are coupled and nonlinear. It is interesting to notice that if $\delta\omega = 0$ we recover the standard Bohmian result that in the case of no interaction each HO is in an eigenstate and therefore has a stationary solution. However, if $\delta\omega \neq 0$, we obtain at once that, after a simple change of variables (both for t and for $x_1$and x_2), the differential equations (18) and (19) are invariant, as we can see from Figure 1 where typical Bohmian trajectories were computed for both particles. In our numerical computations it is not reasonable, from a computational point of view, to use the MKS system as numerical values. So, we will measure time in femtoseconds (1 fs $= 10^{-15}$ s) and distance in Angstroms (1 Å$= 10^{-10}$ m). If we say that the particles in the oscillators are electrons, then $m = 1\,\mathrm{m}_e$, where $\mathrm{m_e}$ is the mass of the electron, then we have

$$\hbar = 10\,\mathrm{m}_e \cdot \text{Å}^2 \cdot \mathrm{fs}^{-1},$$

and

$$k = 1\,\mathrm{m}_e \cdot \mathrm{fs}^{-2},$$

and remembering that

$$\langle(\Delta x)^2\rangle = \frac{\hbar}{2m_e\omega}$$

for the harmonic oscillator. The solutions shown in Fig. 1 was obtained numerically using a 7th-8-th order continuous Runge-Kuta method. Up to now we are still working to understand the role of energies in the bohmian case, and further computations are necessary.