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# Quantum motion with trajectories: beyond the Gaussian beam approximation

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## Abstract

A quantum model based on the Euler–Lagrange variational approach is proposed. Similarly to classical transport, our approach maintains the description of particle motion in terms of trajectories in a configuration space. Our method is designed to provide some corrections to the classical motion of nearly localized particles due to quantum phenomena. We describe the spatial localization of the particles by extending the usual ansatz which is at the basis of the Gaussian beam method. We discuss the completeness of our ansatz and the connection of our results with the Bohm trajectories approach. Our method finds application in the simulation of the motion of light nuclei in *ab initio* calculations.

Keywords: Gaussian beam method, Bohm dynamics, variational method, quantum dynamics

(Some figures may appear in colour only in the online journal)

## 1. Introduction

During the last decade, several numerical methods based on *ab initio* approaches have been developed. Progress made in theoretical modeling and development of new numerical algorithms has facilitated the systematic investigation of the dynamics of molecules and the study of the electronic and optical properties of nanostructures [1–11].

In the framework of such *ab initio* quantum mechanical methods, a system containing  $N$  protons and  $N'$  electrons is described by a single many-body wave function  $\Psi(\mathbf{R}, \mathbf{r}, t)$ . We denote by  $\mathbf{r}(\mathbf{R})$  the collective variable containing the coordinates of all the electrons (nuclei). The wave function  $\Psi$  is extremely hard to compute even for a small number of particles. In order to reduce the complexity of the problem, various approximations of  $\Psi(\mathbf{R}, \mathbf{r}, t)$  have been proposed. The main concern is to find a way to disentangle, to some extent, the electronic from the nuclear component of the wave function [3, 12]. According to the Born–Oppenheimer

ansatz, the total wave function of electrons and nuclei is factorized to the product of the electronic wave functions ( $\Phi_i$ ) and the atomic wave functions ( $\Theta_i$ ):

$$\Psi(\mathbf{R}, \mathbf{r}, t) = \sum_i \Phi_i(\mathbf{R}, \mathbf{r}, t) \Theta_i(\mathbf{R}, t) .$$

A very popular approximation, first proposed by Hartree, is to replace  $\Psi(\mathbf{R}, \mathbf{r}, t)$  by a single term  $\Psi(\mathbf{R}, \mathbf{r}, t) \simeq \Phi(\mathbf{R}, \mathbf{r}, t) \Theta(\mathbf{R}, t)$ . The Hartree approximation is implicitly assumed by the majority of the *ab initio* methods based on the Kohn–Sham density functional theory (DFT) [13]. The second and major approximation which is usually assumed is to limit the quantum mechanical description of the particle motion to the electronic degrees of freedom. The wave function  $\Phi(\mathbf{R}, \mathbf{r}, t)$  is calculated by the solving the quantum Kohn–Sham equation. The nuclei are considered as point-like particles which move along the classical trajectories  $\mathbf{R}(t)$  obtained by solving the Newton equation. Such a two-scale modeling, i.e. classical treatment for the nuclei and quantum description for the electrons, is motivated by the fact that the de Broglie length associated with a proton is usually very small compared with the de Broglie length associated with an electron under equal conditions of temperature and pressure.

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, and that this behavior is at the origin of some complex phenomena. As an example, various chemical reactions are understood in terms of electronic transfer processes assisted by non-adiabatic quantum transitions of protons. Such mechanisms may explain some biological processes related to photosynthesis and to the biosynthesis of DNA [14, 15]. Studying the phase transition of water ice via DFT models, Bronstein *et al* have shown that in order to obtain the experimental value of the transition pressure, it is essential to include in the numerical model the quantum mechanical delocalization of the protons [16].

Motivated by these results, the study of mathematical models for the quantum transport of protons at the nanometric scale has seen renewed interest. The development of new *ab initio* methods applied to the simulation of complex systems, including the description of the quantum motion of light atoms, has a wide array of potential applications. In a large number of molecular configurations, protons are trapped in local minima of the electrostatic potential whose barriers have thicknesses of a few nanometers. In such cases, quantum tunneling and the zero point energy of the protons influence the equilibrium configuration of the system.

New concepts, such as deterministic and stochastic quantum trajectories, have been proposed in order to develop new *ab initio* methods that go beyond the classical description of atomic nuclei [17–23]. A method that extends the concept of classical trajectory to the quantum mechanical context has the clear advantage that it could easily be integrated into the numerical solvers which have been developed for the simulation of molecular dynamics. The Bohm interpretation of quantum mechanics extends in a rigorous way the concept of the deterministic trajectory of a particle [19, 24, 25]. The Bohm approach is potentially able to deal with any quantum phenomenon. Nowadays, methods based on the Bohm formalism are very popular. However, due to the extremely complex structure revealed by the calculations of the quantum Bohm trajectories, the application of the Bohm theory to a real situation suffers from serious limitations. The first attempts in this direction have been proposed by Tully [26] and Wyatt [27]. The dynamics of nuclei is described by a single or by a bundle of quasi-classical trajectories evaluated self-consistently with the electronic density. Such methods have stimulated the study of a few general methods, such as the multiconfiguration time-dependent Hartree method [28], the conditional Born–Oppenheimer dynamics [29] and the extension of Bohm trajectories to the complex plane [30]. Moreover, stochastic methods have also been

addressed. Based on the classical concept of Brownian and Langevin dynamics, some stochastic models are able to reproduce the quantum statistical properties of protons in harmonic traps [31].

In this paper, we propose a quantum model based on the Euler–Lagrange variational approach. Our method is designed to describe the motion of nearly localized particles. Similarly to Gaussian beam methods [32], we assume that the particle wave function is adequately described by a single Gaussian modulated by a polynomial. Our ansatz for the particle wave function contains a complete set of parameters. We derive the evolution equations of such parameters by considering an integral formulation of the evolution equations. Our method shows a strong analogy with the Bohm approach. The integral form of the equations suggests a strategy which is able to tackle the divergences of the Bohm potential.

## 2. Euler–Lagrange variational approach

We derive the motion of a quantum particle by using a variational approach. We assume that the particle is described by a generalized Gaussian wave packet parametrized by a set of time dependent numbers  $\xi_n$ . We formulate the particle evolution in terms of an Euler–Lagrange problem. By minimizing the action of the quantum Lagrangian of the particle, we derive the evolution equations for the parameters  $\xi_n$ . Our ansatz is completely general: every  $L^2$  function can be expressed by the  $\xi_n$ –parametrized Gaussian wave packet. Our interest is to derive approximate models that describe the evolution of particles in the semi-classical regime [33–35]. In standard conditions, a heavy quantum particle has small de Broglie wavelength and can be characterized by just a few parameters—namely, its mean position, velocity and dispersion. Our method is designed to describe the motion of well localized wave packets with Gaussian dispersion, and we focus on neutron and proton motion. As a first approximation, the wave function of a particle in the semi-classical regime is usually described by a minimum uncertainty Gaussian profile [32], [36–38]:

$$\psi(x, t) = \sqrt{\frac{\sigma(t)}{\pi}} e^{-\frac{[x-s(t)]^2}{2\sigma(t)} - i\sigma_i(t)} e^{i[\phi_0(t) + p(t)(x-s(t))]} \quad (1)$$

Here, in order to introduce our model, we have parametrized the particle wave function  $\psi$  by inserting a few real numbers which are associated with the main physical quantities of the particle. In particular,  $s$  is the mean position,  $p$  the mean momentum,  $\phi_0$  the phase and  $\sigma$ ,  $\sigma_i$  respectively the real and imaginary parts of the inverse of the standard deviation. If we assume that the ansatz of equation (1) stays valid for a sufficiently long time interval, by evaluating the evolution of  $s$ ,  $p$ ,  $\phi_0$ ,  $\sigma$  and  $\sigma_i$ , it is possible to obtain an approximate evolution of the particle wave function  $\psi$ . In the following, we generalize the ansatz given in equation (1) by defining a more general set of parameters. Equation (1) constitutes the basic equation and the starting point of the so called Gaussian beam method. The Gaussian beam method has been derived in the framework of the semi-classical WKB approach. In particular, it emerges as an extension of the WKB method in which the second order term of the particle phase may become imaginary, providing Gaussian localization of the wave. Seminal works have been put forward by Heller [39], Lebedev [40] and Popov [41]. Such theories have been extended in various directions, and later reformulations of Gaussian smoothing considered the use of complete polynomial expansion of the wave function [42] and the use of a fixed or variable number of Gaussian functions which are eventually created in correspondence to spatial discontinuities and abrupt interfaces [32]. A number of extensions of the Gaussian wave approach that include non-Gaussian wave functions [43], rotating waves

[44] and formulations which preserve the Hamiltonian structure of the equation of motion [45] have been developed. The investigation of quantum chaos in terms of the semi-classical propagation of Gaussian wave packets and the connection with the Wigner representation have been also considered [46]. A clear introduction to the basic equations of the Gaussian beam approach can be found in [32, 47].

We consider the quantum mechanical evolution of a particle of mass  $m$  in the presence of the potential  $\bar{U}(\bar{x})$ :

$$i\hbar \frac{\partial \psi}{\partial \bar{t}} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \bar{x}^2} + \bar{U}(\bar{x}) \right) \psi. \quad (2)$$

In the following, we will use dimensionless variables for position  $x = \frac{\bar{x}}{L}$ , time  $t = \frac{\bar{t}}{\tau}$  and energy  $U = \frac{\bar{U}}{E_0}$ , where  $L$ ,  $\tau$  and  $E_0$  are suitable scaling factors. In order to simplify the equations, we choose  $\tau = \frac{mL^2}{\hbar}$  and  $E_0 = \frac{\hbar^2}{mL^2}$ . With this, equation (2) becomes

$$i \frac{\partial \psi}{\partial t} = \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + U(x) \right) \psi. \quad (3)$$

For the sake of simplicity, we have considered one-dimensional motion—the major part of this paper is concerned with one-dimensional motion; extension of the main results to two-dimensional space will be considered in section 8. According to the Euler–Lagrange formalism, we define a suitable quantum Lagrangian  $L$  and formulate the quantum motion in terms of a variational problem for  $L$  [48]. We define the quantum Lagrangian

$$L = \int_{\mathbb{R}} \mathcal{L}(\psi, \psi^\dagger, \partial_x \psi, \partial_x \psi^\dagger, \partial_t \psi, \partial_t \psi^\dagger, x, t) dx,$$

where the Lagrangian density  $\mathcal{L}$  is

$$\mathcal{L} = -\frac{i}{2} (\partial_t \psi^\dagger \psi - \psi^\dagger \partial_t \psi) - \frac{1}{2} \partial_x \psi^\dagger \partial_x \psi - U \psi^\dagger \psi.$$

Equation (3) is formally equivalent to the Euler–Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial \psi^\dagger} = \partial_t \frac{\partial \mathcal{L}}{\partial (\partial_t \psi^\dagger)} + \partial_x \frac{\partial \mathcal{L}}{\partial (\partial_x \psi^\dagger)}, \quad (4)$$

where, in accordance with the standard field quantization procedure,  $\psi$  and  $\psi^\dagger$  are considered two independent fields. We write the wave function  $\psi$  as follows:

$$\psi(x) = \sqrt{P(x-s(t), t)} e^{-\frac{(x-s(t))^2}{2} \sigma(t) + i\chi(x-s(t), t)}. \quad (5)$$

Here,  $P$  and  $\chi$  are time-dependent polynomials  $P = P(x, t)$ ,  $\chi = \chi(x, t)$ , and  $s = s(t)$ ,  $\sigma = \sigma(t)$  are two parameters. We treat  $\psi^\dagger$  as the complex conjugate of  $\psi$  [48]. The quantum Lagrangian becomes

$$\begin{aligned} L &= \int_{\mathbb{R}} \left[ \text{Im} (\psi^\dagger \partial_t \psi) - \frac{1}{2} |\partial_x \psi|^2 - U |\psi|^2 \right] dx \\ &= \int_{\mathbb{R}} \left[ P \frac{d\chi}{dx} \dot{s} - P \dot{\chi} - \frac{\sigma^2 x^2 P}{2} - \frac{1}{8P} \left( \frac{dP}{dx} \right)^2 + \frac{x\sigma}{2} \frac{dP}{dx} - \frac{P}{2} \left( \frac{d\chi}{dx} \right)^2 - U_{[s]} P \right] e^{-x^2 \sigma} dx. \end{aligned} \quad (6)$$

Here, the symbol  $U_{[s]}$  denotes  $U(x+s)$ ,  $\text{Im}$  the imaginary part, and the dot the time derivative.

### 2.1. Example: Gaussian wave

We illustrate the application of the Euler–Lagrange method by a textbook example. We consider the standard Gaussian ansatz expressed by equation (1). We note that equation (1) can be obtained as a particular case of equation (5) with  $P = a_0\sigma^{1/2}\pi^{-1/2}$  and  $\chi = \phi_0 + px + \frac{\sigma_i}{2}x^2$ . We write equation (6) in terms of the Lagrangian parameters  $\xi \equiv (a_0, s, \phi_0, p, \sigma_i, \sigma)$

$$L = a_0 \left[ -\dot{\phi}_0 + \dot{s}p - \frac{p^2}{2} - \frac{\dot{\sigma}_i + \sigma_i^2 + \sigma^2}{4\sigma} - \sqrt{\frac{\sigma}{\pi}} \int_{\mathbb{R}} U(s+x)e^{-x^2\sigma} dx \right].$$

The Euler–Lagrange equations are obtained by taking the extremal of the quantum action  $\delta \int L dt = 0$ :

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\xi}_n} = \frac{\partial L}{\partial \xi_n}. \quad (7)$$

We obtain the following closed system of equations:

$$\dot{a}_0 = 0 \quad (8)$$

$$\dot{s} = p \quad (9)$$

$$\dot{p} = -\sqrt{\frac{\sigma}{\pi}} \int_{\mathbb{R}} \frac{dU(s+x)}{ds} e^{-x^2\sigma} dx \quad (10)$$

$$\dot{\sigma} = -2\sigma_i\sigma \quad (11)$$

$$\dot{\sigma}_i = \sigma^2 - \sigma_i^2 - 2\sqrt{\frac{\sigma^3}{\pi}} \int_{\mathbb{R}} (2\sigma x^2 - 1) U(s-x)e^{-x^2\sigma} dx \quad (12)$$

$$\dot{\phi}_0 = \frac{p^2}{2} - \frac{(\sigma - \sigma_i)^2}{4\sigma} - \sqrt{\frac{\sigma}{\pi}} \int_{\mathbb{R}} U(s-x)e^{-x^2\sigma} dx. \quad (13)$$

The first equation ensures that the  $L^2$  norm of the wave function is conserved. In fact, from equation (5) we have  $\|\psi\|_2 = a_0^{1/2}$ . It is interesting to consider the harmonic potential  $U = \frac{\omega^2}{2}x^2$ . Equations (10)–(13) simplify

$$\dot{p} = -\omega^2 s \quad (14)$$

$$\dot{\sigma}_i = \sigma^2 - \sigma_i^2 - \omega^2 \quad (15)$$

$$\dot{\phi}_0 = \frac{p^2}{2} - \frac{\omega^2 s^2}{4} - \frac{\sigma}{2}. \quad (16)$$

We have used

$$\sigma^{3/2}\pi^{-1/2} \int_{\mathbb{R}} (2\sigma x^2 - 1) U(s+x)e^{-x^2\sigma} dx = \frac{\omega^2}{2}.$$

The evolution of the Gaussian packet in the presence of a harmonic potential constitutes a typical test case. It has been considered by various authors [32, 49–51]. The Gaussian ansatz has the remarkable property that in the case of harmonic potential, the solution of equations (8)–(16) provides the exact solution to the Schrödinger equation.

### 2.2. General case

We discuss now the Euler–Lagrange problem in a more general context. We expand the wave function  $\psi$  on a complete set of functions. We write  $P$  and  $\chi$  as follows:

$$P(x, t) = \frac{1}{\pi^{1/4}} \sum_{n=0}^{\infty} h_n^\sigma(x) a_n(t) \quad (17)$$

$$\chi(x, t) = \pi^{1/4} \sum_{n=0}^{\infty} h_n^\sigma(x) \chi_n(t). \quad (18)$$

Here,  $a_n$  and  $\chi_n$  are the coefficients that parametrize the solution, and the symbol  $h_n^\sigma(x)$  denotes the normalized Hermite polynomials:

$$h_n^\sigma(x) \equiv \frac{\sigma^{1/4}}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x\sqrt{\sigma}) = (-1)^n \frac{\sigma^{1/4 - \frac{n}{2}}}{\sqrt{2^n n! \sqrt{\pi}}} e^{x^2 \sigma} \frac{d^{(n)}}{dx^n} e^{-x^2 \sigma}. \quad (19)$$

For the sake of clarity, we have expressed  $h_n^\sigma(x)$  in the previous expression in terms of the more standard definition of Hermite polynomials:

$$H_n(x) \equiv (-1)^n e^{x^2} \frac{d^{(n)}}{dx^n} e^{-x^2}. \quad (20)$$

It is well known that the polynomials  $h_n^\sigma$  form a complete basis set for the inner product:

$$\langle h_n^\sigma, h_m^\sigma \rangle_\sigma \equiv \int_{\mathbb{R}} h_n^\sigma(x) h_m^\sigma(x) e^{-x^2 \sigma} dx = \delta_{n,m}. \quad (21)$$

The symbol  $\delta$  denotes the Kronecker delta. For future reference, we state here some properties of the Hermite polynomials:

$$\frac{dh_n^\sigma}{dx} = \sqrt{2n\sigma} h_{n-1}^\sigma \quad (22)$$

$$\sqrt{\sigma} x h_n^\sigma = \sqrt{\frac{n+1}{2}} h_{n+1}^\sigma + \sqrt{\frac{n}{2}} h_{n-1}^\sigma \quad (23)$$

$$\sqrt{2n\sigma} h_n^\sigma = \left( 2\sigma x - \frac{d}{dx} \right) h_{n-1}^\sigma \quad (24)$$

$$\frac{dh_n^\sigma}{d\sigma} = \frac{2n+1}{4\sigma} h_n^\sigma + \frac{\sqrt{n(n-1)}}{2\sigma} h_{n-2}^\sigma. \quad (25)$$

The following scaling property will be very useful:

$$h_n^\sigma(x) = h_n^1(x\sqrt{\sigma}) \sigma^{1/4}. \quad (26)$$

According to equations (17) and (18), the central assumptions made in our approach concern the expansion of the squared modulus and of the phase of  $\psi$ . We treat such functions in a symmetric way and use the Hermite polynomial set to expand both modulus and phase. Our method shares similarities with other approaches proposed in the past. A popular model has been formulated by Hagedorn [50–52]. Hagedorn’s approach is based on the definition of suitable raising and lowering operators whose basis sets coincide with the Hermite polynomials in the 1D case. Similarly to the Hagedorn approach, the so called time-dependent discrete

variable representation (TDDVR) method uses Hermite polynomials in order to modulate the Gaussian profile (in such context, this is denoted by Gauss–Hermite expansion), the main difference being the choice of the complex parameters appearing in the Gaussian function [49, 53]. Differing from the Hagedorn and the TDDVR approaches in which the phase of the Gaussian wave function contains only linear and quadratic terms, we expand the phase  $\chi$  to all the orders. Our choice is motivated by the possibility of writing the Euler–Lagrange equations in normal form, and by the interesting connection which is found among the time dependent parameters and the Bohm description of the particle motion, which will be discussed in detail in section 3.

### 2.3. Completeness of the expansion

By using the expansion of equations (17) and (18) we have parametrized the particle wave function by the set  $\xi \equiv \{s, \sigma, a_n, \chi_n\}$ . The set  $\xi$  contains all the dynamical variables of our system. The Euler–Lagrange equation (7) for such coefficients are obtained by straightforward computation of the Lagrangian (6). In particular, by analyzing the number of coefficients that we have introduced, it is easy to recognize that our choice of coefficients is redundant. In fact, since the Hermite polynomials form a complete set, it is clear that all functions  $P$  and  $\chi$  can be expanded respectively according to equations (17) and (18). The functions  $P$  and  $\chi$  are sufficient to determine the modulus and phase of  $\psi$ . However, our ansatz contains two additional parameters,  $\sigma$  and  $s$ . This suggests that we can fix the values of two parameters among all the others. Direct computation shows that the quantum Lagrange equations are considerably simplified in a particular case, viz. if the coefficients  $a_1$  and  $a_2$  of the expansion (17) are identically zero. In the following, we will show that every  $L^2$  function can be expanded according to equations (5), (17) and (18) under the constraint  $a_1 = 0$  and  $a_2 = k$  where  $k$  is given.

By writing  $\psi$  in polar coordinates  $\psi = |\psi|e^{i\chi}$ , it is clear that constraints on  $a_1$  and  $a_2$  concern only the expansion of the modulus  $|\psi|$ . In order to show the completeness of our expansion, it is sufficient to show that the modulus  $|\psi(x)|^2 = P(x-s)e^{-(x-s)^2\sigma}$  can be expressed by

$$|\psi(x)|^2 = \frac{e^{-(x-s)^2\sigma}}{\pi^{1/4}} \left( h_0^\sigma a_0 + h_2^\sigma k + \sum_{n=3}^{\infty} h_n^\sigma (x-s)a_n \right). \quad (27)$$

It is well known that for every choice of the parameters  $s \in \mathbb{R}$  and  $\sigma \in \mathbb{R}^+$  the set  $\{h_n^\sigma(x-s)e^{-(x-s)\sigma/2} : n \in \mathbb{N}\}$ , is complete in the space  $L^2(\mathbb{R})$ . Equivalently, the set  $\{h_n^\sigma(x-s) : n \in \mathbb{N}\}$  is complete in the space of the polynomials. The expansion (27) is complete if and only if for every polynomial  $p$ , we can find  $s \in \mathbb{R}$  and  $\sigma \in \mathbb{R}^+$  such that the second and third coefficient of the Hermite expansion of  $p$  are prescribed. This is ensured by the following.

**Lemma 2.1.** *Let  $p$  be a non-negative polynomial of degree  $2n$  with  $n \in \mathbb{N}$ . There is  $k_M \in \mathbb{R}$  such that for each  $k > k_M$  there exist  $\sigma \in \mathbb{R}^+$  and  $s \in \mathbb{R}$  such that*

$$\langle h_1^\sigma(x-s), p \rangle_\sigma = 0 \quad (28)$$

$$\langle h_2^\sigma(x-s), p \rangle_\sigma = k. \quad (29)$$

**Proof.** We prove the lemma by fixed point argument. We define

$$p_1(s, \sigma) \equiv \frac{\sigma^{-1/4}\pi^{-1/4}}{\sqrt{2}} \langle h_1^\sigma(x-s), p \rangle = \frac{\sigma^{3/2}}{\pi^{1/2}} \int_{\mathbb{R}} (x-s)p(x)e^{-(x-s)^2\sigma} dx, \quad (30)$$



$$p_2(s, \sigma) \equiv \sigma^{5/4} \sqrt{2\pi}^{1/4} \langle h_2^\sigma(x-s), p \rangle = \sigma^{3/2} \int_{\mathbb{R}} [2\sigma(x-s)^2 - 1] p(x) e^{-(x-s)^2\sigma} dx. \tag{31}$$

We indicate by  $s = G_1(\sigma)$  the solution of  $p_1(s, \sigma) = 0$  (the variable  $s$  is expressed as a function of  $\sigma$ ) and  $\sigma = G_2(s)$  the solution of  $p_2(s, \sigma) = 0$  (the variable  $\sigma$  is expressed as a function of  $s$ ). We prove that the map

$$\begin{cases} s_i = G_1(\sigma_{i-1}) \\ \sigma_i = G_2(s_i) \end{cases} \quad i = 1, 2, \dots$$

is well defined for every initial value  $\sigma_0$ . We show that the images of the maps  $G_1$  and  $G_2$  are compact. This ensures the existence of a convergent subsequence of the set  $(s_i, \sigma_i)$  and concludes the proof of the lemma.

We start by showing that if we fix  $\bar{\sigma} \in \mathbb{R}^+$ ,  $p_1(s, \sigma) = 0$  always admits a solution  $s = G_1(\bar{\sigma})$ . If  $p(x)$  is constant, the solution is  $s = 0$ . We assume that  $p(x)$  is not constant. From equation (30),  $p_1(s, \sigma) = 0$  can be written as

$$\frac{d}{ds} K_{\bar{\sigma}}(s) = 0, \tag{32}$$

where  $K_{\bar{\sigma}}(s) \in C^\infty(\mathbb{R})$  is given by

$$K_{\bar{\sigma}}(s) \equiv \int_{\mathbb{R}} p(x) e^{-(x-s)^2\bar{\sigma}} dx. \tag{33}$$

It is easy to verify that for every positive definite polynomial of degree  $2n$  there exist  $\bar{x}$  and  $M > 0$  such that, for every  $x \in \mathbb{R}$ ,  $|x| \geq \bar{x} \Rightarrow p(x) \geq Mx^{2n}$ . For  $s > \bar{x} + 1$  we have

$$\begin{aligned} K_{\bar{\sigma}}(s) &= \int_{|x|>\bar{x}} p(x) e^{-(x-s)^2\bar{\sigma}} dx + \int_{|x|\leq\bar{x}} p(x) e^{-(x-s)^2\bar{\sigma}} dx \geq M \int_{|x|>\bar{x}} x^{2n} e^{-(x-s)^2\bar{\sigma}} dx + \sqrt{\frac{\pi}{\bar{\sigma}}} \min_{|x|\leq\bar{x}} p(x) \\ &\geq M e^{-\bar{\sigma}} \int_{s-1}^{s+1} x^{2n} dx + \sqrt{\frac{\pi}{\bar{\sigma}}} \min_{|x|\leq\bar{x}} p(x) = \frac{M e^{-\bar{\sigma}}}{2n+1} [(s+1)^{2n+1} - (s-1)^{2n+1}] + \sqrt{\frac{\pi}{\bar{\sigma}}} \min_{|x|\leq\bar{x}} p(x). \end{aligned}$$

We have used  $e^{-x^2\bar{\sigma}} \geq e^{-\bar{\sigma}} \chi_{|x|<1}$  where  $\chi$  denotes the characteristic function. This shows that

$$\lim_{s \rightarrow +\infty} K(s) = +\infty.$$

In the same way, it is possible to prove that

$$\lim_{s \rightarrow -\infty} K(s) = +\infty,$$

which ensures that  $K$  has at least one stationary point.

As a second step, we find a bound for  $s = G_1(\sigma)$  which is uniform with respect to  $\sigma$ . Here, we assume that  $2n$  (the degree of  $p$ ) is greater than two; otherwise, the result is trivial. Integration by part leads to

$$p_1(s, \sigma) = \frac{\sigma^{1/2}}{2\pi^{1/2}} \int_{\mathbb{R}} \frac{dp}{dx} e^{-(x-s)^2\sigma} dx.$$

In the limit of large  $s$ , we have

$$\frac{\partial p_1}{\partial \sigma} = -s^{2n-3} \frac{d^{2n} p}{dx^{2n}}(0) \frac{(2n-1)(2n-2)\sqrt{\pi}}{(2n)! 2\sigma} + o\left(\frac{1}{s}\right),$$

which is obtained by direct computation of the integral. Since  $\frac{d^{2n} p}{dx^{2n}}(0) > 0$ , for  $s$  sufficiently large, the derivative of  $p_1$  with respect to  $\sigma$  is negative. Thus, there exists  $s_M$  such that  $|s| > s_M$  implies

$$p_1(s, \sigma) \geq \lim_{\sigma \rightarrow \infty} p_1(s, \sigma) = \frac{1}{2} \frac{dp}{dx}(s) > 0.$$

In conclusion, the solutions  $G_1(\sigma)$  belong to a bounded set.

Concerning the second constraint, proceeding in the same way, we fix  $\bar{s}$  and prove that there exists  $k$  such that the equation  $p_2(\bar{s}, \sigma) = k$  admits a solution  $\sigma = G_2(\bar{s})$ . Integrating by parts, from equation (31),  $p_2(\bar{s}, \sigma) = k$  can be written

$$\frac{\sqrt{\sigma}}{2} \int_{\mathbb{R}} \frac{d^2 p}{dx^2} e^{-(x-\bar{s})\sigma} dx = k. \quad (34)$$

If  $p$  is a second order polynomial, equation (34) for  $k = \frac{\sqrt{\pi}}{2} \frac{d^2 p}{dx^2}(0)$  is satisfied for every  $\sigma > 0$ . If the degree of  $p$  is greater than two, it is easy to verify that

$$\begin{aligned} \lim_{\sigma \rightarrow \infty} \frac{\sqrt{\sigma}}{2} \int_{\mathbb{R}} \frac{d^2 p}{dx^2} e^{-(x-\bar{s})\sigma} dx &= \frac{\sqrt{\pi}}{2} \frac{d^2 p}{dx^2}(\bar{s}) \\ \lim_{\sigma \rightarrow 0} \frac{\sqrt{\sigma}}{2} \int_{\mathbb{R}} \frac{d^2 p}{dx^2} e^{-(x-\bar{s})\sigma} dx &= +\infty. \end{aligned}$$

If we take  $k > \frac{\sqrt{\pi}}{2} \frac{d^2 p}{dx^2}(\bar{s})$ , equation (34) always has a solution. Since we have shown that  $\bar{s}$  belongs to a bounded set, there exists  $k_M = \sup_{\bar{s} < s_M} k < \infty$ . The previous limits also show that we can always find a solution of equation (34)  $\sigma \leq \sigma_M$ , where  $\sigma_M$  is the solution of equation (34) for  $k = k_M$ . The solution  $\sigma$  belongs to a bounded domain, and this concludes the proof of the lemma.  $\square$

#### 2.4. Quantum Lagrangian

In this section together with section 4 we derive the relevant evolution equations for our system. The calculation proceeds straightforwardly. The Euler–Lagrange equations are given by equation (7), where the quantum Lagrangian is written in equation (6). We expand the modulus and the phase of  $\psi$  on the complete Hermite basis via equations (17) and (18). For the sake of generality, in our calculations we assume  $a_1 \neq 0$  and  $a_2 \neq 0$ . We obtain

$$\int_{\mathbb{R}} P \dot{\chi} e^{-x^2 \sigma} dx = \sum_{n=0}^{\infty} a_n \left[ \dot{\chi}_n + \frac{\dot{\sigma}}{2\sigma} \left( \frac{2n+1}{2} \chi_n + \sqrt{(n+2)(n+1)} \chi_{n+2} \right) \right] \quad (35)$$

$$\int_{\mathbb{R}} P \frac{d\chi}{dx} e^{-x^2 \sigma} dx = \sqrt{2\sigma} \sum_{n=0}^{\infty} \sqrt{(n+1)} \chi_{n+1} a_n \quad (36)$$

$$\frac{\sigma^2}{2} \int_{\mathbb{R}} x^2 P e^{-x^2 \sigma} dx = \frac{\sigma^{3/4}}{4} (\sqrt{2} a_2 + a_0) \tag{37}$$

$$\int_{\mathbb{R}} \frac{x\sigma}{2} \frac{dP}{dx} e^{-x^2 \sigma} dx = \frac{\sigma^{3/4}}{\sqrt{2}} a_2. \tag{38}$$

We have used the orthogonality condition (21) and equation (25). Moreover,

$$\begin{aligned} \frac{1}{2} \int_{\mathbb{R}} P \left( \frac{d\chi}{dx} \right)^2 e^{-x^2 \sigma} dx &= \pi^{1/4} \sigma \sum_{n=0; r, s=1}^{\infty} \sqrt{rs} a_n \chi_r \chi_s \int_{\mathbb{R}} h_n^\sigma(x) h_{r-1}^\sigma(x) h_{s-1}^\sigma(x) e^{-x^2 \sigma} dx \\ &= \pi^{1/4} \sigma^{5/4} \sum_{n=0; r, s=1}^{\infty} \sqrt{rs} a_n \chi_r \chi_s \int_{\mathbb{R}} h_n^1(x) h_{r-1}^1(x) h_{s-1}^1(x) e^{-x^2} dx, \end{aligned} \tag{39}$$

where we have used equations (26) and (22). We define the matrix

$$A_{r,s,n} = \pi^{1/4} \int_{\mathbb{R}} h_r^1(x) h_s^1(x) h_n^1(x) e^{-x^2} dx = \sqrt{\frac{2^{-(n+s+r)}}{\pi n! s! r!}} \int_{\mathbb{R}} H_r(x) H_s(x) H_n(x) e^{-x^2} dx, \tag{40}$$

where the polynomials  $H_n(x)$  are given in equation (20). Since the matrix  $A_{r,s,n}$  is symmetric with respect to the permutation of the indices, it is convenient to assume that the indices  $r, s, n$ , are ordered increasingly, i.e.  $r \leq s \leq n$ . The integrals (40) can be solved analytically (see for example [54])

$$A_{r,s,n} = \begin{cases} \frac{\sqrt{r! s! n!}}{\left(\frac{r+s-n}{2}\right)! \left(\frac{s+n-r}{2}\right)! \left(\frac{n+r-s}{2}\right)!} & \text{if } n-r \leq s \leq n \text{ and } r+s+n \text{ even} \\ 0 & \text{otherwise.} \end{cases}$$

For future reference, we write the first terms

$$A_{0,s,n} = \delta_{n,s} \tag{41}$$

$$A_{1,s,n} = \sqrt{s+1} \delta_{n,s+1} + \delta_{n,s-1} \sqrt{s} \tag{42}$$

$$A_{2,s,n} = \frac{1}{\sqrt{2}} \left[ (\sqrt{(n+1)(s+1)} + \sqrt{ns} - 1) \delta_{n,s} + \sqrt{(s+1)n} \delta_{n-1,s+1} + \sqrt{(n+1)s} \delta_{n+1,s-1} \right]. \tag{43}$$

At this stage of the calculations, the quantum Lagrangian becomes

$$\begin{aligned} L = \sum_{n=0}^{\infty} a_n \left[ \dot{\chi}_n + \frac{\dot{\sigma}}{2\sigma} \left( \frac{2n+1}{2} \chi_n + \sqrt{(n+2)(n+1)} \chi_{n+2} \right) \right] - \dot{s} \sqrt{2\sigma} \sum_{n=0}^{\infty} \sqrt{(n+1)} \chi_{n+1} a_n \\ + \frac{\sigma^{3/4}}{4} (\sqrt{2} a_2 - a_0) - \sigma^{5/4} \sum_{n=0; r, s=1}^{\infty} \sqrt{rs} a_n \chi_r \chi_s A_{n,r-1,s-1} - \sum_{n=0}^{\infty} \frac{a_n}{\pi^{1/4}} \langle U_{[s]}, h_n^\sigma \rangle_\sigma + \mathcal{B}, \end{aligned} \tag{44}$$

where we have defined

$$\mathcal{B} \equiv -\frac{1}{8} \int_{\mathbb{R}} \frac{1}{P} \left( \frac{dP}{dx} \right)^2 e^{-x^2 \sigma} dx, \tag{45}$$

and

$$\langle U_{[s]}, h_n^\sigma \rangle_\sigma = \int_{\mathbb{R}} U(s+x) h_n^\sigma(x) e^{-x^2 \sigma} dx.$$

### 3. Bohm potential term

In this section, we analyze in detail some properties of the term  $\mathcal{B}$  that appears in the expression of the quantum Lagrangian. This term deserves special attention for two reasons. The first reason is related to the computation of  $\mathcal{B}$ : the presence of  $P$  at the denominator may lead to divergences in the computation of the Lagrangian, and numerical instabilities are expected to appear in the numerical treatment of the evolution equations. The second reason is related to the physical interpretation of  $\mathcal{B}$ . In section 7, we will describe the connection between the term  $\mathcal{B}$  and the so called Bohm's potential. Bohm observed that the quantum transport is formally equivalent to the evolution of a fluid in which the classical force field contains an additional term that accounts for the quantum correction to the motion. Such a force term is expressed by the derivative of the Bohm potential. One of the major limitations of the Bohm representation is related to the highly nonlinear and singular form of the Bohm potential. In our formalism,  $\mathcal{B}$  coincides with the expectation value of the Bohm potential, except for some smooth contributions. For this reason, the analysis of the behaviors of  $\mathcal{B}$ , and in particular the study of the divergence of  $\mathcal{B}$  in correspondence to some particular values of the parameters  $a_n$  and  $\sigma$ , could provide useful information concerning the role played by the Bohm potential in quantum motion. Moreover, our method provides a systematic and stable procedure for the numerical approximation of the Bohm potential, and has a large spectrum of potential applications. We start with the following.

**Lemma 3.1.** *We have*

$$\mathcal{B} = -\frac{\sigma^{3/4}}{4} \sum_{n=1}^{\infty} n R_n a_n, \tag{46}$$

where  $R_s$  are the expansion coefficients of  $\ln(P)$  into the Hermite base. The expansion coefficients of  $|\psi|^2$  (equation (27)) satisfy the following quasi-linear system

$$a_n = \sum_{s=1}^{\infty} B_{n,s}(a) R_s, \quad \text{with } n \geq 1, \tag{47}$$

where the matrix  $B$  depends linearly on the coefficients  $a_n$  and is given by

$$B_{n,s}(a) = \sqrt{\frac{s}{n}} \sum_{r=1}^{\infty} a_r A_{n-1,r,s-1}, \quad \text{with } n \geq 1. \tag{48}$$

**Proof.** We verify the lemma by direct computation. As a first step, we write  $\mathcal{B}$  in the following form:

$$\mathcal{B} = -\frac{1}{8} \int_{\mathbb{R}} P \left( \frac{dR}{dx} \right)^2 e^{-x^2 \sigma} dx, \tag{49}$$

where we have used the fact that the polynomial  $P$  is non-negative and we have defined  $R(x) = \ln(P(x))$ . Proceeding as in equation (39), we obtain

$$\mathcal{B} = -\frac{\sigma^{3/4}}{4} \sum_{n=0;r,s=1}^{\infty} \sqrt{rs} a_n R_s R_r A_{n,s-1,r-1}, \tag{50}$$

where the coefficients  $R_s$  are obtained by expanding  $R(x)$  in the Hermite base  $R(x) = \pi^{1/4} \sigma^{-1/4} \sum_n R_n h_n^\sigma(x)$ . We recall that  $\{a_n\}$  is the set of the expansion coefficients of  $P$  in the Hermite base (see equation (17)). Assuming  $n \geq 1$ , we have

$$\begin{aligned} R_n &= \frac{\sigma^{1/4}}{\pi^{1/4}} \langle \ln(P), h_n^\sigma \rangle_\sigma = \frac{\sigma^{1/2}}{\pi^{1/4}} \int_{\mathbb{R}} h_n^1(x\sqrt{\sigma}) \ln \left( \frac{\sigma^{1/4}}{\pi^{1/4}} \sum_{r=0}^{\infty} h_r^1(x\sqrt{\sigma}) a_r \right) e^{-x^2\sigma} dx \\ &= \frac{1}{\pi^{1/4}} \int_{\mathbb{R}} h_n^1(x) \ln \left( \pi^{-1/4} \sum_{r=0}^{\infty} h_r^1(x) a_r \right) e^{-x^2} dx. \end{aligned} \tag{51}$$

By using the elementary properties of the Hermite polynomials, we write the relationship between  $\{R_n\}$  and  $\{a_n\}$  in algebraic form. We have

$$\begin{aligned} a_n &= \pi^{1/4} \int_{\mathbb{R}} P(x) h_n^\sigma e^{-x^2\sigma} dx \\ &= \pi^{1/4} \int_{\mathbb{R}} e^{-x^2\sigma + R(x)} h_n^\sigma(x) dx = \frac{\sigma^{1/4 - \frac{n}{2}}}{\sqrt{2^n n!}} \int_{\mathbb{R}} e^{R(x)} (-1)^n \frac{d^{(n)}}{dx^n} e^{-x^2\sigma} dx, \end{aligned}$$

where we have used the definition of Hermite polynomials. We proceed by integrating by parts:

$$\begin{aligned} a_n &= - \frac{\sigma^{1/4 - \frac{n}{2}}}{\sqrt{2^n n!}} \int_{\mathbb{R}} \left( \frac{d}{dx} e^{R(x)} \right) (-1)^n \frac{d^{(n-1)}}{dx^{n-1}} e^{-x^2\sigma} dx \\ &= \frac{\pi^{1/4} \sigma^{-\frac{n}{2}}}{\sqrt{2^n n!}} \sum_{s=1}^{\infty} R_s \int_{\mathbb{R}} \frac{dh_s^\sigma}{dx} e^{R(x)} (-1)^{n-1} \frac{d^{(n-1)}}{dx^{n-1}} e^{-x^2\sigma} dx \\ &= \frac{\pi^{1/2} \sigma^{-3/4}}{\sqrt{2n}} \sum_{s=1}^{\infty} R_s \int_{\mathbb{R}} \frac{dh_s^\sigma}{dx} P(x) h_{n-1}^\sigma(x) e^{-x^2\sigma} dx \\ &= \frac{\pi^{1/4}}{\sqrt{n}} \sum_{s=1, r=0}^{\infty} R_s a_r \sqrt{s} \int_{\mathbb{R}} h_{s-1}^1(x) h_r^1(x) h_{n-1}^1(x) e^{-x^2} dx = \frac{1}{\sqrt{n}} \sum_{s=1, r=0}^{\infty} R_s a_r \sqrt{s} A_{s-1, r, n-1}. \end{aligned} \tag{52}$$

In the last line, we have used equation (22). Equation (52) coincides with equations (47) and (48). Finally, inserting equations (52) in (50), we obtain equation (46).  $\square$

This lemma provides an intermediate result that will be used to evaluate the Bohm potential  $\mathcal{B}$  in terms of the coefficients  $a_n$ . Naively, one can calculate the coefficients  $R_n$  by solving equation (51) and obtain  $\mathcal{B}$  from equation (46). However, equation (51) is not suitable for numerical computation. In fact, the calculation of  $R_n$  from equation (51) requires the integration of highly oscillating Hermite polynomials, which becomes a prohibitive task for large values of  $n$ . Moreover, the numerical calculation of the integral is critical around the points where the polynomial inside the logarithm is small.

The advantage of using the formulation of the problem provided by the lemma is that whenever the inverse of the matrix  $B$  exists, the coefficients  $R_s$  are easily obtained from

$$R_s = \sum_{r=1}^{\infty} [B(a)]_{s,n}^{-1} a_n, \quad \text{with } s \geq 1. \tag{53}$$

The proof of the existence of  $B^{-1}$  is given in section 3.1. We write here a useful formula:

$$-\frac{\sigma^{3/4}}{4} \frac{d}{da_n} \sum_{n=1}^{\infty} nR_n a_n = 2nR_n - \sum_{r,s \geq 1}^{\infty} \sqrt{rs} R_s R_r A_{n,r-1,s-1}. \tag{54}$$

We give the derivation of this formula in appendix A.

### 3.1. Invertibility of the matrix B(a)

We study the invertibility of B. This is of primary importance in the design of efficient numerical algorithms.

We define the functional spaces that we use to prove the invertibility of the matrix B. We define by  $\mathcal{S}^N$  the space of polynomials with degree N and by  $\Pi_N$  the projection operator in  $\mathcal{S}^N$ . Let us define by  $\mathcal{S}_M^N \equiv \{P \in \mathcal{S}^N | P = P - \Pi_M P\}$  the space of polynomials with degree N that do not contain terms with degree lower than or equal to M. The space  $\mathcal{S}_M^N$  is spanned by the canonical basis set  $\{x^n | M \leq n \leq N\}$ . In particular, for  $M = 0, 1$ , the spaces  $\mathcal{S}_0^N$  and  $\mathcal{S}_1^N$  are the spans of the following subsets of the Hermite polynomials: respectively  $\{h_n^\sigma | n = 0, \dots, N\}$  and  $\{h_n^\sigma | n = 1, \dots, N\}$ .

We denote by  $\mathcal{F}_N : \mathbb{R}^{N+1} \rightarrow \mathcal{S}_0^N$  the linear operator that maps the sequence  $\{a_n | n = 0, \dots, N\}$  to the polynomial  $P(x) = \frac{1}{\pi^{1/4}} \sum_{n=0}^N h_n^\sigma(x) a_n$ . From the uniqueness of the expansion of a polynomial on the Hermite basis, we have the existence of the inverse map  $\mathcal{F}_N^{-1}$ . We define by  $B(P) \equiv \mathcal{F}_N B \mathcal{F}_N^{-1} : \mathcal{S}_0^N \rightarrow L(\mathcal{S}_1^N)$  the linear operator whose matrix representation is given by equation (48). With the previous definition, equation (47) is equivalent to

$$P(x) = B(P)R(x), \tag{55}$$

where  $P = \mathcal{F}_N(a_n)$  and  $R = \mathcal{F}_N(R_n)$ . We prove that B(P) is invertible by showing that

**Theorem 1.** *Let  $P \in \mathcal{S}_0^N$  be a polynomial such that  $P(0) \neq 0$ . There exists a surjective operator  $\Gamma_P \in L(\mathcal{S}_1^N)$  such that*

$$B(P)\Gamma_P \tilde{P} = \tilde{P} \quad \forall \tilde{P} \in \mathcal{S}_1^N. \tag{56}$$

**Proof.** We fix  $\tilde{P} \in \mathcal{S}_1^N$ . We prove the existence of the operator  $\Gamma_P$  by showing that it is always possible to find a polynomial  $R \equiv \Gamma_P \tilde{P} \in \mathcal{S}_1^N$  such that  $B(P)R = \tilde{P}$ , or equivalently,

$$\tilde{a}_n = \sum_{s=1}^N B_{n,s}(a) R_s, \quad \text{with } n \geq 1, \tag{57}$$

where  $\tilde{a}_n = \mathcal{F}_N^{-1}(\tilde{P})$  and  $R_n = \mathcal{F}_N^{-1}(R)$  as before. We verify that  $\text{span}(\Gamma_P) = \text{Dom}(B(P)) = \mathcal{S}_0^N$ . Equation (57) gives (47) for  $\tilde{P} = P$ . We prove the theorem via one intermediate step. We define an auxiliary polynomial  $G \in \mathcal{S}_0^{N-1}$  and two maps  $M_1, M_2$ , such that  $G = M_1 \tilde{P}$  and  $R = M_2 G$ . In this way,  $\Gamma_P = M_2 M_1$  is the composition of  $M_1$  and  $M_2$ . This is illustrated by the following scheme:

$$\begin{array}{ccccc} & & \Gamma_P & & \\ & & \longrightarrow & & \\ \tilde{P} & \xrightarrow{M_1} & G & \xrightarrow{M_2} & R \\ \in \mathcal{S}_1^N & & \in \mathcal{S}_0^{N-1} & & \in \mathcal{S}_1^N \end{array} \tag{58}$$

We define the polynomial  $G \equiv M_2^{-1}R \in \mathcal{S}_0^{N-1}$  as follows:

$$G(x) = \frac{\pi^{1/4}}{\sigma^{1/4}} \sum_{s=1}^N (\mathcal{F}_N^{-1}R)_s \sqrt{s} h_{s-1}^\sigma(x) = \frac{\pi^{1/4}}{\sigma^{1/4}} \sum_{s=1}^N R_s \sqrt{s} h_{s-1}^\sigma(x). \tag{59}$$

Verification of the bijective nature of the map  $M_2$  follows immediately. By substituting the expression of the matrix  $A$  given by equations (40) in (47), we obtain

$$\sqrt{n} \tilde{a}_n = \frac{\pi^{1/2}}{\sigma^{1/4}} \sum_{s=1}^N R_s \sqrt{s} \int_{\mathbb{R}} P(x) h_{n-1}^\sigma(x) h_{s-1}^\sigma(x) e^{-x^2 \sigma} dx, \quad \text{with } n \geq 1. \tag{60}$$

Equation (60) becomes

$$\frac{\sqrt{n}}{\pi^{1/4}} \tilde{a}_n = \langle G(x)P(x), h_{n-1}^\sigma \rangle_\sigma.$$

By using equation (24), we now write the left-hand side of the equation as follows:

$$\begin{aligned} \frac{\sqrt{n}}{\pi^{1/4}} \tilde{a}_n &= \sqrt{n} \langle \widetilde{P}(x), h_n^\sigma \rangle_\sigma \\ &= \sqrt{2\sigma} \langle \widetilde{P}(x)x, h_{n-1}^\sigma \rangle_\sigma + \frac{1}{\sqrt{2\sigma}} \int_{\mathbb{R}} h_{n-1}^\sigma \left( \frac{d\widetilde{P}(x)}{dx} - 2x\sigma \widetilde{P}(x) \right) e^{-x^2 \sigma} dx \\ &= \frac{1}{\sqrt{2\sigma}} \left\langle \frac{d\widetilde{P}(x)}{dx}, h_{n-1}^\sigma \right\rangle_\sigma. \end{aligned}$$

We have

$$\left\langle \left( GP - \frac{1}{\sqrt{2\sigma}} \frac{d\widetilde{P}}{dx} \right), h_n^\sigma \right\rangle_\sigma = 0 \quad n = 0, \dots, N-1. \tag{61}$$

The set of the first  $N$  Hermite polynomials  $\{h_n^\sigma | n = 0, \dots, N-1\}$  spans  $\mathcal{S}_0^{N-1}$ . Equation (61) ensures that the product  $GP$  is equal to  $\frac{1}{\sqrt{2\sigma}} \frac{d\widetilde{P}(x)}{dx}$  in the polynomial space  $\mathcal{S}_0^{N-1}$ . In order to solve equation (61), it is convenient to write all the polynomials on the canonical basis set  $\{x^n | n = 0, \dots, N-1\}$  of  $\mathcal{S}_0^{N-1}$ . This is equivalent to expanding the polynomials in Taylor series and comparing the coefficients order by order. With this, equation (61) becomes

$$\sum_{k=0}^n \binom{n}{k} G^{(k)}(0) P^{(n-k)}(0) = \frac{\widetilde{P}^{(n+1)}(0)}{\sqrt{2\sigma}} \quad \text{with } n = 0, \dots, N-1. \tag{62}$$

For  $P(0) \neq 0$ , we can solve equation (62) recursively.

$$G^{(n)}(0) = \begin{cases} \frac{\widetilde{P}^{(1)}(0)}{P(0)\sqrt{2\sigma}} & \text{with } n = 0, \\ \frac{1}{P(0)} \left[ \frac{\widetilde{P}^{(n+1)}(0)}{\sqrt{2\sigma}} - \sum_{k=0}^{n-1} \binom{n}{k} G^{(k)}(0) P^{(n-k)}(0) \right] & \text{with } n = 1, \dots, N-1. \end{cases}$$

In conclusion, we have shown that the map  $M_1$  is well defined. For each  $\widetilde{P} \in \mathcal{S}_1^N$ , by solving equation (62), we find a polynomial  $G \in \mathcal{S}_0^{N-1}$ . The map is one-to-one, since if we fix  $G \in \mathcal{S}_0^{N-1}$  we obtain  $\widetilde{P} \in \mathcal{S}_1^N$  by equation (62). From the coefficients  $G^{(n)}(0)$ , we obtain  $G$

by the Taylor expansion  $G(x) = \sum_{n=0}^{N-1} \frac{G^{(n)}(0)}{n!} x^n$ , and from equation (59) the coefficients  $R_s$ :

$$R_s = \frac{\sigma^{1/4}}{\pi^{1/4}\sqrt{s}} \langle G, h_s^\sigma \rangle_\sigma \quad \text{with } s = 1, \dots, N.$$

According to the scheme (58), we have found a map  $\Gamma_P = M_2 M_1$  with  $\text{span}(\Gamma_P) = \mathcal{S}_1^N$ . As a final step, we verify that equation (56) is satisfied. We proceed straightforwardly:

$$\begin{aligned} \sum_{s=1}^N B_{n,s}(a)R_s &= \frac{\sigma^{1/4}}{\pi^{1/4}\sqrt{n}} \sum_{s=1;r=0}^N a_r A_{n-1,r,s-1} \int_{\mathbb{R}} G(x) h_{s-1}^\sigma(x) e^{-x^2\sigma} dx, \quad \text{with } n \geq 1 \\ &= \frac{1}{\sqrt{n}} \sum_{s=1;r=0}^N a_r \int_{\mathbb{R}} h_{n-1}^\sigma(y) h_r^\sigma(y) h_{s-1}^\sigma(y) G(x) h_{s-1}^\sigma(x) e^{-(y^2+x^2)\sigma} dx dy \\ &= \frac{\pi^{1/4}}{\sqrt{n}} \sum_{s=1}^N \int_{\mathbb{R}} P(y) h_{n-1}^\sigma(y) h_{s-1}^\sigma(y) G(x) h_{s-1}^\sigma(x) e^{-(y^2+x^2)\sigma} dx dy. \end{aligned}$$

We use the fact that for each  $G \in \mathcal{S}_0^{N-1}$ ,

$$\sum_{s=1}^N h_{s-1}^\sigma(y) \int_{\mathbb{R}} G(x) h_{s-1}^\sigma(x) e^{-x^2\sigma} dx = G(y).$$

By equation (61),

$$\begin{aligned} \sum_{s=1}^N B_{n,s}(a)R_s &= \frac{\pi^{1/4}}{\sqrt{n}} \int_{\mathbb{R}} P(y) G(y) h_{n-1}^\sigma(y) e^{-y^2\sigma} dy = \frac{\pi^{1/4}}{\sqrt{n}} \langle PG, h_{n-1}^\sigma \rangle_\sigma \\ &= \frac{\pi^{1/4}}{\sqrt{n}\sqrt{2\sigma}} \left\langle \frac{d\widetilde{P}(x)}{dx}, h_{n-1}^\sigma \right\rangle_\sigma = \widetilde{a}_n. \end{aligned}$$

This concludes the proof of theorem 1. □

As a final remark, we note that we apply this theorem to a polynomial of the form  $P(x - s)$  where the spatial variable is shifted by  $s$ . Due to the arbitrary nature of  $s$ , the condition  $P(0) \neq 0$  implies  $P \neq 0$  always.

### 3.2. Calculation of the coefficients $R_n$ : analytic approach

The main source of numerical instabilities of our model of quantum transport arises from the presence of the Bohm term in the Lagrangian. In particular, it is challenging to express the coefficients  $R_i$  that appear in equation (46) in terms of the dynamical parameters  $a_i$ . When the number of parameters is small, it is possible to compute  $R_i$  directly as a function of  $a_i$  via a simple analytical formula. First, we consider a simple test case whose analysis leads to interesting considerations concerning the singularities exhibited by the evolution equations of the parameters. We consider a solution containing only two parameters—namely,  $a_0$  and  $a_3$ :

$$a = (a_0, 0, 0, a_3).$$

The cutoff index in the expansion on Hermite polynomials is  $N = 3$ . We solve by hand the system



$$R_s = \sum_{r=1}^N [B(a)]_{s,n}^{-1} a_n, \quad \text{with } s \geq 1$$

$$B_{n,s}(a) = \sqrt{\frac{s}{n}} \sum_{r=1}^N a_r A_{n-1,r,s-1}, \quad \text{with } n \geq 1.$$

It is convenient to define the matrix  $\tilde{A}_{n,s}^r \equiv A_{n-1,r,s-1}$ . Simple computations lead to (see equation (40))

$$\tilde{A}^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \tilde{A}^3 = \begin{pmatrix} 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 \end{pmatrix}$$

and

$$B(a) = \begin{pmatrix} a_0 & 0 & 3a_3 \\ 0 & a_0 & 0 \\ a_3 & 0 & a_0 \end{pmatrix}.$$

We are interested only in the coefficient  $R_3$ . Cramer's rule provides

$$R_3 = \frac{a_0 a_3}{a_0^2 - 3a_3^2}. \tag{63}$$

In order to show how the complexity of the method increases when other coefficients beyond  $a_0$  and  $a_3$  are considered, we give the results of the computation for the case  $N = 4$ . We proceed in the same way as before, and obtain the coefficients  $R_i$  with  $i = 1, \dots, 4$ :

$$R_1 = a_0(3\sqrt{6}a_3^3 - 2a_0a_3a_4 - 2\sqrt{6}a_3a_4^2)/|B| \tag{64}$$

$$R_2 = (3\sqrt{2}a_3^4 - 3\sqrt{2}a_0^2a_3^2 - 4\sqrt{2}a_0^2a_4^2 + 6\sqrt{3}a_0a_3^2a_4 - 8\sqrt{3}a_0a_4^3)/(2|B|) \tag{65}$$

$$R_3 = a_0(a_3a_0^2 + \sqrt{6}a_3a_0a_4 - a_3^3)/|B| \tag{66}$$

$$R_4 = a_0^2(2a_0a_4 + 2\sqrt{6}a_4^2 - 3\sqrt{6}a_3^2)/(2|B|) \tag{67}$$

$$|B| = a_0^4 + 3a_3^4 - 22a_0^2a_3^2 + 14a_0^2a_4^2 - 4\sqrt{6}a_0a_3^3 + 4\sqrt{6}a_0^3a_4 + 2\sqrt{6}a_0a_3^2a_4. \tag{68}$$

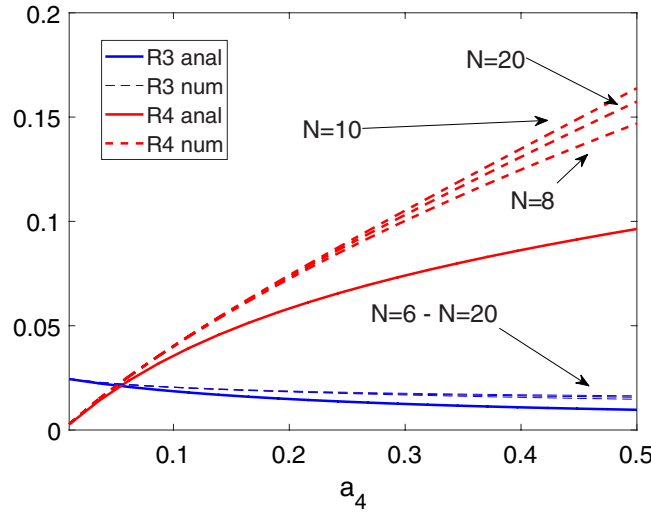
The formulas that express the coefficients  $R_i$  from the parameters  $a_i$  become cumbersome when  $N$  increases. For this reason, in order to improve the precision of the calculations, it is necessary to resort to numerical methods. The most convenient way is to calculate the matrix  $B$  from equation (48) and to obtain  $B^{-1}$  numerically. Theorem 1 ensures that this is always possible.

For the sake of clarity, we summarize the equations and the link among the variables in the following scheme:

$$I: \quad a_n \xrightarrow{\text{equation (17)}} P = \pi^{-1/4} \sum_{n=0}^{\infty} h_n^\sigma a_n \xrightarrow{\text{equation (51)}} R_n = \sigma^{1/4} \pi^{-1/4} \langle \ln(P), h_n^\sigma \rangle_\sigma$$

$$II: \quad a_n \xrightarrow{\text{equation (63)}} R_3 = \frac{a_0 a_3}{a_0^2 - 3a_3^2}; \text{ or equation (64)–(67)}$$

$$III: \quad a_n \xrightarrow{\text{equation (53)}} R_s = \sum_r [B(a)]_{s,r}^{-1} a_r.$$



**Figure 1.** Coefficients  $R_3$  (blue line) and  $R_4$  (red line) as a function of  $a_4$ . Solid lines refer to the equations (64)–(67), and dashed lines refer to the numerical results for two values of  $N$ .

We indicate three possible schemes: in the first case (denoted by  $I$ ), we start from the coefficients  $a_n$ , obtain the polynomial  $P(x)$ , and obtain the coefficients  $R_i$  by projecting the function  $\ln P(x)$  onto the Hermite polynomials. In principle, this procedure provides the coefficients  $R_i$  with greater accuracy. However, the scheme  $I$  has little practical use, since the projection procedure at the end is very expensive from a computational point of view. The other two cases have already been discussed in detail; in case  $II$ , we make use of the analytical approximations, and case  $III$  requires basically only the inversion of the matrix  $B$ .

We investigate the precision of different schemes with two examples. As a first case, we consider the following polynomial:

$$P(x) = \frac{1}{\pi^{1/4}} (2 h_0^\sigma(x) + 0.05 h_3^\sigma(x) + a_4 h_4^\sigma(x)).$$

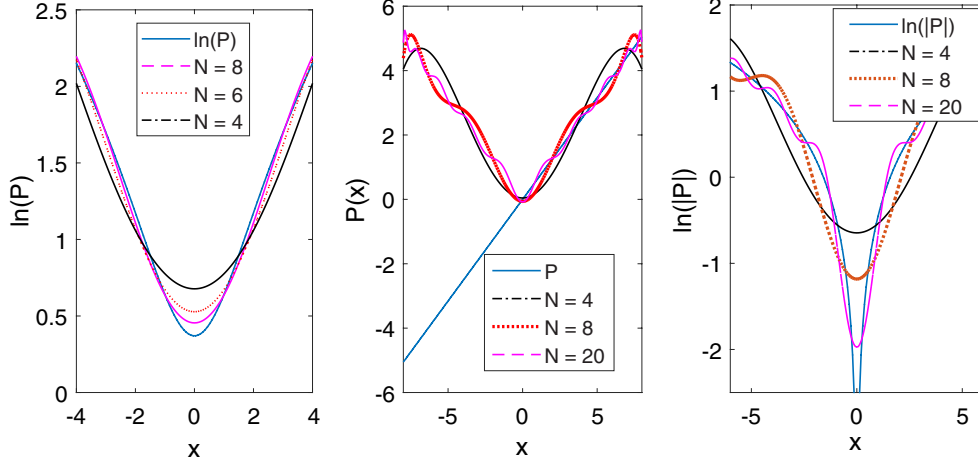
We vary the parameter  $a_4$  in the interval  $[0, 0.5]$  and evaluate the coefficients  $R_3$  and  $R_4$  according to schemes  $II$  and  $III$ . We use  $\sigma = 1/2$ ; however, the results are independent of the value of  $\sigma$ . The results are depicted in figure 1. In the blue (red) line we depict the value of  $R_3$  ( $R_4$ ). We compare the results obtained by using the analytical formulas (64)–(67) (solid lines) with the values obtained by numerical solution (dashed lines) for two values of the expansion cutoff  $N$ , which indicates the precision of the calculation. We find good agreement between the numerical results and the analytical formulas.

As a second example, we consider the following positive polynomial:

$$P(x) = \frac{1}{\pi^{1/4}} (3 h_0^{1/2}(x) + h_2^{1/2}(x)),$$

which corresponds to the vector  $a = (3, 0, 1)$  with  $N = 3$  and  $\sigma = 0.5$ . In figure 2 (first panel from the left), we depict the projection of  $R(x) = \log(P)$  on the Hermite polynomials for various values of the cutoff  $N = 4, 6, 8$ :

$$R(x) = \sum_{n=1}^N \langle \ln(P), h_n^\sigma \rangle_\sigma h_n^\sigma(x).$$



**Figure 2.** First panel:  $R(x)$  calculated up to the order  $N$ , the solid line represents  $\ln(P)$ . Second panel: plot of  $P(x)$  (solid line) used for the calculation of  $R(x)$  depicted in the second panel. The dashed lines represent  $P(x)$  reconstructed from  $R_i$ . Third panel:  $R(x)$  calculated up to the order  $N$ ; the solid line represents  $\ln(|P|)$ .

We see that we already have a good convergence to the exact result for  $N = 8$ . In the second and third panels, we show the results of the same procedure for a non-positive polynomial ( $a_1 = 1$ ):

$$P(x) = \frac{h_1^{1/2}(x)}{\pi^{1/4}} = \frac{1}{2^{1/4}\pi^{1/2}} x.$$

We remark that this is an artificial example, since in our model  $P(x)$  represents the square of the particle density, and thus is necessarily positive. In the second panel of figure 2, we plot the polynomial  $P(x)$  obtained from  $R_i$ . Interestingly, we note that our algorithm converges toward the absolute value of  $P(x)$ . This is a very useful property of our method. In fact, the cutoff in the Hermite expansion of  $P(x)$  necessarily leads to approximations for which the positivity of the particle density is no longer guaranteed. The convergence of the algorithm to the absolute value of  $P(x)$  is a good property that prevents such errors having catastrophic consequences in the dynamics of the quantum particle.

### 3.3. Macroscopic quantities

In order to give the correct physical interpretation to our set of parameters, we investigate the connection of  $a_0$ ,  $s$  and  $\sigma$ , with some relevant physical quantities. By using the conservation of the  $L^2$  norm of the wave function  $\psi$ , we can express the coefficient  $a_0$  as a function of  $\sigma$ :

$$a_0 = \pi^{1/4} h_0^\sigma \int_{\mathbb{R}} P(x) e^{-x^2 \sigma} dx = \pi^{1/4} h_0^\sigma \int_{\mathbb{R}} |\psi|^2 dx = \pi^{1/4} h_0^\sigma \|\psi\|_2^2 = \sigma^{1/4}. \tag{69}$$

The mean particle position is given by

$$\begin{aligned} \langle x \rangle &= \int_{\mathbb{R}} x P(x-s) e^{-(x-s)^2 \sigma} dx = s + \int_{\mathbb{R}} x P(x) e^{-x^2 \sigma} dx = s + \frac{1}{\pi^{1/4}} \sum_{n=0}^{\infty} a_n \int_{\mathbb{R}} x h_n^\sigma(x) e^{-x^2 \sigma} dx \\ &= s + \frac{a_1}{\sigma^{3/4} \sqrt{2}}. \end{aligned}$$

Here, the angle brackets denote the quantum mechanical expectation value. The particle momentum is given by

$$\begin{aligned} \left\langle -i \frac{\partial}{\partial x} \right\rangle &= -i \int_{\mathbb{R}} \bar{\psi}(x) \frac{\partial}{\partial x} \psi(x) dx = -i \int_{\mathbb{R}} \bar{\psi}(x+s) \frac{\partial}{\partial x} \psi(x+s) dx \\ &= \int_{\mathbb{R}} P \frac{\partial \chi}{\partial x} e^{-x^2 \sigma} dx = \sum_{n=0}^{\infty} \sqrt{2\sigma(n+1)} a_n \chi_{n+1}, \end{aligned}$$

where in the last equality we have used the expansions (17) and (18), the orthogonality property (21) and equation (22). The evolution of the mean particle position can be obtained by applying the Ehrenfest theorem:

$$\frac{d \langle x \rangle}{dt} = \left\langle -i \frac{\partial}{\partial x} \right\rangle. \tag{70}$$

In our formalism, this gives

$$\dot{s} = -\frac{1}{\sqrt{2}} \frac{d}{dt} \left( \sigma^{-3/4} a_1 \right) + \sum_{n=0}^{\infty} \sqrt{2\sigma(n+1)} a_n \chi_{n+1}. \tag{71}$$

This equation agrees with equation (77), which will be derived in a more general way by applying the Euler–Lagrange formalism. We remark that, for the sake of generality, we have assumed in equation (71) that all the coefficients of the Hermite expansion of  $P$  are different from zero. In our case,  $a_1 = 0$  by construction, and the first term on the right-hand side vanishes. Other physically relevant quantities are the spatial variance  $\langle \Delta x^2 \rangle$  and the momentum variance  $\langle \Delta p^2 \rangle$ . Concerning  $\langle \Delta x^2 \rangle$ , a simple calculation gives

$$\langle \Delta x^2 \rangle = \left\langle (x-s)^2 \right\rangle = \int_{\mathbb{R}} x^2 P e^{-x^2 \sigma} dx = \frac{\sigma^{-5/4}}{2} \left( \sqrt{2} a_2 + a_0 \right) = \frac{1}{2\sigma}, \tag{72}$$

where we have used equation (37) and we have assumed  $a_2 = 0$ , which is usually a convenient choice. This calculation shows that the variance is always  $\frac{1}{2\sigma}$  and is independent of the other parameters. Due to the presence of the polynomial form of the modulus of the wave function, this result may not appear obvious. Straightforward calculations lead to

$$\begin{aligned} \langle p^2 \rangle &= \int_{\mathbb{R}} |\partial_x \psi|^2 dx = \int_{\mathbb{R}} \left[ \sigma^2 x^2 P + \frac{1}{4P} \left( \frac{dP}{dx} \right)^2 - x\sigma \frac{dP}{dx} + P \left( \frac{d\chi}{dx} \right)^2 \right] e^{-x^2 \sigma} dx \\ &= \frac{\sigma}{2} + 2\sigma^{5/4} \sum_{n=0; r,s=1}^{\infty} \sqrt{rs} a_n \chi_r \chi_s A_{n,r-1,s-1} + \frac{\sigma^{3/4}}{2} \sum_{n=1}^{\infty} n R_n a_n, \end{aligned}$$

and

$$\langle \Delta p^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\sigma}{2} + 2\sigma \sum_{r,s=1}^{\infty} \sqrt{rs} \chi_r \chi_s \left( \sigma^{1/4} \sum_{n=0}^{\infty} a_n A_{n,r-1,s-1} - a_{r-1} a_{s-1} \right) + \frac{\sigma^{3/4}}{2} \sum_{n=1}^{\infty} n R_n a_n.$$

In the simplified case in which we discard the polynomial modulation of the modulus of the function, i.e.  $a_n = 0$  for  $n > 0$ , it is easy to express the Heisenberg minimum uncertainty principle by our formalism:

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle = \frac{1}{4} + \sigma^{1/2} \sum_{r=2}^{\infty} r \chi_r^2 \geq \frac{1}{4},$$

where the equality corresponds to the case of Gaussian wave function modulated by a plane wave. Finally, it is interesting to calculate the total energy of the particle. The energy takes the simple form of a scalar product:

$$H = \int_{\mathbb{R}} \left( \frac{1}{2} |\partial_x \psi|^2 + U |\psi|^2 \right) dx = \frac{\sigma}{4} + \sum_{n=0}^{\infty} a_n v_n \doteq \frac{\sigma}{4} + \langle a, v \rangle_{\ell}, \quad (73)$$

where we have defined the vector

$$v_n = \underbrace{\sigma^{5/4} \sum_{r,s=1}^{\infty} \sqrt{rs} \chi_r \chi_s A_{n,r-1,s-1}}_{\text{Kin.}} + \underbrace{\frac{\sigma^{3/4}}{4} n R_n}_{\text{Bohm}} + \underbrace{\frac{1}{\pi^{1/4}} \langle U_{[s]}, h_n^\sigma \rangle_{\sigma}}_{\text{Pot.}}.$$

In this formula, we have indicated the physical origin of the three contributions to the vector  $v$  namely, the kinetic energy, the Bohm potential and the classical potential.

#### 4. Evolution equations

We complete the expression of the quantum Lagrangian by using equation (46) in equation (44)

$$\begin{aligned} L = & \sum_{n=0}^{\infty} a_n \left[ \dot{\chi}_n + \frac{\dot{\sigma}}{2\sigma} \left( \frac{2n+1}{2} \chi_n + \sqrt{(n+2)(n+1)} \chi_{n+2} \right) \right] - \dot{s} \sqrt{2\sigma} \sum_{n=0}^{\infty} \sqrt{(n+1)} \chi_{n+1} a_n \\ & + \frac{\sigma^{3/4}}{4} \left( \sqrt{2} a_2 - a_0 \right) - \sigma^{5/4} \sum_{n=0; r,s=1}^{\infty} \sqrt{rs} a_n \chi_r \chi_s A_{n,r-1,s-1} \\ & - \frac{\sigma^{3/4}}{4} \sum_{n=1}^{\infty} n R_n a_n - \sum_{n=0}^{\infty} \frac{a_n}{\pi^{1/4}} \langle U_{[s]}, h_n^\sigma \rangle_{\sigma}. \end{aligned}$$

The Euler–Lagrange equations  $\frac{d}{dt} \frac{\partial L}{\partial \dot{a}_n} = \frac{\partial L}{\partial a_n}$  and  $\frac{d}{dt} \frac{\partial L}{\partial \dot{\chi}_n} = \frac{\partial L}{\partial \chi_n}$  lead respectively to

$$\begin{aligned} \dot{\chi}_n = & - \frac{\dot{\sigma}}{2\sigma} \left( \frac{2n+1}{2} \chi_n + \sqrt{(n+2)(n+1)} \chi_{n+2} \right) + \dot{s} \sqrt{2\sigma(n+1)} \chi_{n+1} + \sigma^{3/4} \left( \frac{\delta_{n,2}}{2\sqrt{2}} - \frac{\delta_{n,0}}{4} \right) \\ & - \sum_{r,s \geq 1} \left( \sigma^{5/4} \chi_r \chi_s - \frac{\sigma^{3/4}}{4} R_r R_s \right) \sqrt{rs} A_{n,r-1,s-1} - \frac{\sigma^{3/4}}{2} n R_n + \frac{1}{\pi^{1/4}} \langle U_{[s]}, h_n^\sigma \rangle_{\sigma}, \quad (74) \end{aligned}$$

and

$$\dot{a}_n = \frac{\dot{\sigma}}{2\sigma} \left( a_n \frac{2n+1}{2} + a_{n-2} \sqrt{n(n-1)} \right) - \dot{s} \sqrt{2n\sigma} a_{n-1} + 2\sigma^{5/4} \sqrt{n} \sum_{m,s \geq 1} \sqrt{s} a_m \chi_s A_{m,n-1,s-1}. \quad (75)$$

In order to derive equation (74), we have used equation (54). The evolution equation for the spatial coordinate  $s(t)$  and for the inverse of the variance  $\sigma(t)$  are obtained from the evolution equation (75), for  $n = 1$  and  $n = 2$  respectively. By using equation (41) we have

$$\dot{a}_2 = -2\dot{s} \sqrt{\sigma} a_1 + \frac{5}{4} \frac{\dot{\sigma}}{\sigma} a_2 + \frac{\sqrt{2}}{2} \frac{\dot{\sigma}}{\sigma} a_0 + 2\sqrt{2} \sigma^{5/4} \sum_{n=0}^{\infty} \left( n a_n \chi_n + \sqrt{n+1} \sqrt{n+2} a_n \chi_{n+2} \right).$$

According to the discussion of section 2.3, we set  $a_1 = 0$  and  $a_2$  constant given by the initial condition  $a_2(t_0)$ . We obtain the following equation for the variable  $\sigma$ :

$$\dot{\sigma} = -\frac{16\sigma^2}{4 + 5\sqrt{2}\sigma^{-1/4}a_2(t_0)} \sum_{n=0}^{\infty} a_n \left( n\chi_n + \sqrt{n+1}\sqrt{n+2}\chi_{n+2} \right),$$

where we have used  $a_0 = \sigma^{1/4}$ . Concerning the variable  $a_1$ , the evolution equation is

$$\dot{a}_1 = -\dot{s}\sqrt{2\sigma}a_0 + \frac{3}{4}\frac{\dot{\sigma}}{\sigma}a_1 + 2\sigma^{5/4} \sum_{n=0}^{\infty} \sqrt{n+1}a_n\chi_{n+1}. \quad (76)$$

Imposing  $a_1 = 0$ ,

$$\dot{s} = \sqrt{2}\sigma^{1/2} \sum_{n=0}^{\infty} \sqrt{n+1}a_n\chi_{n+1}. \quad (77)$$

Finally, the evolution equations are

$$\begin{aligned} \dot{\chi}_n = & M \left( \frac{2n+1}{2}\chi_n + \sqrt{(n+2)(n+1)}\chi_{n+2} \right) + 2\sigma S\sqrt{n+1}\chi_{n+1} + \frac{\sigma^{3/4}}{2\sqrt{2}} \left( \delta_{n,2} - \frac{\delta_{n,0}}{\sqrt{2}} \right) \\ & - \frac{\sigma^{3/4}}{2} n R_n - \sigma^{3/4} \sum_{r,s \geq 1} \sqrt{rs} A_{n,r-1,s-1} \left( \sigma^{1/2}\chi_r\chi_s - \frac{R_r R_s}{4} \right) + \pi^{-1/4} \langle U_{[s]}, h_n^\sigma \rangle_\sigma \end{aligned} \quad (78)$$

$$\begin{aligned} \dot{a}_n = & -M \left( a_n \frac{2n+1}{2} + a_{n-2}\sqrt{n(n-1)} \right) - 2\sigma S\sqrt{n}a_{n-1} \\ & + 2\sigma^{3/2}n\chi_n + 2\sigma^{5/4}\sqrt{n} \sum_{m,s \geq 1} \sqrt{s} a_m\chi_s A_{m,n-1,s-1} \end{aligned} \quad (79)$$

$$\dot{\sigma} = -2\sigma M \quad (80)$$

$$\dot{s} = \sqrt{2}\sigma^{1/2}S. \quad (81)$$

We have defined

$$S = \sigma^{1/4}\chi_1 + \sum_{r=1}^{\infty} \sqrt{r+1}a_r\chi_{r+1} \quad (82)$$

$$M = \frac{8\sigma}{4 + 5\sqrt{2}\sigma^{-1/4}a_2(t_0)} \left[ \sqrt{2}\sigma^{1/4}\chi_2 + \sum_{r=1}^{\infty} a_r \left( r\chi_r + \sqrt{(r+1)(r+2)}\chi_{r+2} \right) \right]. \quad (83)$$

Concerning the coefficient  $a_0$ , equation (79) with  $n = 0$  combined with equation (80) gives

$$\frac{\dot{a}_0}{a_0} = \frac{1}{4}\frac{\dot{\sigma}}{\sigma},$$

whose solution is  $a_0(t) = \sigma^{1/4}(t)$  which, as already seen in section 3.3, ensures that the norm of the wave function is conserved.

First, we derive the evolution equation of the Gaussian ansatz given in equation (18) as a particular case of the evolution equations for the complete set of parameters. We express the first three coefficients  $\chi_n$  with the variables  $\phi_0, p$  and  $\sigma_i$ . This can be done by considering the second order polynomials

$$\pi^{1/4} \sum_{n=0}^2 \chi_n h_n^\sigma(x) = \phi_0 - px + \sigma_i \frac{x^2}{2}.$$

We obtain  $\chi_2 = \frac{1}{2\sqrt{2}}\sigma^{-5/4}\sigma_i$ ,  $\chi_1 = -\frac{1}{\sqrt{2}}p\sigma^{-3/4}$ ,  $\chi_0 = \sigma^{-1/4}\phi_0 + \frac{1}{4}\sigma^{-5/4}\sigma_i$ . Direct computation shows that equation (80) reduces to equations (11), and that (78) gives equations (10) and (12) for  $n = 0$  and  $n = 2$  respectively.

The harmonic oscillator  $U(x) = \frac{\omega^2 x^2}{2}$  is a standard example with several applications. In our model, the external potential enters only into the equations for the variables  $\chi_n$  via the scalar product with the Hermite polynomials. For the harmonic potential, this is easily calculated. We have

$$\begin{aligned} \frac{1}{\pi^{1/4}} \langle U_{[s]}, h_2^\sigma \rangle_\sigma &= \frac{1}{\pi^{1/4}} \int_{\mathbb{R}} U(s+x) h_2^\sigma(x) e^{-x^2\sigma} dx = \frac{\omega^2 \sigma^{1/4}}{2\sqrt{2} \pi^{1/4}} \int_{\mathbb{R}} (s+x)^2 (2\sigma x^2 - 1) e^{-x^2\sigma} dx \\ &= \frac{\sigma^{-5/4}}{2\sqrt{2}} \omega^2. \end{aligned} \quad (84)$$

## 5. Examples

We illustrate our method by considering a simple case. In the expansion of the wave function, we keep one coefficient ( $\chi_2$ ) for the phase and two coefficients ( $a_0, a_3$ ) for the modulus. It is more convenient to use the parameter  $\sigma_i$  that appears in the Gaussian ansatz instead of  $\chi_2$ . The change of variable is given by the equation  $\chi_2 = \frac{\sigma^{-5/4}}{2\sqrt{2}}\sigma_i$ . Concerning the potential, we consider the harmonic trap  $U(x) = \frac{\omega^2 x^2}{2}$ . We obtain the following reduced system of equations:

$$\dot{a}_3 = -\frac{7}{2}\sigma_i a_3 \quad (85)$$

$$\dot{\sigma}_i = \sigma^2 - \sigma_i^2 - \omega^2 - \frac{3}{4} \frac{\sigma^2}{\left(1 - \frac{\sigma^{1/2}}{3a_3^2}\right)} \quad (86)$$

$$\dot{\sigma} = -2\sigma\sigma_i, \quad (87)$$

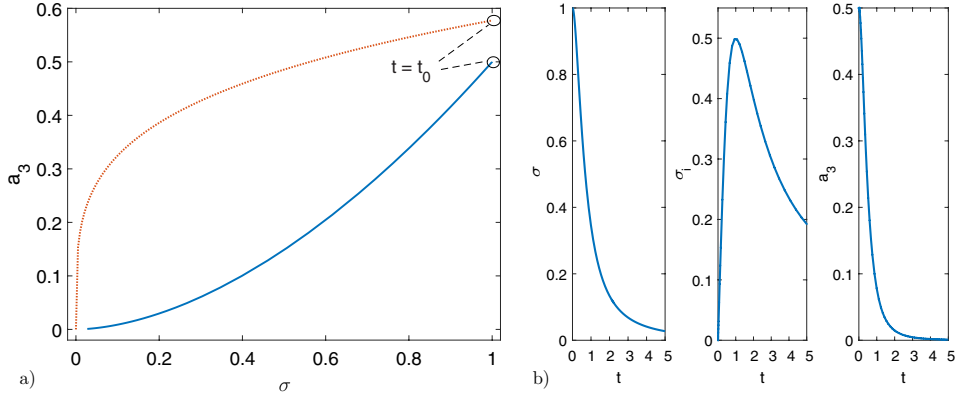
where we have used equations (63) with  $a_0 = \sigma^{1/4}$  and (84). Comparing with equations (11) and (12), we see that the only difference is given by the last term of equation (86). In the limit  $a_3(t_0) \rightarrow 0$ , this term goes to zero, and the system reduces to the evolution of a simple Gaussian beam. In this case, ( $a_3 = 0$ ) it is convenient to represent the solution on the  $\sigma_i - \sigma$  coordinate plane. The trajectories followed by the parameters  $\sigma_i(t)$  and  $\sigma(t)$  are circles with center  $(0, \frac{\xi}{2})$  and radius  $\sqrt{\frac{\xi^2}{4} - \omega^2}$  where  $\xi = \frac{\sigma_i^2(t_0) + \sigma^2(t_0) + \omega^2}{\sigma(t_0)}$  and  $t_0$  is the initial time. From equations (85) and (87), we obtain

$$\frac{d\sigma}{da_3} = \frac{4}{7} \frac{\sigma}{a_3}$$

and

$$a_3(t) = \frac{a_3(t_0)}{\sigma^{7/4}(t_0)} \sigma^{7/4}(t). \quad (88)$$

We interpret the last term in the right-hand side of equation (86) as the first correction to the Gaussian motion induced by the Bohm potential term. As is often the case in Bohm dynamics, the quantum potential shows singular points. It is important to verify that equation (86)



**Figure 3.** Left panel: trajectory of the solution in the plane  $(a_3, \sigma)$  for  $\omega = 0$ . The red curve depicts the pole  $\sigma^{1/2} - 3a_3^2 = 0$ . Right panel: time evolution of the variables.

is always well defined ( $\sigma^{1/2} - 3a_3^2 \neq 0$ ). This is illustrated in figure 3. We prove that this is always the case. Inserting equation (88) into equations (86) and (87), we obtain

$$\dot{\sigma}_i = -\sigma_i^2 - \omega^2 + \sigma^2 \left( 1 - \frac{3}{4} \frac{1}{\left( 1 - \frac{1}{3\sigma^3 \eta_0^2} \right)} \right) \tag{89}$$

$$\dot{\sigma} = -2\sigma\sigma_i, \tag{90}$$

where we have defined  $\eta_0 = \frac{a_3(t_0)}{\sigma^{3/4}(t_0)}$ .

In order to illustrate the behaviors of the solution of equations (89) and (90), we plot in figure 4 the trajectories of the solution on the  $\sigma_i$ - $\sigma$ -coordinate plane for two different initial conditions. We focus on the deformation of the trajectories caused by the Bohm potential term.

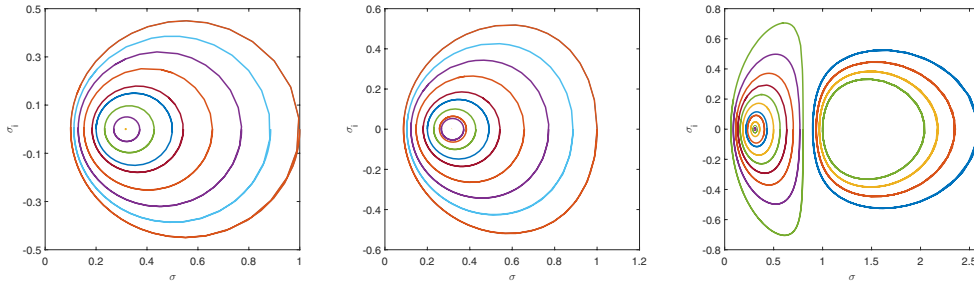
For  $\eta_0 = 0$ , we obtain the simple Gaussian case, and the trajectories are circles (figure 4 panel on the left). For  $\eta_0 \neq 0$ , the vertical line  $\sigma_0 = \frac{\eta_0^{-2/3}}{\sqrt[3]{3}}$  separates the trajectories into two groups, which remain in the left or in the right side of the semi-plane. In particular, our results show that as a function of the initial conditions, the solution may oscillate with two different frequencies.

It is interesting to analyze the behavior of the solution close to the singularity in more detail. In particular, we show that the trajectories do not cross the line  $1 - 3\sigma^3 \eta_0^2 = 0$ . It is convenient to introduce the variables  $y = -\sigma_i$  and  $z = (1 - 3\sigma^3 \eta_0^2)^{1/3}$ . In order to study the behaviour of the system around the singularity  $z = 0$ , we introduce a small parameter  $\varepsilon$  and choose as initial condition a point that approaches the axis  $z = 0$  when  $\varepsilon$  goes to zero. In the new variables, the system of equation (89) and (90) becomes

$$\begin{cases} \dot{y} = y^2 + \omega^2 - \left( \frac{z^3 - 1}{3\eta_0^2} \right)^{2/3} \frac{z^3 + 1}{4z^3} \\ \dot{z} = 2y \frac{z^3 - 1}{z^2} \\ y(t_0) = \bar{y}; \quad z(t_0) = \varepsilon \bar{z}. \end{cases} \tag{91}$$

Here,  $\bar{y} > 0$  and  $\bar{z} > 0$ . It is convenient to use the normalized variables  $\tilde{y}(t) = y\left(\frac{t}{\varepsilon^3}\right)$  and  $\tilde{z}(t) = \frac{1}{\varepsilon} z\left(\frac{t}{\varepsilon^3}\right)$ . With this transformation the small parameter  $\varepsilon$  is removed from the initial condition and appears explicitly in the evolution equations. We obtain





**Figure 4.** Trajectory of the solution of equations (89) and (90) in the plane  $(\sigma, \sigma_i)$  for different initial conditions. From the left, the panels depict the solution for increasing values of the parameter  $\eta_0$ . We have used  $\eta_0 = 0, 0.4, 0.8$  and  $\omega = 0.1$ .

$$\begin{cases} \dot{\tilde{y}} = -\frac{1}{4\tilde{z}^3} \left( \frac{\varepsilon^3 \tilde{z}^3 - 1}{3\eta_0^2} \right)^{2/3} + \varepsilon^3 \left[ \tilde{y}^2 + \omega^2 - \frac{1}{4} \left( \frac{\varepsilon^3 \tilde{z}^3 - 1}{3\eta_0^2} \right)^{2/3} \right] \\ \dot{\tilde{z}} = 2\tilde{y} \left( \varepsilon^3 \tilde{z} - \frac{1}{\tilde{z}^2} \right) \\ \tilde{y}(t_0) = \bar{y}; \quad \tilde{z}(t_0) = \bar{z}. \end{cases} \quad (92)$$

We write the solution by using the Hilbert expansion:

$$\tilde{y} = \tilde{y}_0 + \varepsilon^3 \tilde{y}_3 + o(\varepsilon^3) \quad (93)$$

$$\tilde{z} = \tilde{z}_0 + \varepsilon^3 \tilde{z}_3 + o(\varepsilon^3). \quad (94)$$

At the leading order in  $\varepsilon$ , the system (92) simplifies to

$$\begin{cases} \dot{\tilde{y}}_0 = -\frac{1}{4\tilde{z}_0^3 (3\eta_0^2)^{2/3}} \\ \dot{\tilde{z}}_0 = -2\frac{\tilde{y}_0}{\tilde{z}_0} \\ \tilde{y}(t_0) = \bar{y}; \quad \tilde{z}(t_0) = \bar{z}. \end{cases}$$

The solution of this system can be expressed in closed form. We have

$$\tilde{z}_0(t) = \bar{z} e^{4(\tilde{y}_0^2(t) - \bar{y}^2)(3\eta_0^2)^{2/3}} \geq \bar{z} e^{-4\bar{y}^2(3\eta_0^2)^{2/3}} \equiv \bar{z}_m > 0. \quad (95)$$

Equation (95) shows that the zeroth order trajectory  $(\tilde{y}_0(t), \tilde{z}_0(t))$  does not intersect the axis  $\tilde{z}_0 = 0$ . We verify that this statement remains valid if we also include the first correction to the solution obtained by the expansion given in equation (93)–(94). First, we derive a preliminary bound. We are interested in the behaviour of the solution close to the singularity. We focus on the part of the zeroth order trajectory that starts from the point  $(\bar{y}, \bar{z})$ , reaches the axis  $\tilde{y}_0 = 0$  and—due to the symmetry of the equation—ends at the point  $(-\bar{y}, \bar{z})$ . The time at which the trajectory reaches the axis  $\tilde{y}_0 = 0$  is

$$\Delta_t = \frac{\bar{z}^3}{4(3\eta_0^2)^{2/3}} \int_0^{\bar{y}} e^{12(\tilde{y}_0^2 - \bar{y}^2)(3\eta_0^2)^{2/3}} dy \leq \frac{\bar{z}^3 \bar{y}}{4(3\eta_0^2)^{2/3}}. \quad (96)$$

We have used the bounds  $|\tilde{y}_0| \leq \bar{y}$  and  $\bar{z}_m \leq |\tilde{z}_0| \leq \bar{z}$ . The first order correction to the solution is obtained by the system

$$\begin{cases} \dot{\tilde{y}}_3 = \tilde{y}_0^2 + \omega^2 - \frac{1}{12(3\eta_0^2)^{2/3}} \\ \dot{\tilde{z}}_3 = 2\left(\tilde{z}_0\tilde{y}_0 - \frac{\tilde{y}_3}{\tilde{z}_0}\right) \\ \tilde{y}_3(t_0) = 0; \quad \tilde{z}_3(t_0) = 0. \end{cases} \quad (97)$$

Using equation (97), we find that the solution of equation (91) in the proximity of the singularity has the following expansion:

$$z \geq \varepsilon \left[ \bar{z}_m - \varepsilon^3 \left( 2\Delta_t \bar{z}_y + \frac{\Delta_t^2}{\bar{z}_m^2} \left( \bar{y}^2 + \omega^2 - \frac{1}{12(3\eta_0^2)^{2/3}} \right) \right) \right] + o(\varepsilon^4).$$

This proves that we can find  $\varepsilon$  small enough to ensure that the trajectory does not intersect the axis  $z = 0$ .

### 6. Numerics

We validate the final system of equations (78)–(81) by performing numerical tests. In figure 5, we depict the numerical solution of the equations (solid curves) and compare it with the solution obtained by directly solving the Schrödinger equation (3) (dotted curves). The initial condition is  $\sigma(t_0) = 1$ ,  $a_3(t_0) = 0.1$ , and the other coefficients are set to zero. In panel A, we consider the free evolution of the quantum particle; in panel B, the evolution in the presence of the harmonic potential  $U(x) = \frac{\omega_0^2 x^2}{2}$  with  $\omega_0^2 = 0.5$ . We find agreement with the direct solution of the Schrödinger equation, especially for parameters  $a_n$  and  $\chi_n$  with small  $n$  (we find practically no difference for the coefficients  $\sigma$  and  $\chi_2$ ). Finally, in panels C and D respectively, we depict the particle wave function at the final time  $t = t_0 + 4$  for the free evolution and for the harmonic oscillator case. As indicated in section 2, in our calculations we have used normalized variables. In order to express all the quantities in physical units, it is necessary to multiply the scaled position  $x$ , time  $t$  and energy  $U$  respectively by the scaling factors  $L$ ,  $\tau$  and  $E_0$ . In the case of a proton moving in a confining potential with typical length scale of  $L = 1$  nm, we obtain the following values for the scaling factors  $\tau \simeq 2.5$  ps,  $E_0 \simeq 1.6$  meV.

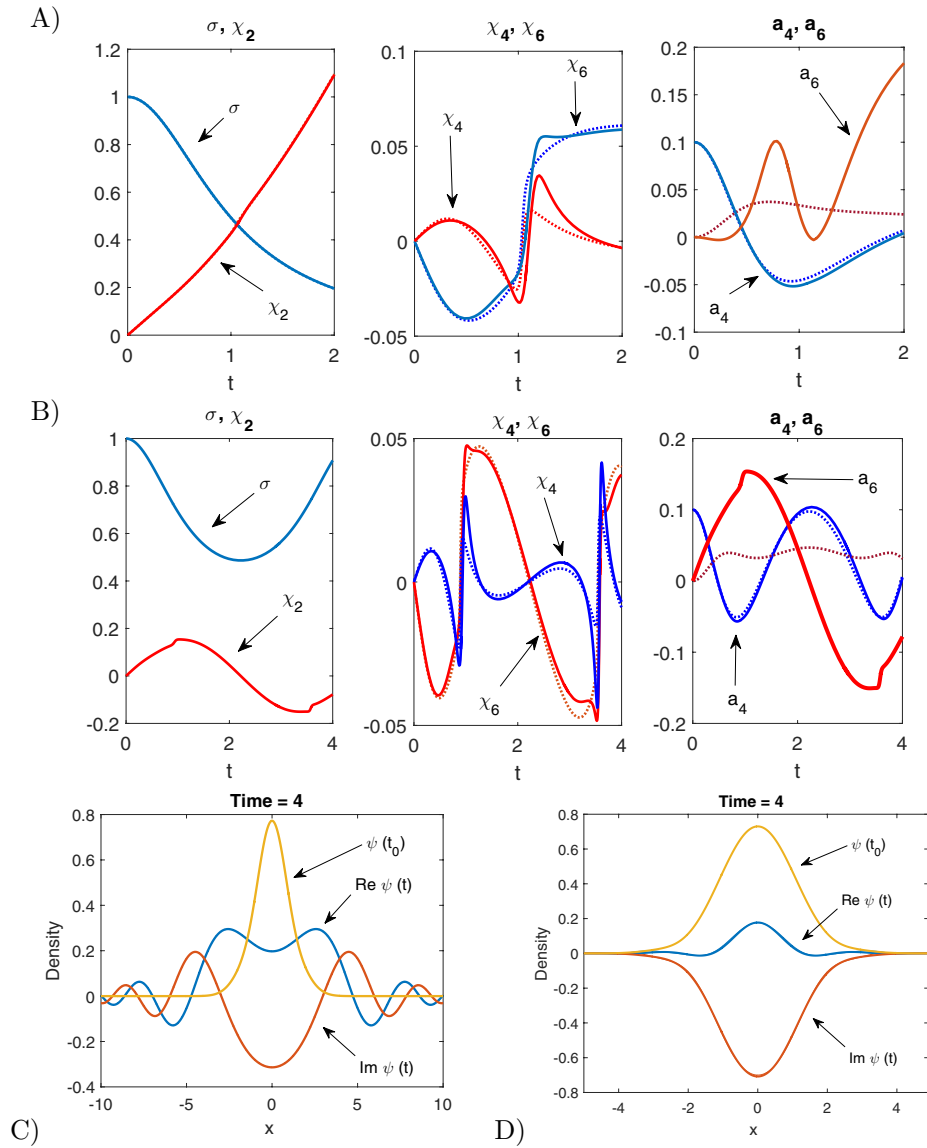
As a second test case, we simulate particle motion in the presence of a non-harmonic potential. We consider the double well structure obtained by taking the sum of a harmonic repulsive potential plus a fourth-order attractive potential:

$$U(x) = -\frac{\omega_0}{2}x^2 + V_4x^4. \quad (98)$$

Here,  $\omega_0$  and  $V_4$  are given parameters. The results of the simulations are depicted in figures 6 and 7. In figure 6, we plot the time evolution of the mean particle position

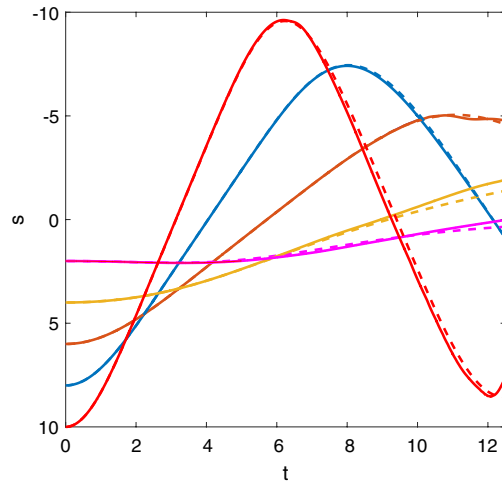
$$\langle x \rangle = \int_{\mathbb{R}} x |\psi(x)|^2 dx = s. \quad (99)$$

We depict the time evolution of  $s$  related to various initial conditions  $s(t_0)$ . We take values of  $s(t_0)$  that span from 2 (solid magenta curve) to 10 (solid red curve). Concerning the shape of the initial wave function, we take a pure Gaussian pulse with  $\sigma(t_0) = 1$ . Our results are obtained by solving the Euler–Lagrange system for  $N = 6$  (which corresponds to evaluating the parameters  $a_0, a_i$ , with  $i = 3, \dots, 6$  and  $\chi_i$  with  $i = 1, \dots, 6$ ) and by taking  $\omega_0 = 4 \cdot 10^{-2}$ ,  $V_4 = 10^{-2}$ . We compare our results with the evolution of the mean particle position obtained by solving directly the Schrödinger equation (dashed curves). The dependence of the oscillation

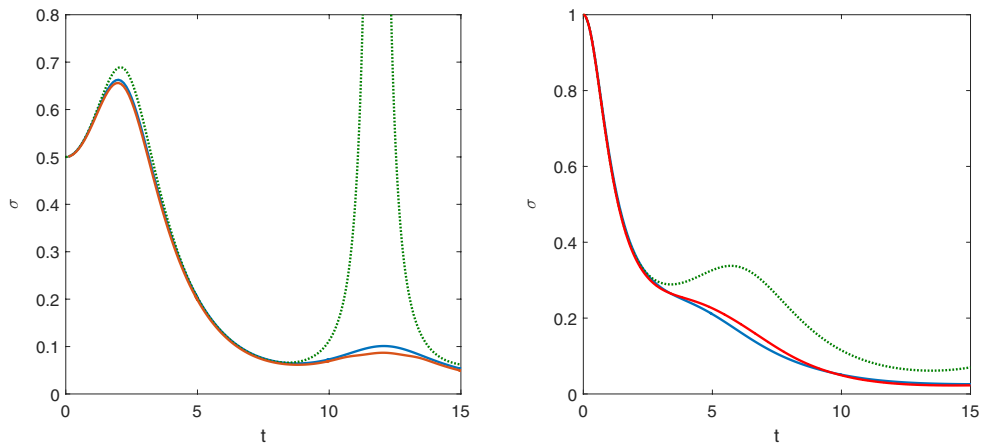


**Figure 5.** Numerical solution of the system (78)–(81) compared with the solution obtained by solving the Schrödinger equation (dotted line). Panel (A): free evolution case. Panel (B): harmonic oscillator with  $\omega = 0.5$ . Panels (C),(D): representation of the solution by the wave function for  $t = t_0 + 4$  for the free evolution (harmonic oscillator) case.

frequency of the center of the Gaussian wave packed from the initial potential energy of the particle is a signature of the presence of a non-harmonic potential. In figure 7 we depict the evolution of the Gaussian width  $\sigma$ . We take the same potential profile as in the previous simulations. The initial conditions are  $s(t_0) = 6$ ,  $\sigma(t_0) = 0.5$  (left panel) and  $\sigma(t_0) = 1$  (right panel). We compare the numerical solution obtained by using Hermite polynomial expansion with  $N = 6$  (red solid curve),  $N = 2$  (green dotted curve) and by solving directly the



**Figure 6.** Evolution of the mean particle position  $\langle x \rangle = s$  for  $\omega_0 = 4 \cdot 10^{-2}$ ,  $V_4 = 10^{-2}$ . Solid curves: solution of Euler-Lagrange system with  $N = 6$ . Dashed curves: direct solution of the Schrödinger equation.



**Figure 7.** Time evolution of the Gaussian width  $\sigma$ . The solid red curve is obtained by solving the system (78)–(81) with  $N = 6$ , the solid blue curve by solving the Schrödinger equation, and the dotted green curve by taking the standard Gaussian approximation (the value of the maximum of the function in correspondence to the pick located around  $t = 12$  is 3.4). We use the parameters  $\omega_0 = 4 \cdot 10^{-2}$ ,  $V_4 = 10^{-2}$ ,  $s(t_0) = 6$ , and  $\sigma(t_0) = 0.5$  (left panel),  $\sigma(t_0) = 1$  (right panel).

Schrödinger equation (blue solid curve). The case  $N = 2$  corresponds to the standard Gaussian approximation. Our simulations show that in the presence of non-harmonic terms, the simple Gaussian approximation leads to large errors in the estimation of the evolution of the variance of the Gaussian shape, and a finer description of the particle motion is required.

## 7. Bohm dynamics

We discuss the connection of our procedure with the quantum hydrodynamic formalism based on the definition of the so called Bohm potential. In particular, we show how the Bohm potential can be expressed by our set of variables. The Bohm mechanics can be viewed as the physical interpretation given to the quantum hydrodynamic equations obtained from the application of the Madelung transform at the Schrödinger equation. According to Madelung, the particle wave function is represented in polar coordinates:

$$\psi(x) = \sqrt{n(x-s)}e^{i\chi(x-s)}.$$

In agreement with our previous notations, we have maintained the translation of amount  $s$  in the spatial coordinate. The function  $\psi$  is the single particle wave function, and  $n(x)$  represents the particle density. According to our notations,  $n$  is written as

$$n(x) = P(x)e^{-x^2\sigma}.$$

In this section, for the sake of simplicity, we will assume  $s = 0$ . The Madelung transform leads to the well known quantum hydrodynamic equations

$$\frac{\partial n}{\partial t} = -\frac{dJ}{dx} \quad (100)$$

$$\frac{\partial J}{\partial t} = -\frac{d}{dx} \left( \frac{J^2}{n} \right) + n \frac{d}{dx} (Q + U). \quad (101)$$

Here,  $J = n \frac{d\chi}{dx}$  is the quantum current and  $Q(x)$  is the quantum Bohm potential:

$$\begin{aligned} Q &\equiv \frac{1}{2} \frac{d^2 \sqrt{n}}{\sqrt{n}} = \frac{1}{4n} \frac{d^2 n}{dx^2} - \frac{1}{8} \frac{1}{n^2} \left( \frac{dn}{dx} \right)^2 \\ &= \frac{1}{4} \left[ \frac{1}{P} \frac{d^2 P}{dx^2} - \frac{1}{2P^2} \left( \frac{dP}{dx} \right)^2 - 2x\sigma \frac{1}{P} \frac{dP}{dx} + 2\sigma(x^2\sigma - 1) \right]. \end{aligned} \quad (102)$$

The expectation value of the Bohm potential is

$$\int_{\mathbb{R}} Q(x) |\psi|^2 dx = \int_{\mathbb{R}} \left( \frac{1}{4} \frac{d^2 P}{dx^2} - \frac{x\sigma}{2} \frac{dP}{dx} + \frac{\sigma(x^2\sigma - 1)P}{2} \right) e^{-x^2\sigma} dx - \frac{1}{8} \int_{\mathbb{R}} \frac{1}{P} \left( \frac{dP}{dx} \right)^2 e^{-x^2\sigma} dx.$$

The last term of this equation contains the non-regular part of the Bohm potential (see equation (49)). In the intervals where the density  $P(x)$  goes to zero, this term is a source of numerical troubles. From equation (101), with some algebra, we obtain the evolution equation for the phase  $\chi$ :

$$\frac{\partial \chi}{\partial t} = -\frac{1}{2} \left( \frac{d\chi}{dx} \right)^2 + Q + U. \quad (103)$$

As a possible alternative to our variational procedure, equation (103) can be taken as a starting point to derive the evolution equation of the parameters  $\chi_n$  obtained by expanding the function  $\chi(x)$  on the Hermite polynomials. We multiply equation (103) by  $h_n^\sigma e^{-x^2\sigma}$  and integrate. We obtain

$$\begin{aligned} \frac{\partial \chi_n}{\partial t} = & -\pi^{-1/4} \frac{1}{2} \int_{\mathbb{R}} \left( \frac{d\chi}{dx} \right)^2 h_n^\sigma e^{-x^2 \sigma} dx + \pi^{-1/4} \int_{\mathbb{R}} (Q + U) h_n^\sigma e^{-x^2 \sigma} dx \\ & - \frac{d\sigma}{dt} \sum_r \chi_r \int_{\mathbb{R}} h_n^\sigma \frac{dh_r^\sigma}{d\sigma} e^{-x^2 \sigma} dx. \end{aligned}$$

For the first term, we have (see equation (39))

$$-\frac{1}{2\pi^{1/4}} \int_{\mathbb{R}} \left( \frac{d\chi}{dx} \right)^2 h_n^\sigma e^{-x^2 \sigma} dx = -\sigma^{5/4} \sum_{r,s} \sqrt{rs} \chi_r \chi_s A_{n,r-1,s-1}.$$

For the other terms, we proceed as in equation (49). First, we note that

$$\frac{1}{P} \frac{d^2 P}{dx^2} - \frac{1}{2P^2} \left( \frac{dP}{dx} \right)^2 = \frac{d^2 R}{dx^2} + \frac{1}{2} \left( \frac{dR}{dx} \right)^2.$$

We have introduced the auxiliary variable  $R(x) = \ln(P(x))$ . The integral containing the Bohm potential becomes

$$\int_{\mathbb{R}} Q h_n^\sigma e^{-x^2 \sigma} dx = \int_{\mathbb{R}} \left( \frac{1}{4} \frac{d^2 R}{dx^2} + \frac{1}{8} \left( \frac{dR}{dx} \right)^2 - \frac{x\sigma}{2} \frac{dR}{dx} + \frac{\sigma}{2} (x^2 \sigma - 1) \right) h_n^\sigma e^{-x^2 \sigma} dx.$$

By using the expansion  $R(x) = \pi^{1/4} \sigma^{-1/4} \sum_m R_m h_m^\sigma(x)$ , we obtain the explicit form of the previous terms. For the sake of completeness, we give the result of the computations:

$$\begin{aligned} \frac{1}{4\pi^{1/4}} \int_{\mathbb{R}} \frac{d^2 R}{dx^2} h_n^\sigma e^{-x^2 \sigma} dx &= \frac{\sigma^{3/4}}{2} \sum_m R_m \sqrt{m(m-1)} \int_{\mathbb{R}} h_{m-2}^\sigma h_n^\sigma e^{-x^2 \sigma} dx \\ &= \frac{\sigma^{3/4}}{2} R_{n+2} \sqrt{(n+2)(n+1)} \\ \frac{1}{8\pi^{1/4}} \int_{\mathbb{R}} \left( \frac{dR}{dx} \right)^2 h_n^\sigma e^{-x^2 \sigma} dx &= \frac{\sigma^{3/4}}{4} \sum_{r,s} \sqrt{rs} R_r R_s A_{n,r-1,s-1} \\ -\frac{1}{2\pi^{1/4}} \int_{\mathbb{R}} x\sigma \frac{dR}{dx} h_n^\sigma e^{-x^2 \sigma} dx &= -\frac{\sigma^{3/4}}{2} \left( \sqrt{(n+1)(n+2)} R_{n+2} + n R_n \right) \\ \frac{\sigma}{2\pi^{1/4}} \int_{\mathbb{R}} (x^2 \sigma - 1) h_n^\sigma e^{-x^2 \sigma} dx &= \frac{\sigma^{3/4}}{4} \left( \sqrt{2} \delta_{n,2} - \delta_{n,0} \right) \\ \sum_r \chi_r \int_{\mathbb{R}} h_n^\sigma \frac{dh_r^\sigma}{d\sigma} e^{-x^2 \sigma} dx &= \frac{2n+1}{4\sigma} \chi_n + \frac{\sqrt{(n+2)(n+1)}}{2\sigma} \chi_{n+2}. \end{aligned}$$

In conclusion,

$$\begin{aligned} \frac{d\chi_n}{dt} = & \sum_{r,s} \sqrt{rs} A_{n,r-1,s-1} \left( -\sigma^{5/4} \chi_r \chi_s + \frac{\sigma^{3/4}}{4} R_r R_s \right) + \pi^{-1/4} \int_{\mathbb{R}} U h_n^\sigma e^{-x^2 \sigma} dx \\ & - \frac{\sigma^{3/4}}{2} n R_n + \frac{1}{4} \sigma^{3/4} \left( \sqrt{2} \delta_{n,2} - \delta_{n,0} \right) - \frac{d\sigma}{dt} \left( \frac{2n+1}{4\sigma} \chi_n + \frac{\sqrt{(n+2)(n+1)}}{2\sigma} \chi_{n+2} \right) \end{aligned}$$

which agrees with equation (78). The evolution equation for  $a_n$  and  $\sigma$  can be obtained by using the continuity equation. It is easy to verify that

$$\frac{\partial n}{\partial t} = -\frac{dJ}{dx} = -\frac{dn}{dx} \frac{d\chi}{dx} - n \frac{d^2\chi}{dx^2}$$

leads to

$$\left(\frac{dP}{dt} - x^2 P \frac{d\sigma}{dt}\right) e^{-x^2\sigma} = -\frac{d}{dx} \left(P \frac{d\chi}{dx} e^{-x^2\sigma}\right).$$

We proceed by considering the expansion on the Hermite polynomial of  $P$ . The equation

$$\int_{\mathbb{R}} h_n^\sigma(x) \left(\frac{dP}{dt} - x^2 P \frac{d\sigma}{dt}\right) e^{-x^2\sigma} dx = \int_{\mathbb{R}} \frac{dh_n^\sigma}{dx} P \frac{d\chi}{dx} e^{-x^2\sigma} dx$$

gives

$$\begin{aligned} &\sum_{r=0}^{\infty} \int_{\mathbb{R}} h_n^\sigma(x) \left(a_r \frac{d\sigma}{dt} \frac{\partial h_r^\sigma(x)}{\partial \sigma} + h_r^\sigma(x) \frac{da_r}{dt}\right) e^{-x^2\sigma} dx - \frac{d\sigma}{dt} \sum_{r=0}^{\infty} a_r \int_{\mathbb{R}} h_n^\sigma(x) x^2 h_r^\sigma(x) e^{-x^2\sigma} dx \\ &= \pi^{1/4} \sum_{r,s=0}^{\infty} \chi_s a_r \int_{\mathbb{R}} \frac{dh_n^\sigma}{dx} h_r^\sigma(x) \frac{dh_s^\sigma(x)}{dx} e^{-x^2\sigma} dx. \end{aligned} \tag{104}$$

We have

$$\sum_{r=0}^{\infty} \int_{\mathbb{R}} h_n^\sigma(x) \left(a_r \frac{d\sigma}{dt} \frac{\partial h_r^\sigma(x)}{\partial \sigma}\right) e^{-x^2\sigma} dx = \frac{d\sigma}{dt} \left(\frac{2n+1}{4\sigma} a_n + \frac{\sqrt{(n+2)(n+1)}}{2\sigma} a_{n+2}\right).$$

Moreover,

$$\begin{aligned} \sum_{r=0}^{\infty} a_r \int_{\mathbb{R}} h_n^\sigma(x) x^2 h_r^\sigma(x) e^{-x^2\sigma} dx &= \frac{1}{\sigma} \sum_{r=0}^{\infty} a_r \int_{\mathbb{R}} (x\sqrt{\sigma} h_n^\sigma(x)) (x\sqrt{\sigma} h_r^\sigma(x)) e^{-x^2\sigma} dx \\ &= \frac{1}{2\sigma} \left[ a_n(2n+1) + a_{n-2} \sqrt{n(n-1)} + a_{n+2} \sqrt{(n+1)(n+2)} \right]. \end{aligned}$$

The last term of equation (104) gives

$$\begin{aligned} \sum_{r,s=0}^{\infty} \chi_s a_r \int_{\mathbb{R}} \frac{dh_n^\sigma}{dx} h_r^\sigma(x) \frac{dh_s^\sigma(x)}{dx} e^{-x^2\sigma} dx &= 2\sigma^{5/4} \sqrt{n} \sum_{r,s=0}^{\infty} \sqrt{s} \chi_s a_r \int_{\mathbb{R}} h_{n-1}^1 h_r^1 h_{s-1}^1 e^{-x^2} dx \\ &= \frac{2\sigma^{5/4}}{\pi^{1/4}} \sqrt{n} \sum_{r,s=0}^{\infty} \sqrt{s} \chi_s a_r A_{n-1,r,s-1}. \end{aligned}$$

We obtain

$$\frac{da_n}{dt} = \frac{1}{2\sigma} \frac{d\sigma}{dt} \left(\frac{2n+1}{2} a_n + a_{n-2} \sqrt{n(n-1)}\right) + 2\sigma^{5/4} \sqrt{n} \sum_{r,s=0}^{\infty} \sqrt{s} \chi_s a_r A_{n-1,r,s-1},$$

which agrees with equation (79) for  $s = 0$ .

### 8. Euler–Lagrange method in dimension two

The Hermite–Gaussian beam method that we have developed in the preceding sections can be extended straightforwardly to spaces with dimension greater than one. In this section, we

derive the Euler–Lagrange evolution equations for a two-dimensional space. We generalize the ansatz for the wave function  $\psi$  given in equation (5) as follows:

$$\psi(\mathbf{r}, t) = \sqrt{P(\mathbf{r} - \mathbf{s}(t), t)} e^{-\frac{\langle \sigma, \mathbf{r} - \mathbf{s}(t) \rangle}{2} + i\chi(\mathbf{r} - \mathbf{s}(t), t)}. \quad (105)$$

Here,  $\mathbf{r} \in \mathbb{R}^2$ . As before, the parameters  $\mathbf{s}$  and  $\sigma$  provide, respectively, the center of the Hermite polynomial expansion and the width of the Gaussian packet. We indicate the components of the vectors along the coordinate axis as follows:  $\mathbf{s} = (s_x, s_y)$ ,  $\sigma = (\sigma_x, \sigma_y)$  and  $\mathbf{r} = (x, y)$ . For the sake of compactness, we have introduced the notation

$$\langle \sigma, \mathbf{r} - \mathbf{s} \rangle \doteq (x - s_x)^2 \sigma_x + (y - s_y)^2 \sigma_y. \quad (106)$$

According to equations (17) and (18), we expand the time dependent polynomials  $P = P(\mathbf{r}, t)$  and  $\chi = \chi(\mathbf{r}, t)$ , on the Hermite basis:

$$P(\mathbf{r}, t) = \frac{1}{\pi^{1/2}} \sum_{n, n'=0}^{\infty} a_{n, n'}(t) h_n^{\sigma_x}(x) h_{n'}^{\sigma_y}(y) \quad (107)$$

$$\chi(\mathbf{r}, t) = \pi^{1/2} \sum_{n, n'=0}^{\infty} \chi_{n, n'}(t) h_n^{\sigma_x}(x) h_{n'}^{\sigma_y}(y). \quad (108)$$

Similarly to the one dimensional case, the set of parameters  $a_{n, n'}$  appearing in expansion (107) is overcomplete, and we are free to fix some of them. In the present case, the choice  $a_{0,1} = a_{1,0} = a_{2,1} = a_{1,2} = 0$  is convenient. In this way, the evolution equations of the vectors  $\mathbf{s}$  and  $\sigma$  have a particularly simple form. Proceeding as in section 2, we define the quantum Lagrangian:

$$\begin{aligned} L &= \int_{\mathbb{R}^2} \left[ \text{Im}(\psi^\dagger \partial_t \psi) - \frac{1}{2} |\nabla \psi|^2 - U(x, y) |\psi|^2 \right] dx dy \\ &= \int_{\mathbb{R}^2} \left[ \dot{\mathbf{s}} \cdot \nabla \chi - \dot{\chi} - \frac{1}{2} |\nabla \chi|^2 - \frac{(\sigma_x)^2 x^2 + (\sigma_y)^2 y^2}{2} - U(\mathbf{r} + \mathbf{s}) \right] P e^{-\langle \sigma, \mathbf{r} \rangle} dx dy \\ &\quad + \int_{\mathbb{R}^2} \left( \frac{x \sigma_x}{2} \frac{dP}{dx} + \frac{y \sigma_y}{2} \frac{dP}{dy} - \frac{|\nabla P|^2}{8P} \right) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy. \end{aligned}$$

We evaluate the various terms that appear in the expression of the quantum Lagrangian in the same way as we have done in equations (35)–(39). We obtain

$$\begin{aligned} \int_{\mathbb{R}^2} P \dot{\chi} e^{-\langle \sigma, \mathbf{r} \rangle} dx dy &= \sum_{n, n'=0}^{\infty} a_{n, n'} \left[ \dot{\chi}_{n, n'} + \chi_{n, n'} \left( \frac{\dot{\sigma}_x}{\sigma_x} \frac{2n+1}{4} + \frac{\dot{\sigma}_y}{\sigma_y} \frac{2n'+1}{4} \right) \right] \\ &\quad + \frac{1}{2} \sum_{n, n'=0}^{\infty} a_{n, n'} \left( \frac{\dot{\sigma}_x}{\sigma_x} \sqrt{(n+2)(n+1)} \chi_{n+2, n'} + \frac{\dot{\sigma}_y}{\sigma_y} \sqrt{(n'+2)(n'+1)} \chi_{n, n'+2} \right) \\ \dot{\mathbf{s}} \cdot \int_{\mathbb{R}^2} (\nabla \chi) P e^{-\langle \sigma, \mathbf{r} \rangle} dx dy &= \sum_{n, n'=0}^{\infty} a_{n, n'} \left( \dot{s}_x \sqrt{2\sigma_x(n+1)} \chi_{n+1, n'} + \dot{s}_y \sqrt{2\sigma_y(n'+1)} \chi_{n, n'+1} \right) \\ \frac{1}{2} \int_{\mathbb{R}^2} P |\nabla \chi|^2 e^{-\langle \sigma, \mathbf{r} \rangle} dx dy &= \sigma_x^{1/4} \sigma_y^{1/4} \sum_{n, n'=0; r_1, r_2, r'_1, r'_2=1}^{\infty} a_{n, n'} \chi_{r_1, r'_1} \chi_{r_2, r'_2} \\ &\quad \times \left( A_{n, r_1-1, r_2-1} A_{n', r'_1, r'_2} \sigma_x \sqrt{r_1 r_2} + A_{n, r_1, r_2} A_{n', r'_1-1, r'_2-1} \sigma_y \sqrt{r'_1 r'_2} \right), \end{aligned}$$



and

$$\int_{\mathbb{R}^2} P \left( \frac{\sigma_x^2 x^2 + \sigma_y^2 y^2}{2} \right) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy = \frac{\sigma_x^{3/4}}{4} (\sqrt{2} a_{2,0} + a_{0,0}) + \frac{\sigma_y^{3/4}}{4} (\sqrt{2} a_{0,2} + a_{0,0})$$

$$\int_{\mathbb{R}^2} \left( \sigma_x x \frac{\partial P}{\partial x} + \sigma_y y \frac{\partial P}{\partial y} \right) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy = \sqrt{2} (\sigma_x^{3/4} a_{2,0} + \sigma_y^{3/4} a_{0,2}).$$

The Bohm term

$$\mathcal{B}_2 \doteq -\frac{1}{8} \int_{\mathbb{R}^2} \frac{|\nabla P|^2}{P} e^{-\langle \sigma, \mathbf{r} \rangle} dx dy,$$

requires the same treatment as  $\mathcal{B}$  in section 3. We define  $R(\mathbf{r}) = \log(P)$  and we assume the expansion

$$R(\mathbf{r}, t) = \frac{\pi^{1/2}}{(\sigma_x \sigma_y)^{1/4}} \sum_{n,n'=0}^{\infty} R_{n,n'}(t) h_n^{\sigma_x}(x) h_{n'}^{\sigma_y}(y) \tag{109}$$

$$R_{r,r'} = \frac{(\sigma_x \sigma_y)^{1/4}}{\pi^{1/2}} \int_{\mathbb{R}^2} R(\mathbf{r}) h_r^{\sigma_x}(x) h_{r'}^{\sigma_y}(y) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy. \tag{110}$$

In appendix B we derive the following simple expression for  $\mathcal{B}_2$ :

$$\mathcal{B}_2 = -\frac{1}{4(\sigma_y \sigma_x)^{1/4}} \sum_{n,n'=1}^{\infty} R_{n,n'} a_{n,n'} (\sigma_x n + \sigma_y n'). \tag{111}$$

By inserting the previous terms in the expression of the quantum Lagrangian, we can proceed to calculate the Euler–Lagrange evolution equations. It is easy to verify that

$$\frac{\partial L}{\partial \dot{a}_{n,n'}} = 0$$

$$\frac{\partial L}{\partial \dot{\chi}_{n,n'}} = -a_{n,n'}.$$

The Euler–Lagrange equations take the form

$$\dot{a}_{n,n'} = -\frac{\partial L}{\partial \chi_{n,n'}} \tag{112}$$

$$\frac{\partial L}{\partial a_{n,n'}} = 0. \tag{113}$$

At first, it is convenient to evaluate the evolution equation of the parameter  $a_{0,0}$ . Equation (112) gives

$$\dot{a}_{0,0} = \frac{a_{0,0}}{4} \left( \frac{\dot{\sigma}_x}{\sigma_x} + \frac{\dot{\sigma}_y}{\sigma_y} \right),$$

whose solution is

$$a_{0,0}(t) = (\sigma_x(t)\sigma_y(t))^{1/4}. \tag{114}$$

We now consider the evolution equation of the parameter  $a_{0,1}$ . We have

$$\begin{aligned} \dot{a}_{0,1} = & -\dot{s}_y\sqrt{2\sigma_y} a_{0,0} + \frac{a_{0,1}}{4} \left( \frac{\dot{\sigma}_x}{\sigma_x} + 3\frac{\dot{\sigma}_y}{\sigma_y} \right) \\ & + 2\sigma_x^{1/4}\sigma_y^{3/4} \sum_{m,m'=0;r,r'=1}^{\infty} a_{m,m'}\chi_{r,r'}\sqrt{r'} A_{m,0,r}A_{m',0,r'-1}. \end{aligned}$$

We fix  $a_{0,1} = 0$  and obtain

$$\dot{s}_y = \sqrt{2\sigma_y} \sum_{m,m'=0}^{\infty} a_{m,m'}\chi_{m,m'+1}\sqrt{m'+1}.$$

Applying the same procedure to  $a_{1,0}$  (now  $a_{1,0} = 0$ ), we obtain

$$\dot{s}_x = \sqrt{2\sigma_x} \sum_{m,m'=0}^{\infty} a_{m,m'}\chi_{m+1,m'}\sqrt{m+1}.$$

As a next step, we consider the parameter  $a_{0,2}$ . Equation (112) gives

$$\begin{aligned} \dot{a}_{0,2} = & -2\dot{s}_y\sqrt{\sigma_y} a_{0,1} + \frac{a_{0,2}}{4} \left( \frac{\dot{\sigma}_x}{\sigma_x} + 5\frac{\dot{\sigma}_y}{\sigma_y} \right) + \frac{a_{0,0}}{\sqrt{2}} \frac{\dot{\sigma}_y}{\sigma_y} \\ & + 2\sqrt{2}\sigma_x^{1/4}\sigma_y^{5/4} \sum_{m,m'=0;r,r'=1}^{\infty} a_{m,m'}\chi_{r,r'}\sqrt{r'} A_{m,0,r}A_{m',1,r'-1}. \end{aligned}$$

Fixing  $a_{0,2} = 0$  and using equation (114) we obtain

$$\dot{\sigma}_y = -4\sigma_y^2 \sum_{m,m'=0}^{\infty} a_{m,m'} \left( \chi_{m,m'+2}\sqrt{(m'+1)(m'+2)} + \chi_{m,m'}m' \right).$$

Analogously, for  $a_{2,0}$  we obtain

$$\dot{\sigma}_x = -4\sigma_x^2 \sum_{m,m'=0}^{\infty} a_{m,m'} \left( \chi_{m+2,m'}\sqrt{(m+1)(m+2)} + \chi_{m,m'}m \right).$$

We now calculate the evolution equations for the other parameters  $a_{n,n'}$  and  $\chi_{n,n'}$ . After straightforward calculations, we obtain

$$\begin{aligned} \dot{a}_{n,n'} = & -2\sigma_x S_x \sqrt{n} a_{n-1,n'} - 2\sigma_y S_y \sqrt{n'} a_{n,n'-1} \\ & - a_{n,n'} \left( \frac{2n+1}{2} M_x + \frac{2n'+1}{2} M_y \right) - a_{n-2,n'} M_x \sqrt{n(n-1)} - a_{n,n'-2} M_y \sqrt{n'(n'-1)} \\ & + 2(\sigma_x\sigma_y)^{1/4} \sum_{m,m'=0;r,r'=1}^{\infty} a_{m,m'}\chi_{r,r'} \left( \sigma_x\sqrt{nr} A_{m,n-1,r-1}A_{m',n',r'} + \sigma_y\sqrt{n'r'} A_{m,n,r}A_{m',n'-1,r'-1} \right), \end{aligned} \tag{115}$$

and

$$\begin{aligned}
 \dot{\chi}_{n,n'} &= 2\sigma_x S_x \sqrt{(n+1)} \chi_{n+1,n'} + 2\sigma_y S_y \sqrt{(n'+1)} \chi_{n,n'+1} \\
 &+ \chi_{n,n'} \left( \frac{2n+1}{2} M_x + \frac{2n'+1}{2} M_y \right) + M_x \sqrt{(n+2)(n+1)} \chi_{n+2,n'} + M_y \sqrt{(n'+2)(n'+1)} \chi_{n,n'+2} \\
 &+ \frac{\sigma_x^{3/4}}{2\sqrt{2}} \delta_{n,2} \delta_{n',0} + \frac{\sigma_y^{3/4}}{2\sqrt{2}} \delta_{n',2} \delta_{n,0} - \left( \frac{\sigma_x^{3/4} + \sigma_y^{3/4}}{4} \right) \delta_{n,0} \delta_{n',0} \\
 &- (\sigma_x \sigma_y)^{1/4} \sum_{r_1, r_2, r'_1, r'_2=1}^{\infty} \chi_{r_1, r'_1} \chi_{r_2, r'_2} \left( \sigma_x \sqrt{r_1 r_2} A_{n, r_1-1, r_2-1} A_{n', r'_1, r'_2} + \sigma_y \sqrt{r'_1 r'_2} A_{n, r_1, r_2} A_{n', r'_1-1, r'_2-1} \right) \\
 &- \frac{\sigma_x n + \sigma_y n'}{4(\sigma_y \sigma_x)^{1/4}} R_{n,n'} - \frac{1}{4\pi} \sum_{r, r'=1; m, m'=0}^{\infty} (\sigma_x r + \sigma_y r') a_{r, r'} R_{m, m'} A_{m, r, n} A_{m', r', n'} \\
 &- \frac{1}{\pi^{1/2}} \int_{\mathbb{R}^2} U(\mathbf{r} + \mathbf{s}) h_n^{\sigma_x}(x) h_{n'}^{\sigma_y}(y) e^{-(\sigma, \mathbf{r})} d\mathbf{x} d\mathbf{y}. \tag{116}
 \end{aligned}$$

In particular, in the fifth line of equation (116), we have used equation (B.3) given in appendix B. We have defined

$$\begin{aligned}
 M_y &= 2\sigma_y \sum_{m, m'=0}^{\infty} a_{m, m'} \left( \chi_{m, m'+2} \sqrt{(m'+1)(m'+2)} + \chi_{m, m'} m' \right) \\
 M_x &= 2\sigma_x \sum_{m, m'=0}^{\infty} a_{m, m'} \left( \chi_{m+2, m'} \sqrt{(m+1)(m+2)} + \chi_{m, m'} m \right) \\
 S_y &= \sum_{m, m'=0}^{\infty} a_{m, m'} \chi_{m, m'+1} \sqrt{m'+1} \\
 S_x &= \sum_{m, m'=0}^{\infty} a_{m, m'} \chi_{m+1, m'} \sqrt{m+1}.
 \end{aligned}$$

By using the previous definitions, the evolution equations of the coordinates of the center of expansion  $\mathbf{s}$  and of  $\boldsymbol{\sigma}$  can be written

$$\begin{aligned}
 \dot{s}_i &= \sqrt{2\sigma_i} S_i \\
 \dot{\sigma}_i &= -2M_i \sigma_i \quad \text{with } i = x, y.
 \end{aligned}$$

With these equations, the Euler–Lagrange system is closed. For the sake of simplicity, in this section we have restricted the calculations to the two dimensional case. It is easy to verify that by increasing the number of indexes in the parameters, it is possible to extend the previous calculations and to obtain the Euler–Lagrange evolution equations in the case of higher dimensional spaces.

### 9. Conclusions

We have presented a model designed to describe the motion of nearly localized particles. From a mathematical point of view, such particles are characterized by wave functions localized around a Gaussian packet. The oscillations of the particle wave functions around the mean particle positions are reproduced by Hermite polynomials. The particle motion is described by a set of time dependent parameters whose evolution equation is obtained by the Euler–Lagrange variational approach. Differing from other approaches that have been proposed in the past which investigate the evolution of Gaussian packed modulated by Hermite polynomials, as for

example by Hagedorn in [52] and by Billig in [49] where the time-dependent discrete variable representation method was proposed, our choice of the dynamical parameters is characterized by the expansion in Hermite polynomials of both the squared modulus and the quantum mechanical phase of the wave function. Such a symmetric treatment of modulus and phase proves very convenient in writing the Euler–Lagrange equations in a normal form. Moreover, our approach shows an interesting connection with the description of particle motion provided by the Bohm theory. We have applied our method to investigate the divergences induced by the Bohm potential. In particular, we were able to describe the evolution of the variance of the Gaussian beam in a simple case by showing the existence of two classes of trajectory separated by a singularity. Finally, in the case of 1D dynamics, we have validated our method by numerical tests. The extension of our results to a two dimensional space has also been discussed.

### Appendix A. Derivation of equation (54)

We derive equation (54). We start with equation (46):

$$\mathcal{B} \equiv -\frac{1}{8} \int_{\mathbb{R}} \frac{1}{P} \left( \frac{dP}{dx} \right)^2 e^{-x^2\sigma} dx = -\frac{\sigma^{3/4}}{4} \sum_{n=1}^{\infty} n a_n R_n.$$

We differentiate with respect to  $a_n$  and use the expansion (17):

$$\frac{d\mathcal{B}}{da_n} = -\frac{1}{4\pi^{1/4}} \int_{\mathbb{R}} \frac{dR}{dx} \frac{dh_n^\sigma}{dx} e^{-x^2\sigma} dx + \frac{1}{8\pi^{1/4}} \int_{\mathbb{R}} \left( \frac{dR}{dx} \right)^2 h_n^\sigma e^{-x^2\sigma} dx,$$

where we have used (recall that  $R = \ln(P)$ )

$$\frac{d}{da_n} \left[ P(x) \left( \frac{dR}{dx} \right)^2 \right] = 2 \frac{dR}{dx} \frac{dP(x)}{da_n} - \frac{dP(x)}{da_n} \left( \frac{dR}{dx} \right)^2.$$

Proceeding as in equation (39),

$$\begin{aligned} \frac{1}{8\pi^{1/4}} \int_{\mathbb{R}} \left( \frac{dR}{dx} \right)^2 h_n^\sigma e^{-x^2\sigma} dx &= \frac{\pi^{1/4}}{8\sigma^{1/2}} \sum_{r,s} R_r R_s \int_{\mathbb{R}} \frac{dh_r^\sigma(x)}{dx} \frac{dh_s^\sigma(x)}{dx} h_n^\sigma e^{-x^2\sigma} dx \\ &= \frac{\pi^{1/4} \sigma^{1/2}}{4} \sum_{r,s} \sqrt{rs} R_r R_s \int_{\mathbb{R}} h_{r-1}^\sigma h_{s-1}^\sigma h_n^\sigma e^{-x^2\sigma} dx \\ &= \frac{\sigma^{3/4}}{4} \sum_{r,s} \sqrt{rs} R_r R_s \pi^{1/4} \int_{\mathbb{R}} h_{r-1}^1 h_{s-1}^1 h_n^1 e^{-x^2} dx \\ &= \frac{\sigma^{3/4}}{4} \sum_{r,s \geq 1} \sqrt{rs} R_r R_s A_{n,r-1,s-1}, \end{aligned}$$

and (using equation (22))

$$\frac{1}{4\pi^{1/4}} \int_{\mathbb{R}} \frac{dR}{dx} \frac{dh_n^\sigma}{dx} e^{-x^2\sigma} dx = \frac{\sigma^{3/4}}{2} \sum_s \sqrt{sn} R_s \int_{\mathbb{R}} h_{s-1}^\sigma h_{n-1}^\sigma e^{-x^2\sigma} dx = \frac{\sigma^{3/4}}{2} n R_n.$$

Finally

$$\frac{d\mathcal{B}}{da_n} = -\frac{\sigma^{3/4}}{2}nR_n + \frac{\sigma^{3/4}}{4} \sum_{r,s \geq 1} \sqrt{rs}R_rR_sA_{n,r-1,s-1}.$$

## Appendix B. Derivation of equation (111)

We evaluate the expression of the Bohm term in the two dimensional case:

$$\mathcal{B}_2 \equiv -\frac{1}{8} \int_{\mathbb{R}^2} \frac{|\nabla P|^2}{P} e^{-\langle \sigma, \mathbf{r} \rangle} dx dy = -\frac{1}{8} \int_{\mathbb{R}^2} P |\nabla R|^2 e^{-\langle \sigma, \mathbf{r} \rangle} dx dy.$$

Proceeding in the same way as we have done for equation (50), we calculate

$$\frac{1}{8} \int_{\mathbb{R}^2} P \left( \frac{\partial R}{\partial x} \right)^2 e^{-\langle \sigma, \mathbf{r} \rangle} dx dy = \frac{\sigma_x^{3/4}}{4\sigma_y^{1/4}} \sum_{n,n'=0;r_1,r_2,r'_1,r'_2=1}^{\infty} a_{n,n'} R_{r_1,r'_1} R_{r_2,r'_2} \sqrt{r_1 r_2} A_{n,r_1-1,r_2-1} A_{n',r'_1,r'_2}.$$

A similar expression is obtained if in the left side of the previous formula we take the derivative of  $R$  with respect to  $y$ . We obtain

$$\begin{aligned} \mathcal{B}_2 = & -\frac{1}{4(\sigma_y \sigma_x)^{1/4}} \sum_{n,n'=0;r_1,r_2,r'_1,r'_2=1}^{\infty} a_{n,n'} R_{r_1,r'_1} R_{r_2,r'_2} \\ & \times \left( \sigma_x \sqrt{r_1 r_2} A_{n,r_1-1,r_2-1} A_{n',r'_1,r'_2} + \sigma_y \sqrt{r'_1 r'_2} A_{n,r_1,r_2} A_{n',r'_1-1,r'_2-1} \right). \end{aligned} \quad (\text{B.1})$$

With a few manipulations, the previous expression can be simplified. We write  $\mathcal{B}_2$  in a form which is more useful for the computation of the Euler–Lagrange equations. Proceeding as in equation (52), we obtain

$$\begin{aligned} a_{n,n'} &= \frac{\pi^{1/2}}{\sqrt{2n\sigma_x}} \int_{\mathbb{R}^2} \frac{\partial R}{\partial x} P h_{n'}^{\sigma_y}(y) h_{n-1}^{\sigma_x}(x) h_{n'-1}^{\sigma_y}(y) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy \\ &= \frac{\pi^{1/2}}{(\sigma_x \sigma_y)^{1/4}} \sum_{r,r',m,m'=0}^{\infty} R_{m,m'} a_{r,r'} \sqrt{\frac{m}{n}} \int_{\mathbb{R}^2} h_{m-1}^{\sigma_x}(x) h_r^{\sigma_x}(x) h_{n-1}^{\sigma_x}(x) h_{m'}^{\sigma_y}(y) h_{r'}^{\sigma_y}(y) h_{n'}^{\sigma_y}(y) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy \\ &= \frac{1}{\sqrt{n}} \sum_{r,r',m,m'=0}^{\infty} \sqrt{m} a_{r,r'} R_{m,m'} A_{m-1,r,n-1} A_{m',r',n'}. \end{aligned}$$

As before, by taking in the previous equation the derivative of  $R$  with respect to  $y$  instead of  $x$ , we obtain a similar expression

$$a_{n,n'} = \frac{1}{\sqrt{n}} \sum_{r,r',m,m'=0}^{\infty} \sqrt{m'} a_{r,r'} R_{m,m'} A_{m,r,n} A_{m'-1,r',n'-1}.$$

Comparing with equation (B.1), we obtain

$$\mathcal{B}_2 = -\frac{1}{4(\sigma_y \sigma_x)^{1/4}} \sum_{n,n'=1}^{\infty} R_{n,n'} a_{n,n'} (\sigma_x n + \sigma_y n'). \quad (\text{B.2})$$

In order to derive the Euler–Lagrange equations, it is necessary to calculate the derivative of  $\mathcal{B}_2$  with respect to  $a_{n,n'}$ . From equation (B.2) we see that the computational difficulties arise from the term  $\frac{\partial R_{r,r'}}{\partial a_{n,n'}}$ . We take the derivative of equation (110) and obtain

$$\begin{aligned}\frac{\partial R_{r,r'}}{\partial a_{n,n'}} &= \frac{(\sigma_x \sigma_y)^{1/4}}{\pi^{1/2}} \int_{\mathbb{R}^2} \frac{\partial e^{P(\mathbf{r})}}{\partial a_{n,n'}} h_r^{\sigma_x}(x) h_{r'}^{\sigma_y}(y) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy \\ &= \frac{(\sigma_x \sigma_y)^{1/4}}{\pi} \int_{\mathbb{R}^2} R(\mathbf{r}) h_r^{\sigma_x}(x) h_{r'}^{\sigma_y}(y) h_n^{\sigma_x}(x) h_{n'}^{\sigma_y}(y) e^{-\langle \sigma, \mathbf{r} \rangle} dx dy \\ &= \frac{(\sigma_x \sigma_y)^{1/4}}{\pi} \sum_{m,m'=0}^{\infty} R_{m,m'} A_{m,r,n} A_{m',r',n'}.\end{aligned}$$

In conclusion,

$$\frac{\partial \mathcal{B}_2}{\partial a_{n,n'}} = -\frac{R_{n,n'} (\sigma_x n + \sigma_y n')}{4(\sigma_y \sigma_x)^{1/4}} - \frac{1}{4\pi} \sum_{r,r'=1; m,m'=0}^{\infty} a_{r,r'} R_{m,m'} (\sigma_x r + \sigma_y r') A_{m,r,n} A_{m',r',n'}.$$
 (B.3)

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