Quantum Model for the Transport of Nearly Localized Particles

Omar Morandi

Abstract A quantum model based on the Gaussian-Hermite expansion of the wave function of a system of n particles is proposed. The dynamics is described by trajectories in a configuration space. Our method is designed to provide some corrections to the classical motion of nearly localized particles. As an application of our model we describe the motion of a nearly localized particle in a 2D confining structure.

1 Introduction

During the last decade, the dynamics of molecules inside gases or nanostructures have been extensively investigated. New concepts such as deterministic and stochastic quantum trajectories have been proposed to develop new ab initio methods that go beyond the classical description of the atomic nuclei[1–12].

Such approaches are mainly based on the Bohm interpretation of the quantum mechanics where the concept of the deterministic trajectory of a particle is extended to the quantum dynamics in a rigorous way [13]. One of the first attempts to apply Bohm theory to a real nanostructure, have been proposed by Tully [14] and Wyatt [15]. Nowadays, methods based on the Bohm formalism are very popular and are at the basis of few general methods such as the multiconfiguration time-dependent Hartree method [16] and the Bohm trajectories extended to the complex plane [17]. Moreover, stochastic methods have also been employed [18]. Based on the classical concept of Brownian and Langevin dynamics, stochastic models are able to reproduce the quantum statistical properties of protons in harmonic traps [19].

O. Morandi (✉)
University of Florence, Florence, Italy
e-mail: omar.morandi@unifi.it

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In this paper, we derive the motion of a system of quantum particles. We assume that every particle is described by a Gaussian-like wave packet parametrized by a set of numbers that depend on time. Our approach is designed to describe the motion of heavy particles as for example neutrons and protons. We will discuss the application of our method to the 2D motion of a particle in the presence of a confining non harmonic potential. In particular, the connection with the Bohm interpretation of the quantum mechanics will be discussed.

2 Particle Motion: Beyond the Gaussian Beam Approximation

We consider the quantum mechanical evolution of a system defined by the wave function $\psi(\mathbf{r}) \in L^2(\mathbb{R}^d)$. Our system consists of $n \leq d$ particles, where d is the dimension of the space. We focus on the physical situation in which each particle is localized around a spatial coordinate. We assume that the probability dispersion of the particle wave function is modulated by a Gaussian function centred on mean particle positions. Moreover, we assume that all the particles are identical and have mass $m = 1$. The particles move in the presence of an external potential $U(\mathbf{r})$. We discard the direct particle-particle interaction. However, $U(\mathbf{r})$ may contains some nonlinear terms that describe the particle-particle interaction at the mean field level. We develop a model that preserves the classical description of particle motion in terms of trajectories. In particular, in our model the particle motion is expressed by a system of nonlinear ODE for a set of physically relevant parameters. This is obtained by parametrizing the particle wave function by a complete set of parameters which extend the classical dynamical quantities position and momentum. Similarly to the coherent state projection technique [20–22], we project the wave function of the system on the basis set of the Harmonic oscillator shifted at the mean particle positions. The Gaussian beam approximation is a popular method used to describe nearly localized particles [23–25] Similarly to the Gaussian beam approximation, our expansion procedure is based on the projection of the solution over a set of functions which are modulated by a Gaussian whose width changes in time according to the quantum evolution equation.

In this paper we extend the results obtained in Ref. [26], where the 1D case with some extension to the 2D problem, was considered. In Ref. [26] the evolution equations for the parameters have been obtained by applying a integral approach based on the Euler-Lagrange formalism. Here, we proceed in a more direct way. We calculate the evolution equations by using the Madelung decomposition in which the particle wave function is expressed in polar coordinates. In particular, in Sect. 2.2 we calculate the expression of the projection of the potential on the Hermite basis in a closed form. This is an important step toward the implementation of a efficient numerical solver for the particle motion.

We start by considering the time dependent Schrödinger equation of a quantum system of dimension d

$$i\frac{\partial \psi}{\partial t} = \left(-\frac{1}{2}\Delta_{\mathbf{r}} + U(\mathbf{r})\right)\psi \ . \tag{1}$$

We have normalized the Planck constant $\hbar = 1$. According to Madelung, we represent the particle wave function in polar coordinates $\psi(\mathbf{r}) = \sqrt{n(\mathbf{r}-\mathbf{s})}e^{i\chi(\mathbf{r}-\mathbf{s})}$. We have introduced the parameter $\mathbf{s} \in \mathbb{R}^d$ which represents the mean particle position. In particular, $\mathbf{s}$ is the centre of the Hermite expansion that will be performed in the following. The evolution equation of $\mathbf{s}$ (see Eq. (22) below) can be interpreted as a Newton equation with quantum corrections. We assume that the density $n(x)$ is a Gaussian function modulated by the polynomial P

$$n(\mathbf{r}, t) = P(\mathbf{r}, t)e^{-\langle \sigma, \mathbf{r}\rangle} \ .$$

The parameter $\boldsymbol{\sigma} \in \mathbb{R}^d$ provides the width of the Gaussian packed. For the sake of compactness, we have introduced the notation $\langle \boldsymbol{\sigma}, \mathbf{r}\rangle \doteq \sum_{n=1}^{d} r_i^2\sigma_i$, where the lower indexes indicate the components of the vectors along the coordinate axis. The Madelung transform leads to the well known quantum hydrodynamic equations

$$\frac{\partial n}{\partial t} = -\nabla \cdot \boldsymbol{J} + \frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \cdot \nabla n \tag{2}$$

$$\frac{\partial \boldsymbol{J}}{\partial t} = -\nabla\left(\frac{\boldsymbol{J}\otimes\boldsymbol{J}}{n}\right) + n\nabla\left(Q + U_{[\mathbf{s}]}\right) + \frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \cdot \nabla\chi \ . \tag{3}$$

Here, we have introduced the notation $U_{[\mathbf{s}]} \doteq U(\mathbf{r}+\mathbf{s})$, $J = n\nabla\chi$ is the quantum current and $Q(\mathbf{r})$ is the quantum Bohm potential

$$Q \equiv \frac{1}{2}\frac{\Delta\sqrt{n}}{\sqrt{n}} = \frac{1}{4}\left[\frac{\Delta P}{P} - \frac{|\nabla P|^2}{2P^2} - 2\sum_{i=1}^{d}\sigma_i\frac{r_i\frac{\partial P}{\partial r_i}}{P} + 2\sum_{i=1}^{d}\sigma_i(r_i^2\sigma_i - 1)\right] . \tag{4}$$

Concerning the physical meaning of the Bohm potential, we refer to [15, 26]. By introducing the auxiliary variable $R(x) = \ln(P(x))$, the previous expression becomes

$$Q = \frac{1}{4}\left[\Delta R + \frac{|\nabla R|^2}{2} - 2\sum_{i=1}^{d}\sigma_i r_i\frac{\partial R}{\partial r_i} + 2\sum_{i=1}^{d}\sigma_i(r_i^2\sigma_i - 1)\right] .$$

From Eq. (3) with some algebra we obtain to the evolution equation for the phase χ

$$\frac{\partial \chi}{\partial t} = -\frac{1}{2}|\nabla\chi|^2 + Q + U_{[\mathbf{s}]} + \frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \cdot \nabla\chi \ . \tag{5}$$

The main interest of our approach is to derive the evolution equation of the parameters obtained by expanding the functions χ and P on the Hermite polynomial basis set. We write the expansion as follows

$$P(\mathbf{r},t) = \sum_{\{n\}=0}^{\infty} a_{\{n\}}(t) h^{\boldsymbol{\sigma}}_{\{n\}}(\mathbf{r}) \tag{6}$$

$$\chi(\mathbf{r},t) = \sum_{\{n\}=0}^{\infty} \chi_{\{n\}}(t) h^{\boldsymbol{\sigma}}_{\{n\}}(\mathbf{r}) \; . \tag{7}$$

We have introduced the compact notation $\{n\}$ to indicate the sequence of d integers $\{n\} \doteq (n_1, n_2, \ldots, n_d)$ and

$$h^{\boldsymbol{\sigma}}_{\{n\}}(\mathbf{r}) \doteq \prod_{i=1}^{d} h^{\sigma_i}_{n_i}(r_i) \; . \tag{8}$$

The functions $h^{\sigma_i}_{n_i}(r_i)$ are the normalized Hermite functions. For the details concerning the definition of $h^{\sigma_i}_{n_i}(r_i)$ we refer to [26], Eq. (19). In order to clarify the notation, we write explicitly Eq. (7) in the 3D case

$$\chi(\mathbf{r},t) = \sum_{n_x,n_y,n_z=0}^{\infty} \chi_{n_x,n_y,n_z}(t) h^{\sigma_x}_{n_x}(x) h^{\sigma_y}_{n_y}(y) h^{\sigma_z}_{n_z}(z) \; . \tag{9}$$

By using the property of orthonormality of the Hermite functions, it is easy to invert the previous equations. As un example, we give the inversion formula for P

$$a_{\{n\}} = \int P(\mathbf{r}) h^{\boldsymbol{\sigma}}_{\{n\}}(\mathbf{r}) e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} \; . \tag{10}$$

Hereafter, all the integrals are considered over all the space $\mathbb{R}^d$. Finally, it is useful to expand the variable $R(x) = \ln(P(x))$ in the Hermite basis set

$$R(\mathbf{r}) = \sum_{m} R_{\{m\}} h^{\boldsymbol{\sigma}}_{\{m\}}(\mathbf{r}) \; . \tag{11}$$

In order to clarify our approach, in the following expression we indicate all the parameters that we have introduced

$$\psi(\mathbf{r}) = \sqrt{n(\mathbf{r}-\mathbf{s})} e^{i\chi(\mathbf{r}-\mathbf{s})} \Rightarrow \begin{cases} a_{\{n\}} \in \ell^2(\mathbb{N}^d) & : \text{modulus} \\ \chi_{\{n\}} \in \ell^2(\mathbb{N}^d) & : \text{phase} \\ \mathbf{s} \in \mathbb{R}^d & : \text{mean position} \\ \boldsymbol{\sigma} \in \mathbb{R}^d & : \text{Gaussian width} \\ R_{\{n\}} = R_{\{n\}}(a_{\{n\}}) \in \ell^2(\mathbb{N}^d) & \end{cases} .$$

In particular, in the last line we have indicated that the parameters R_n are not independent and obtained by $a_{\{n\}}$. The details concerning this point are given in Ref. [26]. We calculate now the evolution equations for our set of parameters. We give some technical details concerning the expansion coefficients of the phase χ. The calculations proceed straightforwardly. We multiply Eq. (5) by $h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle}$ and we integrate over $\mathbb{R}^d$. We obtain

$$\frac{\mathrm{d}\chi_{\{n\}}}{\mathrm{d}t} = \underbrace{-\frac{1}{2}\int |\nabla\chi|^2 \, h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r}}_{I} + \underbrace{\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \cdot \int \nabla\chi \, h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r}}_{II}$$

$$\underbrace{-\sum_{i=1}^{d} \frac{\mathrm{d}\sigma_i}{\mathrm{d}t} \sum_{\{n'\}} \chi_{\{n'\}} \int h^{\sigma}_{\{n\}} \frac{\mathrm{d}h^{\sigma}_{\{n'\}}}{\mathrm{d}\sigma_i} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} + \int \left(Q + U_{[\mathbf{s}]}\right) h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r}}_{III} .$$

For the first term we have

$$\begin{aligned} I &= -\frac{1}{2} \sum_{\{r\},\{s\}} \chi_{\{r\}} \chi_{\{s\}} \sum_{i=1}^{d} \int \frac{\mathrm{d}h^{\sigma}_{\{r\}}}{\mathrm{d}r_i} \frac{\mathrm{d}h^{\sigma}_{\{s\}}}{\mathrm{d}r_i} h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} \\ &= -\sum_{\{r\},\{s\}} \chi_{\{r\}} \chi_{\{s\}} \sum_{i=1}^{d} \sigma_i \sqrt{r_i s_i} \int h^{\sigma}_{\{r; r_i \to r_i - 1\}} h^{\sigma}_{\{s; s_i \to s_i - 1\}} h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} \\ &= -\sum_{\{r\},\{s\}} \chi_{\{r\}} \chi_{\{s\}} \sum_{i=1}^{d} \sigma_i \sqrt{r_i s_i} \mathbb{A}^{\sigma_i}_{n_i, r_i - 1, s_i - 1} \prod_{j \neq i} \mathbb{A}^{\sigma_j}_{n_j, r_j, s_j} . \end{aligned} \tag{12}$$

The matrix $\mathbb{A}$ is defined as

$$\mathbb{A}^{\sigma}_{n,r,s} = \pi^{1/4} \int_{\mathbb{R}} h^{\sigma}_n(x) h^{\sigma}_r(x) h^{\sigma}_s(x) e^{-x^2\sigma} \, \mathrm{d}x .$$

Details concerning the calculation of $\mathbb{A}^{\sigma}_{n,r,s}$ are given in [26]. We have used the following property of the Hermite functions (see Eq. (22) of Ref. [26])

$$\frac{\mathrm{d}h^{\sigma}_{\{n\}}(\mathbf{r})}{\mathrm{d}r_i} = \sqrt{2n_i\sigma_i} h^{\sigma_i}_{n-1}(r_i) \prod_{j \neq i, j=1}^{d} h^{\sigma_j}_{n_j}(r_j) = \sqrt{2n_i\sigma_i} h^{\sigma}_{\{n; n_i \to n_i - 1\}}(\mathbf{r}) . \tag{13}$$

Finally, we have introduced the following notation $\{r; r_i \to a\} \doteq (r_1, \ldots, r_{i-1}, a, r_{i+1}, \ldots, r_d)$ where the i-th term is substituted by a. For the second term, we have

$$II = \sum_{\{r\}} \chi_{\{r\}} \sum_{i=1}^{d} \frac{\mathrm{d}s_i}{\mathrm{d}t} \int \frac{\mathrm{d}h^{\sigma}_{\{r\}}}{\mathrm{d}r_i} h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} = \sum_{i=1}^{d} \chi_{\{n; n_i \to n_i + 1\}} \frac{\mathrm{d}s_i}{\mathrm{d}t} \sqrt{2(n_i + 1)\sigma_i} . \tag{14}$$

Furthermore,

$$III = -\sum_{i=1}^{d} \frac{\mathrm{d}\sigma_i}{\mathrm{d}t} \left(\frac{2n_i+1}{4\sigma_i} \chi_{\{n\}} + \frac{\sqrt{(n_i+2)(n_i+1)}}{2\sigma_i} \chi_{\{n;n_i\to n_i+2\}} \right) . \tag{15}$$

We consider now the term that contains the Bohm potential

$$\int Q h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} = \frac{1}{4} \int \left[\Delta R + \frac{|\nabla R|^2}{2} - 2 \sum_{i=1}^{d} \sigma_i r_i \frac{\partial R}{\partial r_i} + 2 \sum_{i=1}^{d} \sigma_i (r_i^2 \sigma_i - 1) \right] h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r}$$

By using the expansion of R we obtain the explicit form of the previous terms. After cumbersome algebra we obtain

$$\begin{aligned} \int Q h^{\sigma}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r} \rangle} \, \mathrm{d}\mathbf{r} = & \frac{1}{4} \sum_{\{r\},\{s\}} R_{\{r\}} R_{\{s\}} \sum_{i=1}^{d} \sigma_i \sqrt{r_i s_i} \mathbb{A}^{\sigma_i}_{n_i, r_i - 1, s_i - 1} \prod_{j \neq i} \mathbb{A}^{\sigma_j}_{n_j, r_j, s_j} - \sum_{i=1}^{d} \frac{\sigma_i}{2} n_i R_{\{n\}} \\ & + \pi^{d/4} \frac{1}{4} \sum_{i=1}^{d} \sigma_i^{3/4} \left(\sqrt{2} \delta_{n_i, 2} - \delta_{n_i, 0} \right) \prod_{j \neq i}^{d} \sigma_j^{-1/4} \delta_{n_j, 0} \, . \end{aligned}$$

Here, δ denotes the Kronecker's delta. The final expression of the evolution equation for χ is given in Eq. (19). The evolution equations for a, $\mathbf{s}$ and σ can be obtained by using the continuity equation. It is easy to verify that

$$\frac{\partial n}{\partial t} = -\nabla \cdot \boldsymbol{J} + \frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \cdot \nabla n = \nabla \cdot \left[n \left(-\nabla \chi + \frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} \right) \right] . \tag{16}$$

Proceeding in similar way as we have done for χ, from Eq. (16) we obtain

$$\begin{aligned} \frac{\mathrm{d}a_{\{n\}}}{\mathrm{d}t} = & \sum_{i=1}^{d} \frac{\mathrm{d}\sigma_i}{\mathrm{d}t} \frac{1}{2\sigma_i} \left[a_{\{n\}} \frac{2n_i+1}{2} + a_{\{n;n_i\to n_i-2\}} \sqrt{n_i(n_i-1)} \right] \\ & - \sum_{i=1}^{d} a_{\{n;n_i\to n_i-1\}} \frac{\mathrm{d}s_i}{\mathrm{d}t} \sqrt{2n_i\sigma_i} \\ & + 2 \sum_{\{r\},\{s\}} a_{\{r\}} \chi_{\{s\}} \sum_{i=1}^{d} \sigma_i \sqrt{n_i s_i} \mathbb{A}^{\sigma_i}_{n_i - 1, r_i, s_i - 1} \prod_{j \neq i} \mathbb{A}^{\sigma_j}_{n_j, r_j, s_j} \, . \end{aligned}$$

It is easy to verify that the first coefficient $a_{\{0,\ldots,0\}}$ is directly related to the L2 norm of ψ. It can be integrated analytically. From the previous equation we have

$$\frac{\mathrm{d}a_{\{0,\ldots,0\}}}{\mathrm{d}t} = \sum_{i=1}^{d} \frac{\mathrm{d}\sigma_i}{\mathrm{d}t} \frac{1}{4\sigma_i} a_{\{0,\ldots,0\}} \, ,$$

whose solution is $a_{\{0,\ldots,0\}} = \pi^{-d/4}\prod_{i=1}^{d}\sigma_i^{1/4}(t)$. According to the discussion of Ref. [26], it is possible to verify that the number of expansion coefficients that we have introduced so far is redundant. In particular, it is always possible to fix some of the coefficients a that multiply the linear and the quadratic terms of the expansion (6). For the linear terms, the evolution equation is

$$\frac{\mathrm{d}a_{\{0,\ldots,1,\ldots,0\}}}{\mathrm{d}t} = \sum_{j=1}^{d}\frac{\mathrm{d}\sigma_j}{\mathrm{d}t}\frac{1}{2\sigma_j}\left[a_{\{0,\ldots,1,\ldots,0\}}\frac{2n_j+1}{2}\right] - \sum_{j=1}^{d}a_{\{n;n_j\to n_j-1\}}\frac{\mathrm{d}s_j}{\mathrm{d}t}\sqrt{2n_j\sigma_j}$$

$$+2\sum_{\{r\},\{s\}}a_{\{r\}}\chi_{\{s\}}\sigma_i\sqrt{s_i}\mathbb{A}^{\sigma_i}_{0,r_i,s_i-1}\prod_{j\neq i}\mathbb{A}^{\sigma_j}_{0,r_j,s_j}$$

$$= a_{\{0,\ldots,1,\ldots,0\}}\sum_{j=1}^{d}\frac{\mathrm{d}\sigma_j}{\mathrm{d}t}\frac{2n_j+1}{4\sigma_j} - a_{\{0,\ldots,0\}}\frac{\mathrm{d}s_i}{\mathrm{d}t}\sqrt{2\sigma_i}$$

$$+\frac{2\sigma_i\sqrt{r_i+1}\prod_k\sigma_k^{1/4}}{\pi^{d/4}}\sum_{\{r\}}a_{\{r\}}\chi_{\{r;r_i\to r_i+1\}}\,.$$

By imposing $a_{\{0,\ldots,1,\ldots,0\}} = 0$ we obtain the evolution equation for $\mathbf{s}$

$$\frac{\mathrm{d}s_i}{\mathrm{d}t} = \sqrt{2\sigma_i}\sum_{\{m\}}a_{\{m\}}\chi_{\{m;m_i\to m_i+1\}}\sqrt{m_i+1}\,.$$

The evolution equation of the width of the Gaussian $\boldsymbol{\sigma}$ is obtained by setting the quadratic terms to zero: $a_{\{0,\ldots,2,\ldots,0\}} = 0$. From

$$\frac{\mathrm{d}a_{\{0,\ldots,2,\ldots,0\}}}{\mathrm{d}t} = \frac{\mathrm{d}\sigma_i}{\mathrm{d}t}\frac{1}{2\sigma_i}a_{\{0\}}\sqrt{2} + \sum_{i=1}^{d}\frac{\mathrm{d}\sigma_i}{\mathrm{d}t}\frac{1}{2\sigma_i}\left[a_{\{0,\ldots,2,\ldots,0\}}\frac{2n_i+1}{2}\right]$$

$$-a_{\{0,\ldots,1,\ldots,0\}}\frac{\mathrm{d}s_i}{\mathrm{d}t}2\sqrt{\sigma_i}$$

$$+2\left(\prod_j\sigma_j^{1/4}\right)\sum_{\{r\},\{s\}}a_{\{r\}}\chi_{\{s\}}\sigma_i\sqrt{2s_i}\mathbb{A}^{1}_{1,r_i,s_i-1}\prod_{j\neq i}\mathbb{A}^{1}_{0,r_j,s_j}\,,$$

we obtain

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}t} = -4\sigma_i^2\sum_{\{m\}}a_{\{m\}}\left(\chi_{\{m\}}m_i + \chi_{\{m;m_i\to m_i+2\}}\sqrt{(m_i+1)(m_i+2)}\right)\,.$$

2.1 Evolution Equations

We give here the final form of the evolution equations for the phase $\chi_{\{n\}}$, the modulus $a_{\{n\}}$, the Gaussian width $\boldsymbol{\sigma}$ and the center of the expansion $\mathbf{s}$ of the particle wave function.

$$\frac{\mathrm{d}\chi_{\{n\}}}{\mathrm{d}t} = \left(\prod_j^d \sigma_j^{1/4}\right) \sum_{\{r\},\{s\}} \left(-\chi_{\{r\}}\chi_{\{s\}} + \frac{1}{4} R_{\{r\}} R_{\{s\}}\right) \sum_{i=1}^d \sigma_i \sqrt{r_i s_i}\, \mathbb{A}^1_{n_i, r_i - 1, s_i - 1} \tag{17}$$

$$\times \prod_{j\neq i} \mathbb{A}^1_{n_j, r_j, s_j} - \sum_{i=1}^d \frac{\sigma_i}{2} n_i R_{\{n\}} + \pi^{d/4} \frac{1}{4} \sum_{i=1}^d \sigma_i^{3/4} \left(\sqrt{2}\delta_{n_i,2} - \delta_{n_i,0}\right) \left(\prod_{j\neq i}^d \sigma_j^{-1/4} \delta_{n_j,0}\right) \tag{18}$$

$$+ \sum_{i=1}^d \chi_{\{n; n_i \to n_i + 1\}} \frac{\mathrm{d}s_i}{\mathrm{d}t} \sqrt{2(n_i+1)\sigma_i}$$

$$+ \sum_i M_i \left(\frac{2n_i + 1}{2} \chi_{\{n\}} + \sqrt{(n_i+2)(n_i+1)}\, \chi_{\{n; n_i \to n_i + 2\}}\right) + \int U_{[\mathbf{s}]} h^{\boldsymbol{\sigma}}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r}\rangle}\, \mathrm{d}\mathbf{r} \tag{19}$$

$$\frac{\mathrm{d}a_{\{n\}}}{\mathrm{d}t} = \sum_{i=1}^d \frac{\mathrm{d}\sigma_i}{\mathrm{d}t} \frac{1}{2\sigma_i} \left[a_{\{n\}} \frac{2n_i + 1}{2} + a_{\{n; n_i \to n_i - 2\}} \sqrt{n_i (n_i - 1)}\right] - \sum_{i=1}^d a_{\{n; n_i \to n_i - 1\}} \frac{\mathrm{d}s_i}{\mathrm{d}t} \times$$

$$\sqrt{2n_i\sigma_i} + 2 \left(\prod_j^d \sigma_j^{1/4}\right) \sum_{\{r\},\{s\}} a_{\{r\}} \chi_{\{s\}} \sum_{i=1}^d \sigma_i \sqrt{n_i s_i}\, \mathbb{A}^1_{n_i - 1, r_i, s_i - 1} \prod_{j\neq i} \mathbb{A}^1_{n_j, r_j, s_j} \tag{20}$$

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}t} = -2 M_i \sigma_i \tag{21}$$

$$\frac{\mathrm{d}s_i}{\mathrm{d}t} = \sqrt{2\sigma_i}\, S_i\ , \tag{22}$$

where $M_i = 2\sigma_i \sum_{\{m\}} a_{\{m\}} \left(\chi_{\{m\}} m_i + \chi_{\{m; m_i \to m_i + 2\}} \sqrt{(m_i+1)(m_i+2)}\right)$ and $S_i = \sum_{\{m\}} a_{\{m\}} \chi_{\{m; m_i \to m_i + 1\}} \sqrt{m_i + 1}$.

2.2 Projection Coefficients of the Potential

By looking at the final system of evolution equations we see that the external potential appears only in the evolution equation for the phase (19) via the term $\int U_{[\mathbf{s}]} h^{\boldsymbol{\sigma}}_{\{n\}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r}\rangle}\, \mathrm{d}\mathbf{r}$ which, from a mathematical point of view, represents the projection of the potential on the Hermite basis set. In the general case, this term can be evaluated only numerically; since its calculation can be very costly, it is convenient to consider the case in which external potential is a polynomial. In this case, the calculations can be done explicitly. We proceed by assuming that the

potential U can be written in the following form which, from the point of view of the applications, is very general

$$U(\mathbf{r}) = \prod_{i}^{d} U^i(x_i) = \prod_{i}^{d} \sum_{n}^{N} \alpha_n^i x_i^n \ . \tag{23}$$

Here, $U^i(x_i) \doteq \sum_n^N \alpha_n^i x_i^n$, α_n^i are a set of given coefficients and N is the maximum degree at which the coordinate appears in the polynomial expansion of U. We obtain

$$\begin{aligned}\int U(\mathbf{r}+\mathbf{s}) h_{\{m\}}^{\boldsymbol{\sigma}} e^{-\langle \boldsymbol{\sigma}, \mathbf{r}\rangle} =& \sum_i \int h_{m_i}^{\sigma_i} e^{-\sigma_i r_i} U^i(x_i + s_i)\, \mathrm{d}x_i \prod_{j\neq i}^{d} \int h_{m_j}^{\sigma_j} e^{-\sigma_j r_j}\, \mathrm{d}x_j \\ =& \pi^{\frac{d-1}{4}} \sum_i \left(\prod_{j\neq i}^{d} \sigma_j^{-1/4} \right) \int h_{m_i}^{\sigma_i} U^i(x_i + s_i) e^{-\sigma_i r_i}\, \mathrm{d}x_i \ .\end{aligned}$$

The previous equation can be elaborated by inserting the polynomial expansion of Eq. (23). In particular, it is convenient to order the terms according to the degree with respect to the parameter s_i. At the end of the computation, we obtain

$$\begin{aligned}\int U_{[s]} h_{2r}^{\sigma} e^{-x^2\sigma}\, \mathrm{d}x =& \frac{\pi^{1/4} 2^r \sigma^{-1/4}}{\sqrt{(2r)!}} \left(\sum_{u=0}^{\left\lfloor \frac{N}{2} \right\rfloor - r} s^{2u} \frac{\sigma^u 2^{2u}}{(2u)!} \Gamma(u, r, \sigma) + 2\sigma^{\frac{1}{2}} \right. \\ & \left. \times \sum_{u=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor - r} s^{2u+1} \frac{\sigma^u 2^{2u}}{(2u+1)!} \widetilde{\Gamma}(u, r, \sigma) \right)\end{aligned}$$

$$\begin{aligned}\int U_{[s]} h_{2r+1}^{\sigma} e^{-x^2\sigma}\, \mathrm{d}x =& \frac{\pi^{1/4} 2^r \sigma^{-3/4}}{\sqrt{2}\sqrt{(1+2r)!}} \left(\sum_{u=1}^{\left\lfloor \frac{N}{2} \right\rfloor - r} s^{2u-1} \frac{\sigma^u 2^{2u}}{(2u-1)!} \Gamma(u, r, \sigma) + 2\sigma^{\frac{1}{2}} \right. \\ & \left. \times \sum_{u=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor - r} s^{2u} \frac{2^{2u} \sigma^u}{(2u)!} \widetilde{\Gamma}(u, r, \sigma) \right) \ ,\end{aligned}$$

where $r \in \mathbb{N}$, the symbol $\lfloor x \rfloor$ denotes the integer part of x and we have defined

$$\Gamma(u,r,\sigma) \doteq \sum_{n=2(u+r)+(0,2,4,\ldots)}^{N} \alpha_n \frac{n!\sigma^{-\frac{n}{2}}2^{-n}}{(\frac{n}{2}-u-r)!}$$

$$\widetilde{\Gamma}(u,r,\sigma) \doteq \sum_{n=2(u+r)+(1,3,5,\ldots)}^{N} \alpha_n \frac{n!\sigma^{-\frac{n}{2}}2^{-n}}{(\frac{n-1}{2}-u-r)!} \,.$$

The symbols under the sums indicate that the index n takes the value $2(u+r)$ plus the numbers indicated inside the parenthesis (even numbers for the first equation and odd numbers for the second equations).

3 Numerical Simulations: 2D Case

We apply the model that has been introduced in the previous sections to the motion of heavy quantum particles (typically atoms with few protons). In this section, we provide some motivations to our work and we describe the results obtained by solving the evolution equations in the case of a two-dimensional system. There exist many cases in which electrons are delocalized in a solid structure. The electron wave function may extend over various atomic cells and has typically a very complex shape. For this reason, the simulation of electron motion in solids in a realistic case requires the application of complex many body full quantum methods like the DFT [27] or the Green function approach. On the other side, nuclei are well localized quantum particles. They are typically considered as point-like particles which move along the classical trajectories obtained by solving the Newton equation. The De Broglie wave length provides a simple estimate of the degree of localization of the quantum wave function of a particle. It is well known that De Broglie wave length provides the spatial scale on which the probability to find a particle around the position expectation value decays. Since the Broglie wave length is proportional to the inverse of the particle mass, heavy particles may have very small localization length. This is the case of atoms inside a solid. For this reason, the spread of the atomic wave function around the mean particle position is typically neglected. However, recent theoretical and experimental studies reveal the existence of physical conditions for which the previous approximation is violated. They suggest that slightly bound protons and the hydrogen molecule behave as quantum particles. In particular, we focus on the study of the phase transition of ice of water and we analyse the so called VIII-X transition. The physical phenomena concerns the modification of the atomic structure of the ice in the presence of an external pressure. In particular, the VIII-X phase transition concerns the behaviour of the protons. At low pressure, every protons of the H_2O crystal remain close to one oxygen atom. By increasing the pressure a phase transition is observed. At the

critical pressure, the protons migrate to the middle of the O-O bound. This behaviour is explained by assuming that the electrostatic potential between two oxygen atoms at low pressure has a double well structure. Due to this potential profile the protons are trapped inside one of the two minima of the potential. By increasing the pressure, the two wells merge together and form a single central well. The equilibrium position of the proton is thus shifted to the middle of the two atoms. Even if the qualitative behaviour of the transition has been clarified, theoretical estimations of the transition pressure are not in agreement with the experiments. Bronstein et al. have shown that in order to obtain the experimental value of the transition pressure, it is essential to include the quantum mechanical delocalization of the protons in the numerical model [28]. Recent results [29] suggest that tunneling of protons plays a essential role in this process. Classical simulations ignore the possibility to overcome thin barriers by tunneling and tend to overestimate the transition pressure. Quantum corrected model are thus essential for simulating this kind of phenomena.

In particular, in Ref. [29], ab initio calculations indicate that the shape of the electrostatic potential around two oxygen atoms can be approximated by a simple expression. The potential is fitted by a harmonic term plus a non harmonic correction which is proportional to the macroscopic pressure applied to the sample.

Motivated by these results, we have applied our method to reproduce the two-dimensional motion of a single particle in a non harmonic potential. In the simulations we use the following double well potential

$$U(x, y) = -\frac{\omega_x}{2}x^2 + V_4 x^4 + \frac{\omega_y}{2}y^2 \,. \tag{24}$$

We take the following values of the parameters $\omega_x = 1$, $\omega_y = 1$ $V_4 = 0.05$. As initial condition, we have considered a Gaussian beam localized around the left minimum of the potential profile and initial momentum $\mathbf{p} = (0, 1)$. The results of the simulations are shown in Fig. 1, where the panels refer to different times, $t = 1, 2, 3.5, 6$. In our simulation, we have solved the system of Eqs. (19)–(22) by choosing a cutoff on n_1 and n_2. More precisely, we evaluate the following parameters: a_{n_1,n_2}, χ_{n_1,n_2} with $0 \leq n_1 \leq 3$, $0 \leq n_2 \leq 3$. We plot by solid blue curves the contour of the solution. In order to follow the evolution of the particle, we have represented the trajectory of the mean particle position by a solid light blue line. In order to appreciate the difference between the classical and the quantum corrected dynamics, we have depicted the classical trajectories obtained by solving the Newton equation by red solid lines. Our simulations show the relevance of the tunneling effect on the localization of the particle inside the two well structure. We see that in the classical case the particle has not enough energy to overcome the potential barrier. The classical trajectory is confined in the left well. Quantum calculations show that the particle tends to bounce back and forth between the two potential minima. This indicate, as expected, that there exists a range of pressure in which, according to classical dynamics, the proton is trapped in a minima near one of the oxygen atoms, while, according to quantum dynamics, the proton can be found on the left or on the right well with similar probability.

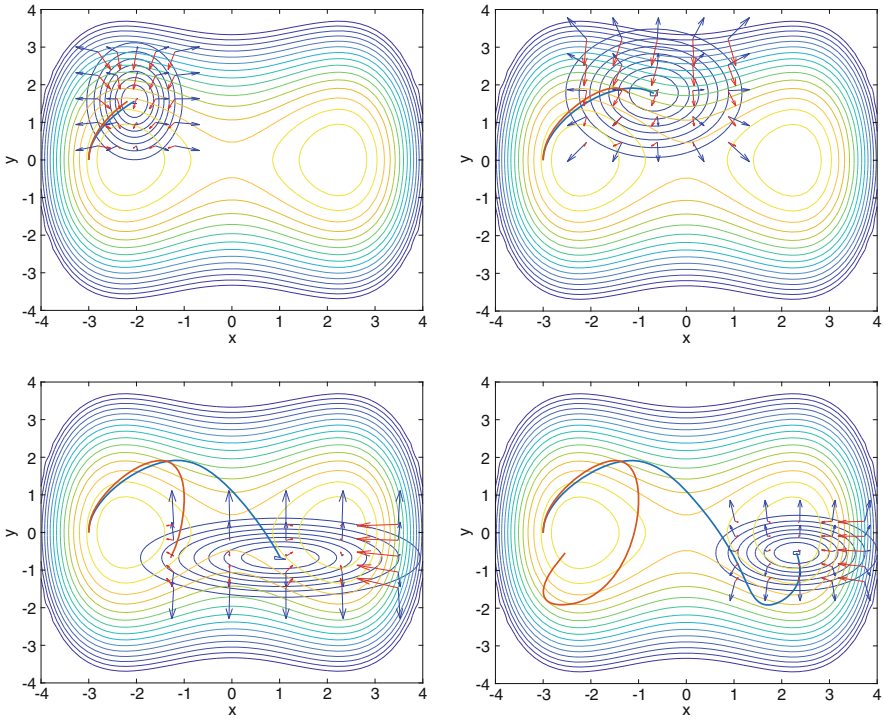

Fig. 1 Evolution of a initially localized Gaussian pulse inside the potential profile (24) (Coloured lines represent the contour plot of U). The panels refer to different times: upper-left $t = 1$ upper-right $t = 2$ bottom-left $t = 3.5$ bottom-right $t = 6$. The contour plot of the solution is depicted by blue lines, the trajectory of the centre of the wave function and the trajectory of the classical motion are depicted by, respectively, light blue and red lines. Arrows depict the classical force field (red arrows) and the Bohm force field (blue arrows)

By looking at the Bohm force we see some interesting features of the quantum behaviour of the nearly localized particles. In Fig. 1 we have represented by red arrows the classical force field obtained by the taking the gradient of the potential given in Eq. (24). According to the Bohm description of quantum mechanics, the quantum motion of a particle can be understood in terms of the evolution of a fluid whose volume elements move along integral curves of the total force field $\mathbf{F} = \nabla(U + Q)$, where Q is the Bohm potential defined in Eq. (4). This point of view provides a simple interpretation of the Bohm force field and can help to visualize the particle motion. In our plots, the gradient of the Bohm potential is represented by blue arrows. According to the Bohm framework every material point is accelerated by two force fields, the classical force and the Bohm one. In particular, the simulations show that the Bohm field is responsible of the spread of the particle wave packed, which allows the particle to overcome the potential barrier.

4 Conclusions

We have presented a quantum model for particles characterized by Gaussian wave packets. The oscillations of the wave function around the mean particle positions are represented by Hermite polynomials. The particle motion is described by a set of time dependent parameters. Our approach shows an interesting connection with the description of the particle motion provided by the Bohm theory. We have applied our method to investigate the motion of a nearly localized particle in a 2D confining structure.

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