Gauss-Hermite wavepacket dynamics: convergence of the spectral and pseudo-spectral approximation

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Abstract

The time dependent linear Schrödinger equation for nuclei on the whole space is semi-discretised using Hermite and Gauss-Hermite basis functions. These are well suited on the one hand for the conservation properties of the numerical solution and, on the other hand, for their remarkable approximation properties. We investigate theoretically and numerically the convergence of the spectral and pseudo-spectral Gauss-Hermite semi-discretisation schemes. Schrödinger equation, Gauss-Hermite approximation, spectral and pseudo-spectral methods

1 Introduction

The numerical approximation of the Schrödinger equation on the whole space using Gauss-Hermite basis functions is the subject of our paper. The particularity of this method is that the basis functions of the finite dimensional approximation space are defined on an unbounded domain, while standard numerical schemes are classically best developed for bounded domains. In the last years, numerical methods based on orthogonal basis functions that live on unbounded domains gained increasing attention, see Boyd (2000) and Bernardi & Maday (1997). Hermite functions are a natural choice for many fields, as testify the citations in Tang (1993) and Boyd (2000). Weideman (1992) showed that in the case of the first and second Hermite differentiation, we need rather weak stability restrictions for the time step in the discretisation of parabolic differential equations. Funaro & Kavian (1990) studied the stability and convergence properties of the Hermite method for the heat equation. Further, Tang (1993) evidenced the need to choose a scaling factor in the basis functions in order to get accurate approximation results using only a reasonable number of Hermite functions. Ma *et al.*

(2005) employed a time dependent scaling factor in the Hermite expansions for the viscous Burgers' equation in unbounded domains.

As quantum dynamics concerns, Billing (1999) used a time-dependent Gauss-Hermite basis in order to formulate approximations in which the classical limit arises in a natural fashion and that scale moderately with the number of particles. Vijay *et al.* (1999) compared the Hermite approach to quantum dynamics with the Chebyshev method. They evidenced that it may be possible to achieve a faster convergence with Hermite based method for finite time propagation, by a proper choice of scaling parameter.

In the spirit of these ideas, we are interested in a mathematical justification of the spectral and pseudo-spectral method in the context of a time-adaptive Gauss-Hermite basis. Regarding the time discretisation, we introduce in Faou *et al.* (2007) an algorithm to compute the solution of the time-dependent Schrödinger equation using Hagedorn wavepackets approximations, see Hagedorn (1998). The Hagedorn wavepackets are better suited for the dynamics in higher dimensional spaces as the tensor product of Gauss-Hermite functions. The Hagedorn wavepackets can be written in terms of Gauss-Hermite functions and hence the approximation properties are equivalent, see Hagedorn (1998) .

Here, we stick to the investigation of the convergence of the spectral and pseudo-spectral method in the context of the parameter dependent Gauss-Hermite basis. We start from the basic approximation results using Hermite functions on $\mathbb{R}$ of Guo *et al.* (2003). In comparison to earlier papers Guo (1999), Guo & Xu (2000), they insist on the importance of avoiding non-uniform weighted Sobolev norms. As for the Dirac equation, this fact is important for us, too, since we are very concerned about the conservation properties of the numerical solution.

We consider the reduced Schrödinger equation for the nuclei, see for instance Teufel (2003), Hagedorn & Joye (2006) on the whole space $\mathbb{R}$

$$i\varepsilon\partial_t u = -\frac{\varepsilon^2}{2m}\Delta u + Vu \tag{1.1}$$

with initial value u^0, where m denotes the mass of the particle, $\Delta = \partial_{xx}$ is the Laplace operator on $\mathbb{R}$, $V = V(x) \in \mathbb{R}$ is the potential function, and ε denotes the Planck constant. This equation is a hamiltonian partial differential equation, and it is well known that the L^2-norm of its solution remain constant in time.

Assume given a finite dimensional linear approximation manifold $\mathscr{V}_N \subset L^2$. The corresponding variational approximation problem (see Lubich (2004, 2005)) can be stated as follows: Find $u_N(t,\cdot) \in \mathscr{V}_N$ such that for all time $t \geq 0$,

$$\begin{aligned} &i\varepsilon\frac{d}{dt}\langle u_N(t), v_N\rangle = \langle Hu_N(t), v_N\rangle \text{ for all } v_N \in \mathscr{V}_N\,, \\ &u_N(0,\cdot) = u_N^0(\cdot)\,, \end{aligned} \tag{1.2}$$

where $u_N^0 \in \mathscr{V}_N$. Here, $H = -\frac{\varepsilon^2}{2m}\Delta + V$ and $\langle u, v\rangle = \int_{\mathbb{R}} u(x)\bar{v}(x)\mathrm{d}x$ denotes the L^2 hermitian product on $\mathbb{R}$. It can be easily shown that if $\mathscr{V}_N$ is a complex subspace of L^2 in the sense where for all $v_N \in \mathscr{V}_N$, we have $iv_N \in \mathscr{V}_N$, then the L^2-norm of the solution is preserved: $\|u_N(t)\| = \|u_N^0\|$ for all $t \geq 0$.

The goal of this paper is to give error estimates between the solution $u(t)$ of the Schrödinger equation (1.1) and the solution of (1.2) in the case where $\mathscr{V}_N$ is the complex space spanned by Gauss-Hermite function $\varphi_n(x)$, $n = 0, \ldots, N$, of the form

$$\varphi_n(x) = \pi_n(x) \exp\left(\frac{i}{\varepsilon}(a|x-q|^2 + p(x-q))\right), \tag{1.3}$$

where $a = \alpha + i\beta$ is a complex parameter (with $\beta > 0$ denoting the width of the Gaussian), $q \in \mathbb{R}$ and $p \in \mathbb{R}$ the position and momentum parameter of the Gaussian. The terms $\pi_n(x)$ are polynomials of degree n depending on the parameters a, p, q, and of the classical Hermite polynomials. We also address the same question when (1.2) is approximated by using a pseudo-spectral discretisation, i.e. when the L^2 product is replaced by a discrete product involving collocation points associated with the Gauss-Hermite polynomials.

The convergence results obtained below give bounds for the numerical approximation of (1.1) using Gauss-Hermite functions, with estimates depending explicitly of the parameters a, q, p, ε and m. Allowing the parameters a, p and p to evolve with time would give the approximation of (1.1) by Gauss-Hermite wavepacket for which we give a numerical algorithm in Faou *et al.* (2007). Our result can hence been understood as a first step to show the convergence of the fully discrete algorithm in Faou *et al.* (2007). Note that the extension of these results to higher space dimensions and the approximation by Hagedorn polynomials (see Hagedorn (1998)) may be made using the same techniques. However, the practical implementation in higher dimensions uses *sparse* decompositions of the wave function, making the approach rather different from the one-dimensional case, see Faou *et al.* (2007).

The paper is organised as follows: In Section 2, we consider a simplified situation, where $\varepsilon = m = 1$ and $a = i/2$, $p = q = 0$. This allows us to introduce the basic concepts of the approximation results. We then deal with the general Gauss-Hermite functions (1.3) and give estimates depending explicitly on the various parameters. Note that one of the difficulties comes from the oscillatory part in the Gaussian (1.3). In both cases, the convergence estimates rely on a regularity assumption on the exact solution of (1.1). In Section 3, we consider the pseudo-spectral approximation of (1.2) using quadrature collocation points, and show similar estimates. Finally, we give numerical examples for fixed parameters a, p and q and we compare them with the simulations obtained by the algorithm in Faou *et al.* (2007).

2 Decomposition and spectral method

We start with a general approximation estimate. Let $\mathscr{V}_N$ be a finite dimensional subspace of L^2, and let $P_N : L^2 \longrightarrow \mathscr{V}_N$ be the L^2-orthogonal projector onto $\mathscr{V}_N$ defined by the relation

$$\langle P_N u, v_N \rangle = \langle u, v_N \rangle, \quad \forall v_N \in \mathscr{V}_N,$$

and let R_N be the approximation error operator defined by $R_N u = u - P_N u$.

Let $u(t)$ and $u_N(t)$ be solutions of (1.1) and (1.2) respectively, and let $e_N(t) =$

$P_N u(t) - u_N(t)$. If u^0 is smooth enough, the solution $u(t)$ satisfies in particular

$$i\varepsilon \frac{d}{dt} \langle u(t), v_N \rangle = \langle Hu(t), v_N \rangle \text{ for all } v_N \in \mathscr{V}_N . \tag{2.1}$$

Substracting this equality from (1.2), we get

$$i\varepsilon \left\langle \frac{d}{dt} e_N(t), v_N \right\rangle = \langle He_N(t), v_N \rangle + \langle HR_N u(t), v_N \rangle \text{ for all } v_N \in \mathscr{V}_N .$$

This shows that

$$\begin{aligned} \frac{\varepsilon}{2} \frac{d}{dt} \|e_N(t)\|^2 &= \varepsilon \Re \left\langle \frac{d}{dt} e_N(t), e_N(t) \right\rangle \\ &= \Re \langle -iHe_N(t), e_N(t) \rangle + \Re \langle -iHR_N u(t), e_N(t) \rangle . \end{aligned}$$

As the left hand side is real as well as $\langle He_N(t), e_N(t) \rangle$ for real potential V, it must hold

$$\frac{\varepsilon}{2} \frac{d}{dt} \|e_N(t)\|^2 = \Re \langle -iHR_N u(t), e_N(t) \rangle .$$

If we are able to write now $H = L + W$ such that for all t,

$$\langle LR_N u(t), e_N(t) \rangle = 0 , \tag{2.2}$$

then the problem is reduced to the estimation of $\|WR_N u(t)\|$, because

$$\frac{\varepsilon}{2} \frac{d}{dt} \|e_N(t)\|^2 = \Re \langle -iWR_N u(t), e_N(t) \rangle \leq \|WR_N u(t)\| \, \|e_N(t)\| . \tag{2.3}$$

As it will be of constant use throughout the rest of this work, we recall here the following comparison result:

LEMMA 2.1 let $f : \mathbb{R} \to \mathbb{R}_+$ a continuous function, and $y : \mathbb{R} \to \mathbb{R}_+$ a differentiable function satisfying the inequality

$$\forall t \in \mathbb{R}, \quad \frac{d}{dt} y(t) \leq 2 f(t) \sqrt{y(t)}.$$

Then we have the estimate

$$\forall t \in \mathbb{R}, \quad \sqrt{y(t)} \leq \sqrt{y(0)} + \int_0^t f(s) ds.$$

Proof. For all $\eta > 0$, we easily show (see e.g. Hairer *et al.* (2006), Sec. I.10)

$$\forall t \in \mathbb{R}, \quad \sqrt{y(t)} \leq \sqrt{(y(0) + \eta)} + \int_0^t f(s) ds,$$

which yields the result by letting $\eta \to 0$. ∎

Using this lemma, Eqn. (2.3) with a bounded function W yields

$$\|u(t) - u_N(t)\| \leq \|e_N(0)\| + \|R_N u(t)\| + \frac{1}{\varepsilon} C_W \int_0^t \|R_N u(s)\| \, ds , \tag{2.4}$$

with $C_W = \|W\|_{L^\infty}$. Hence, we see that the error due to the space discretisation in the Schrödinger equation is controlled by the operator R_N. Let us note that the condition of a bounded W may be relaxed to the integrability of $\|WR_N u(s)\|$ with the corresponding change in the constants.

Note that the condition (2.2) will be satisfied if L send $\mathscr{V}_N^\perp$ to itself. This will be the case in the simplified situation studied in the next section, where L will be the hamiltonian associated with the harmonic oscillator. For general Gaussian wave packets with arbitrary parameters, the orthogonality condition (2.2) will not be exactly fulfilled for the natural splitting between the kinetic and potential operators. Nevertheless, the induced error will be small allowing us to obtain an error estimate.

2.1 Spectral Hermite Method

In this subsection, we consider the simplified situation where $\varepsilon = m = 1$ in the equation (1.1). We consider the **Hermite functions**:

$$\chi_n(x) = e^{-x^2/2} H_n(x)\,, \tag{2.5}$$

where for all $n \geq 0$, H_n denotes the nth Hermite polynomial defined recursively by the formula

$$H_{n+1} - 2xH_n + 2nH_{n-1} = 0\,, \quad H_0 = 1 \quad \text{and} \quad H_1 = 2x. \tag{2.6}$$

The functions (2.5) are the eigenfunctions of the problem

$$e^{x^2/2}\partial_x(e^{-x^2/2}\partial_x\chi_n + xe^{-x^2/2}\chi_n) + \lambda_n\chi_n = 0$$

associated with the eigenvalue $\lambda_n = 2n$. The derivative of the Hermite function may be written in terms of other Hermite functions:

$$\chi_n' = 2n\chi_{n-1} - x\chi_n = x\chi_n - \chi_{n+1} = n\chi_{n-1} - \frac{1}{2}\chi_{n+1}\,, \text{ for } n \geq 1\,. \tag{2.7}$$

Clearly, the Hermite functions are orthogonal in $L^2(\mathbb{R})$:

$$\int_{\mathbb{R}} \chi_n(x)\chi_m(x)dx = 2^n n!\sqrt{\pi}\delta_{nm}\,, \tag{2.8}$$

Moreover, a careful computation shows that

$$\left(-\frac{1}{2}\partial_{xx}^2 + \frac{1}{2}x^2\right)\chi_n(x) = (n+\frac{1}{2})\chi_n(x)\,, \tag{2.9}$$

that is, the Hermite basis diagonalises the problem of the harmonic oscillator.
We consider $\mathscr{V}_N = \text{span}\{\chi_0, \ldots, \chi_N\}$ and see any $u \in L^2$ as

$$u(x) = \sum_{k\leq N} \hat{u}_k\chi_k(x) + \sum_{k\geq N+1} \hat{u}_k\chi_k(x) = P_N u(x) + R_N u(x)\,, \tag{2.10}$$

where for all $k \geq 0$,

$$\hat{u}_k = \frac{1}{2^k k! \sqrt{\pi}} \langle u, \chi_k \rangle .$$

Let us denote the differential operator related to the Hermite functions by $Au = u' + xu$. Guo *et al.* (2003) proved that the approximation error is of order $N^{-r/2}$ with r depending on smoothness assumptions on u. Since it is a result of fundamental importance for our paper we give here the proof, together with a previously unexposed estimation of the optimal constant:

LEMMA 2.2 Assume that for $r \geq 1$, we have $A^r u \in L^2$. Then for $N \geq r-1$ we have the estimate

$$\|R_N u\| \leq C_r N^{-r/2} \|A^r u\| ,$$

with the constant $(C_1)^2 < 0.5$, $(C_2)^2 < 0.25$ and

$$(C_{2+p})^2 = 0.25 \cdot 2^{-p} \frac{(p+1)^{p+2}}{(p+2)!} , \text{ if } p \geq 1.$$

Proof. The orthogonality of the Hermite functions gives

$$\|R_N u\|^2 = \sum_{k \geq N+1} c_k |\hat{u}_k|^2 ,$$

with $c_k = 2^k k! \sqrt{\pi}$. By the orthogonality of the Hermite functions and the eigenvalue property we have for $k \geq 1$:

$$\hat{u}_k = \frac{1}{c_k} \int_{\mathbb{R}} u(x) \chi_k(x) dx = -\frac{1}{2k} \frac{1}{c_k} \int_{\mathbb{R}} u(x) e^{x^2/2} \partial_x \left(e^{-x^2/2} A \chi_k(x) \right) dx .$$

Integration by parts and the decay conditions at ∞ for u give

$$\hat{u}_k = \frac{1}{2k} \frac{1}{c_k} \int_{\mathbb{R}} Au(x) A\chi_k(x) dx = \frac{1}{c_k} \int_{\mathbb{R}} Au(x) \chi_{k-1} dx ,$$

using the first relation (2.7) which can be written $A\chi_k = 2k\chi_{k-1}$ for $k \geq 1$. This argument repeats giving

$$c_k \hat{u}_k = \int_{\mathbb{R}} A^r u(x) \chi_{k-r}(x) dx \text{ with } r \geq 1.$$

We substitute this expression in $\|R_N u\|^2$ in order to get

$$\|R_N u\|^2 = \sum_{k \geq N+1} \frac{c_{k-r}}{c_k} \cdot c_{k-r} \left| \frac{1}{c_{k-r}} \int_{\mathbb{R}} A^r u(x) \chi_{k-r}(x) dx \right|^2 .$$

Hence, we have

$$\|R_N u\|^2 = \sum_{k \geq N+1} \frac{c_{k-r}}{c_k} \cdot c_{k-r} |\widehat{(A^r u)}_{k-r}|^2 .$$

As $A^r u$ is in L^2, we obtain

$$\|R_N u\|^2 \leq \max_{k \geq N+1} \frac{c_{k-r}}{c_k} \cdot \|A^r u\|^2 .$$

We then get $\|R_N u\|^2 \leq g(N,r)\,\|A^r u\|^2$, where

$$g(N,r) := \max_{k\geq N+1} \frac{c_{k-r}}{c_k} = \frac{2^{-r}}{(N+1)N\ldots(N-r+2)} \text{ for } r \geq 1\,. \tag{2.11}$$

In the cases $r=1$ and $r=2$ we easily get the announced bounds for the constants C_r. If $r = 2+p$, with $p \geq 1$, one can show that

$$g(N,r)\cdot N^r = \frac{1}{4}\frac{N}{N+1}\prod_{j=0}^{p}\frac{N}{2(N-j)}$$

is decreasing in $N \geq p+1$. This yields the general expression of C_{2+p}. Let us note that for reasonable moderate $p \in \{1,2,\ldots,14\}$ we have really small constants, such that $C_{2+p} < 0.5$. ■

Assume now that the potential can be written $V = \frac{1}{2}x^2 + W$ with a bounded function W. Denoting $L = -\frac{1}{2}\Delta + \frac{1}{2}x^2$, the hamiltonian H splits into $H = L + W$, and we have using (2.9), for all u sufficiently smooth,

$$LR_N u = L\sum_{k\geq N+1}\hat{u}_k\chi_k(x) = \sum_{k\geq N+1}\hat{u}_k(k+\frac{1}{2})\chi_k(x)$$

that is orthogonal on $\mathscr{V}_N$.

Using the previous lemma and (2.4), we easily get the following result:

THEOREM 2.1 Let $u(t)$ be a solution of (1.1) with $\varepsilon = m = 1$, and with a potential $V(x) = \frac{1}{2}x^2 + W(x)$ where W is bounded. Let $u_N(t)$ be the solution of (1.2) associated with the manifold $\mathscr{V}_N = \text{span}\{\chi_0,\ldots,\chi_n\}$, and with initial value $u_N^0 = P_N u(0)$. Let $r \geq 1$, and assume that the function $t \mapsto A^r u(t)$ is continuous from $\mathbb{R}$ to L^2, then we have the following bound, for all $t \geq 0$,

$$\|u(t) - u_N(t)\| \leq C_r N^{-r/2}\Big(\,\|A^r u(0)\| + \|A^r u(t)\| + C_W\int_0^t \|A^r u(s)\|\,ds\Big),$$

provided the right-hand side makes sense, where $C_W = \|W\|_{L^\infty} < \infty$ and where C_r is the constant appearing in Lemma 2.2.

2.2 Gauss-Hermite Wave-packet

For fixed numbers $a = \alpha + i\beta \in \mathbb{C}$ with $\beta > 0$, $p \in \mathbb{R}$ and $q \in \mathbb{R}$, let $\varphi(x)$ be the Gaussian function

$$\varphi(x) = \exp\left(\frac{i}{\varepsilon}(a|x-q|^2 + p(x-q))\right). \tag{2.12}$$

In Faou *et al.* (2006), such functions are used to approximate the Schrödinger equation (1.1) using Gaussian-wave packets dynamics. A natural extension is to consider the natural Hermite basis associated with (2.12): For all $N \geq 0$, we consider the linear subspace $\mathscr{V}_N$ spanned by

$$\varphi_n(x) = \varphi(x)\cdot\sqrt{\zeta}\,d_n H_n(\zeta(x-q))\,, \quad n = 0,1,\ldots,N\,, \tag{2.13}$$

with $\zeta = \sqrt{\frac{2\beta}{\varepsilon}}$, where H_n are the hermite polynomials defined by (2.6), and where $d_n = 1/\sqrt{2^n n! \sqrt{\pi}}$ is a normalising constant. The functions (2.13) are generalisations of the Hermite functions (2.5). Note that the shift in the functions (2.13) corresponds to the shift made in the Gaussian (2.12), whose real part is $\exp(-\beta(x-q)^2/\varepsilon)$. We then expect the previous functions to satisfy orthogonality properties inherited from the structure of Hermite functions.

Denoting $y = \sqrt{\frac{2\beta}{\varepsilon}}(x-q) = \zeta(x-q)$, we write the basis function

$$\varphi_n(x) = \sqrt{\zeta} d_n H_n(y) e^{-\frac{1}{2}y^2} \omega(y) = \sqrt{\zeta} d_n \chi_n(y) \omega(y), \tag{2.14}$$

where $\omega(y)$ is the oscillatory part of the Gaussian wave packet, namely

$$\omega(y) = \exp\left(\frac{i}{\varepsilon}\left(\frac{\alpha}{\zeta^2}y^2 + \frac{p}{\zeta}y\right)\right).$$

In this situation, the basis functions φ_n are no longer the eigenfunctions of an obvious operator as in the previous case. However, as $|\omega| = 1$, we see that for all $n, m \geq 0$, $\langle \varphi_n, \varphi_m \rangle = \delta_{nm}$ using the change of variable $x \mapsto y$ and the properties of the Hermite functions χ_n.

For any $u \in L^2$, we decompose

$$u(x) = \sum_{k \leq N} \tilde{u}_k \varphi_k(x) + \sum_{k \geq N+1} \tilde{u}_k \varphi_k(x) = \tilde{P}_N u(x) + \tilde{R}_N u(x),$$

with the coefficients $\tilde{u}_k = \langle \varphi_k, u \rangle$, where $\tilde{P}_N$ and $\tilde{R}_N$ are the corresponding projection and error operators.

Let us consider the transformation Tu defined by

$$Tu(y) = (\omega(y)\sqrt{\zeta})^{-1} u(q + \frac{1}{\zeta}y). \tag{2.15}$$

As $|\omega|^2 = 1$ and $dy = \zeta dx$, we see that T is an isometry of L^2: for functions f and g,

$$\langle Tf, Tg \rangle = \langle f, g \rangle.$$

Moreover, from (2.14), we have

$$T\varphi_n = d_n \chi_n.$$

This implies that

$$\tilde{u}_n = \langle \varphi_n, u \rangle = \langle T\varphi_n, Tu \rangle = d_n \langle \chi_n, v \rangle = d_n^{-1} \hat{v}_n, \tag{2.16}$$

where $v = Tu$ and where $\hat{v}_k$ denotes as before the coefficients in the decomposition $v = \sum_{k \geq 0} \hat{v}_k \chi_k$, see (2.10).

With these notations, we have for all $k \geq 0$, $\tilde{u}_k T\varphi_k = \hat{v}_k \chi_k$, and hence

$$\tilde{P}_N = T^{-1} P_N T \quad \text{and} \quad \tilde{R}_N = T^{-1} R_N T. \tag{2.17}$$

Using Lemma 2.2, the approximation error reads then in the parameter dependent setting, for $N \geq r-1$,

$$\left\|\tilde{R}_N u\right\| = \left\|T\tilde{R}_N u\right\| = \|R_N T u\| \leq C_r N^{-r/2} \|A^r v\| . \tag{2.18}$$

We require now some regularity on the solution of the continuous Schrödinger equation:

$$|u|_r^2 := \sum_{n\geq r} 2^r n(n-1)\dots(n-r+1)|\tilde{u}_n|^2 < \infty. \tag{2.19}$$

This condition is linked to the Hermite decomposition and the regularity of the related function $v = Tu$. Remember the differential operator related to the Hermite functions $Au = u' + xu$. By the recursion formula (2.6) we have that $A\chi_n = 2n\chi_{n-1}$ and hence $Av = \sum_{n\geq 0} \hat{v}_n A\chi_n = \sum_{n\geq 1} 2n\hat{v}_n\chi_{n-1}$. Using this iteratively, we get using (2.8) and (2.16),

$$\begin{aligned}
\|A^r v\|^2 &= \sum_{n\geq r} \left(2^r n(n-1)\dots(n-r+1)\right)^2 c_{n-r}|\hat{v}_n|^2 \\
&= \sum_{n\geq r} \left(2^r n(n-1)\dots(n-r+1)\right)^2 c_{n-r}c_n^{-1}|\tilde{u}_n|^2 \\
&= \sum_{n\geq r} 2^r n(n-1)\dots(n-r+1)|\tilde{u}_n|^2 ,
\end{aligned}$$

where as before $c_k = 2^k k!\sqrt{\pi} = d_k^{-2}$. Shortly, this means that

$$\|A^r Tu\| = |u|_r . \tag{2.20}$$

Hence, the norm $|u|_r$ is just equivalent to the norm $\|A^r v\|$ applied to the scaled function $v = Tu$ (note that the regularity assumptions on u and $v = Tu$ are equivalent). This observation brings the approximation error in the parameter dependent case from (2.18) to the form

$$\left\|\tilde{R}_N u\right\| \leq cN^{-r/2}|u|_r . \tag{2.21}$$

Here, and in the following, c denote a generic constant independent of N.

We now want to derive an estimate similar to (2.4).We begin with the following result:

LEMMA 2.3 The kinetic part of the basis function φ_n may be split:

$$-\frac{\varepsilon^2}{2m}\Delta\varphi_n(x) = \frac{1}{2m}\left[2\bar{a}(x-q)+p\right]^2\varphi_n(x) + \mathscr{L}(\varphi_n, \varphi_{n+1}, \varphi_{n+2}) ,$$

where $\mathscr{L}(\varphi_n, \varphi_{n+1}, \varphi_{n+2})$ is a linear combination of φ_n, φ_{n+1} and φ_{n+2} with coefficients depending on a, p, q, n and ε.

Proof. Using (2.14), we have

$$\Delta\varphi_n = \zeta^{5/2} d_n \left[\Delta\chi_n(y)\omega(y) + 2\partial_x\chi_n(y)\cdot\partial_x\omega(y) + \chi_n(y)\Delta\omega(y)\right] .$$

The second derivative of the Hermite function may be computed using the recurrence relations (2.7) and (2.6) as

$$\begin{aligned}\Delta\chi_n(y) &= \partial_x(y\chi_n(y)-\chi_{n+1}(y))\\ &= \chi_n(y)+y\partial_x\chi_n(y)-\partial_x\chi_{n+1}(y)\\ &= \chi_n(y)+y(y\chi_n(y)-\chi_{n+1}(y))-((n+1)\chi_n(y)-\frac{1}{2}\chi_{n+2}(y))\,.\end{aligned}$$

We focus only on the terms that contain the factors y or y^2, since the other are just linear combinations of Hermite functions χ_m with $m \geq n$. Remark that

$$y\chi_{n+1}(y) = (n+1)\chi_n(y)+\frac{1}{2}\chi_{n+2}(y)\,,$$

and consequently, the first term in $\Delta\varphi_n$ is

$$d_n\Delta\chi_n(y)\omega(y)\zeta^{5/2} = \varphi_n(x)\zeta^2y^2+\text{linear}(\varphi_n,\varphi_{n+1},\varphi_{n+2})\,,$$

where the last term will enter into the definition of the operator $\mathscr{L}$. The second term in $\Delta\varphi_n$ is

$$\begin{aligned}2d_n\partial_x\chi_n(y)\cdot\partial_x\omega(y)\zeta^{5/2} &= 2d_n(y\chi_n(y)-\chi_{n+1}(y))\omega(y)(2\alpha y+p\zeta)\frac{i}{\varepsilon}\sqrt{\zeta}\\ &= \frac{i}{\varepsilon}\varphi_n(x)\cdot 2y(2\alpha y+p\zeta)+\text{linear}(\varphi_n,\varphi_{n+1},\varphi_{n+2})\,.\end{aligned}$$

The last term in $\Delta\varphi_n$ is

$$d_n\chi_n(y)\Delta\omega(y)\zeta^{5/2} = \varphi_n(x)\left(\frac{2\alpha}{\zeta}y+p\right)^2\left(\frac{i}{\varepsilon}\right)^2+\varphi_n(x)\cdot 2\alpha\frac{i}{\varepsilon}\,.$$

Altogether, we obtain

$$\Delta\varphi_n(x) = \varphi_n(x)\left[\left(\zeta+\frac{2\alpha}{\zeta}\frac{i}{\varepsilon}\right)y+p\frac{i}{\varepsilon}\right]^2+\text{linear}(\varphi_n,\varphi_{n+1},\varphi_{n+2})\,,$$

that gives the result of the lemma. ■

In comparison with the previous subsection, we cannot decompose the hamiltonian H, which is independent on p and q, into $L+W$ with L acting on $\mathscr{V}_N^\perp$. However, we can always split the operator H as $H = K+V$ where V is the potential and $K = -\frac{\varepsilon^2}{2m}\Delta$. In the following, we assume that the potential V is bounded. In this situation, the orthogonal condition (2.2) is no longer exactly fulfilled:

LEMMA 2.4 Let c_n, $n = 0,\ldots,N$ be given complex numbers, and let $w_N = \sum_{n=0}^{N} c_n\varphi_n \in \tilde{\mathscr{V}}_N$.Then we have

$$\begin{aligned}\left\langle K\tilde{R}_N u, w_N\right\rangle &= s_1\sqrt{N+1}\tilde{u}_{N+1}\bar{c}_N+\\ &\quad s_2\left(\sqrt{N(N+1)}\tilde{u}_{N+1}\bar{c}_{N-1}+\sqrt{(N+1)(N+2)}\tilde{u}_{N+2}\bar{c}_N\,,\right)\end{aligned}$$

with $s_1 = \frac{\bar{a}p\sqrt{2}}{m\zeta}$ and $s_2 = \frac{\vec{a}^2}{m\zeta^2}$.

Proof. The previous Lemma gives

$$\left\langle K\tilde{R}_N u, w_N \right\rangle = \frac{2\bar{a}p}{m}\left\langle \sum_{n\geq N+1}(x-q)\tilde{u}_n\varphi_n, w_N \right\rangle + \frac{2\vec{a}^2}{m}\left\langle \sum_{n\geq N+1}(x-q)^2\tilde{u}_n\varphi_n, w_N \right\rangle .$$

Using standard Gaussian calculus, we compute the following momenta integrals:

$$\langle \varphi_n \,|\, (x-q) \,|\, \varphi_m \rangle = \begin{cases} \dfrac{1}{\zeta}\sqrt{\dfrac{n+1}{2}} & \text{if} \quad m = n+1, \\ 0 & \text{otherwise,} \end{cases} \tag{2.22}$$

$$\langle \varphi_n \,|\, (x-q)^2 \,|\, \varphi_m \rangle = \begin{cases} \dfrac{1}{2\zeta^2}(2n+1) & \text{if} \quad m = n, \\ \dfrac{1}{2\zeta^2}\sqrt{(n+1)(n+2)} & \text{if} \quad m = n+2, \\ 0 & \text{otherwise,} \end{cases} \tag{2.23}$$

and the result follows. ∎

We make the smoothness assumption $|u|_{2+r} < \infty$, with $r \geq 1$. Even if the first part of the splitting is no longer zero, the previous lemma gives us the upper bound, for $N \geq r$,

$$|\left\langle K\tilde{R}_N u, w_N \right\rangle|^2 \leq f(N,r)\left[\frac{|s_1|^2}{N} + |s_2^2|\right]\cdot |u|_{2+r}^2 \cdot \|w_N\|^2 ,$$

with $f(N,0) = 2^{-1}$ and (see (2.11))

$$f(N,r) = \frac{2^{-(r+1)}}{(N-1)\ldots(N-r)} = \frac{1}{2}g(N-2,r) \text{ for } r \geq 1 .$$

This justify again the use of the regularity condition (2.19). The upper bound for $g(N-2,r)$ yields finally

$$|\left\langle K\tilde{R}_N u, w_N \right\rangle|^2 \leq CN^{-r}\left[\frac{|s_1|^2}{N} + |s_2|^2\right]\cdot |u|_{2+r}^2 \|w_N\|^2 , \tag{2.24}$$

where C is a constant depending on r and $C < 1$ for $r \in \{1,\ldots,14\}$.

Now, let $u(t)$ be a solution of (1.1) and $v_N(t)$ be the solution of (1.2) associated with the manifold $\tilde{\mathscr{V}_N}$ and initial value $v_N(0) = \tilde{P}_N u(0)$, and let $e_N(t) = \tilde{P}_N u(t) - v_N(t)$. We obtain

$$\begin{aligned} \varepsilon\frac{d}{dt}\|e_N(t)\|^2 &= \Re\left\langle -i(K+V)\tilde{R}_N u(t), e_N(t)\right\rangle \\ &\leq |\left\langle (K+V)\tilde{R}_N u(t), e_N(t)\right\rangle| \\ &\leq \sqrt{C}N^{-r/2}\sqrt{\frac{|s_1|^2}{N} + |s_2|^2}\cdot |u(t)|_{2+r}\|e_N(t)\| \\ &\qquad + C_V\left\|\tilde{R}_N u(t)\right\|\|e_N(t)\| , \end{aligned}$$

with the upper bound $C_V = \|V\|_{L^\infty}$ and the regularity $r \geq 1$. We now use the upper bound for the spectral approximation (2.18) with $r+2$ in order to get, using Lemma 2.1,

$$\varepsilon \|e_N(t)\| \leq \varepsilon \|e_N(0)\| + cN^{-r/2} \left(\frac{C_V}{N} + \sqrt{\frac{|s_1|^2}{N} + |s_2|^2} \right) \int_0^t |u(\xi)|_{2+r} d\xi \,.$$

The conclusion is that under the $(r+2)$-regularity assumption on the exact solution $u(t)$ for a bounded potential V, the error in the Gauss-Hermite spectral discretisation of the Schrödinger equation stay of order $N^{-r/2}$. Note that there is a lose of accuracy when compared to (2.18), where less regularity is required to obtain this rate of convergence.

THEOREM 2.2 Let $u(t)$ be a solution of (1.1) such that $|u|_r$ is continuous, and $|u|_{r+2} \in L^1(0,t)$, for $r \geq 1$ and $t > 0$. Let $v_N(t)$ be the solution of (1.2) associated with the manifold $\tilde{\mathscr{V}}_N$ and initial value $v_N(0) = \tilde{P}_N u(0)$. Then for $t \geq 0$ and $N \geq r$, the estimate of the error reads

$$\begin{aligned} \|u(t) - v_N(t)\| \quad \leq \quad & cN^{-r/2}(|u(t)|_r + |u(0)|_r) + \\ & cN^{-r/2} \left(\frac{C_V}{N\varepsilon} + \frac{|a|}{2m} \sqrt{\frac{2}{N\varepsilon} \frac{p^2}{\beta} + \frac{1}{\beta^2}} \right) \int_0^t |u(\xi)|_{2+r} d\xi \,, \end{aligned}$$

with global constant c independent of N and t, and upper bound C_V for the potential V.

3 Pseudo-spectral method

In concrete applications, we cannot in general compute exactly the right hand side of (1.2), and we use a quadrature rule for the part involving the potential.

3.1 Pseudo-spectral Hermite Method for the simplified Schrödinger equation

Consider again the case of the simplified Schrödinger equation ($\varepsilon = 1$ and $m = 1$) with the potential $V(x) = \frac{1}{2}x^2 + W(x)$ with a bounded function W. Note that the Hermite basis diagonalises the operator $L = -\frac{1}{2}\Delta + \frac{1}{2}x^2$, but the integral $\langle Wu_N, v_N \rangle$ has to be approximated by the Gauss quadrature. This involves the grid $\Gamma_M = \{\gamma_0^M, \ldots \gamma_M^M\}$ formed by the $(M+1)$-zeros of the Hermite polynomial H_{M+1} and the Hermite-Gauss weights $\omega_\gamma = \rho_\gamma e^{\gamma^2}$ with the Christoffel-numbers (ρ_γ)t, with $\gamma \in \Gamma_M$. (see Tang (1993) and Section 3.3 below).

Let f be a polynomial of degree less or equal with $2M+1$ and $g(x) = f(x)e^{-x^2}$. The Gauss-Hermite quadrature is then exact:

$$\int_{\mathbb{R}} g(x)dx = \int_{\mathbb{R}} f(x)e^{-x^2}dx = \sum_{\gamma \in \Gamma_M} f(\gamma)\rho_\gamma =: G_M(g) \,.$$

Denote by $\|\cdot\|_M$ the discrete norm induced by the Gauss-Hermite quadrature formula

$$(u,v)_M = \sum_{\gamma\in\Gamma_M} u(\gamma)v(\gamma)\omega_\gamma, \qquad \|u\|_M = (u,u)_M^{1/2} \tag{3.1}$$

and by $\mathscr{I}_M$ the Hermite interpolant on the points Γ_M:

$$\begin{aligned} \mathscr{I}_M v &\in \mathscr{V}_M := \text{span}\{\chi_0,\ldots,\chi_M\} \\ \mathscr{I}_M v(\gamma) &= v(\gamma), \text{ for } \gamma\in\Gamma_M. \end{aligned}$$

Clearly $\|\mathscr{I}_M v\| = \|\mathscr{I}_M v\|_M = \|v\|_M$. We need the following two results for the Hermite-interpolation from Guo *et al.* (2003):

$$\|\mathscr{I}_M v - v\|_{H^\mu} \leq cM^{1/3+(\mu-r)/2}\|A^r v\|, \text{ for } 0\leq\mu\leq r, \text{ and } r\geq 1; \tag{3.2}$$

$$\|v\|_M \leq c(\|v\| + M^{-1/6}|v|_{H^1}), \tag{3.3}$$

with Sobolev semi-norm $|\cdot|_{H^1}$ and norm $\|\cdot\|_{H^\mu}$. The derivation of the constants is less obvious here that in the previous section. This is why from now on we denote by c a generic constant. However, it is not difficult to see from Guo *et al.* (2003) that for $\mu = 0$ and moderate $r\in\{1,\ldots,14\}$ the constant in (3.2) is strictly less than 1, while it rapidly deteriorates for $\mu > 2$.

We consider now again a solution $u(t)$ of (1.1) with $\varepsilon = m = 1$. Let us now carry out the error analysis of the collocation on the points from Γ_M of the simplified Schrödinger equation. Let $M\geq N$ be fixed. We consider the problem :

$$\begin{aligned} &\text{find } u_N^c(t)\in\mathscr{V}_N \text{ such that} \\ &i\frac{d}{dt}(u_N^c(t),v_N)_M = (Lu_N^c(t),v_N)_M + (Wu_N^c(t),v_N)_M \text{ for all } v_N\in\mathscr{V}_N, \\ &u_N^c(0) = P_N\mathscr{I}_M u(0), \end{aligned} \tag{3.4}$$

where P_N is the projection operator defined in (2.10). Note that due to the exactness property of the Gauss quadrature, we have for all function u,

$$P_N\mathscr{I}_M u = \sum_{k=0}^{N}\frac{1}{c_k}\langle\mathscr{I}_M u,\chi_k\rangle\chi_k = \sum_{k=0}^{N}\frac{1}{c_k}(u,\chi_k)_M\chi_k,$$

with $c_k = 2^k k!\sqrt{\pi}$. Similarly, we rewrite the previous collocation equation as

$$\begin{aligned} &\text{find } u_N^c(t)\in\mathscr{V}_N \text{ such that} \\ &i\frac{d}{dt}\langle u_N^c(t),v_N\rangle = \langle Lu_N^c(t),v_N\rangle + \langle\mathscr{I}_M(Wu_N^c(t)),v_N\rangle \text{ for all } v_N\in\mathscr{V}_N, \\ &u_N^c(0) = P_N\mathscr{I}_M u(0). \end{aligned} \tag{3.5}$$

Remember from the decomposition method that we have for the exact solution $u(t) = P_N u(t) + R_N u(t)$ with both $R_N u(t)$ and $LR_N u(t)$ being orthogonal on the approximation space $\mathscr{V}_N$. Hence

$$i\frac{d}{dt}\langle P_N u(t),v_N\rangle = \langle LP_N u(t),v_N\rangle + \langle Wu(t),v_N\rangle \text{ for all } v_N\in\mathscr{V}_N.$$

Subtracting the last two equations, we obtain the equation for the error $e_N^c(t) = P_N u(t) - u_N^c(t)$:

$$i\frac{d}{dt}\langle e_N^c(t), v_N\rangle = \langle Le_N^c(t), v_N\rangle + \langle Wu(t) - \mathscr{I}_M(Wu_N^c(t)), v_N\rangle \text{ for all } v_N \in \mathscr{V}_N\,. \quad (3.6)$$

We derive now an upper bound for the error, as in the previous section.

LEMMA 3.1 With the previous notations, the following inequality holds

$$\|e_N^c(t)\| \le \|e_N^c(0)\| + cN^{1/3-r/2}\int_0^t (\|A^r(Wu(s))\| + \|A^r u(s)\|)\,ds + C_W\int_0^t \|e_N^c(s)\|\,ds,$$

where $C_W = \|W\|_{L^\infty}$.

Proof. The decomposition (3.6) implies

$$\begin{aligned}\frac{d}{dt}\|e_N^c\|^2 &\le \|Wu - \mathscr{I}_M(Wu_N^c)\|\,\|e_N^c\| &(3.7)\\ &\le \left(\|Wu - \mathscr{I}_M(WP_N u)\| + \|\mathscr{I}_M(We_N^c)\|\right)\|e_N^c\|\,. &(3.8)\end{aligned}$$

We deal now with the first term in this sum, that is

$$\|Wu - \mathscr{I}_M(WP_N u)\| \le \|Wu - \mathscr{I}_M(Wu)\| + \|\mathscr{I}_M(WR_N u)\|\,.$$

Using (3.2) with $\mu = 0$ for the first term, and (3.3) for the second term, we obtain for $r \ge 1$,

$$\|Wu - \mathscr{I}_N(WP_N u)\| \le cM^{1/3-r/2}\|A^r(Wu)\| + c(\|WR_N u\| + M^{-1/6}|WR_N u|_{H^1})\,.$$

If W and its derivative are bounded, we use again the results on the upper bound of the spectral approximation from Guo *et al.* (2003):

$$|R_N u|_{H^1} \le \|R_N u\|_{H^1} \le cN^{1/2-r/2}\|A^r u\|\,, \quad (3.9)$$

and hence, as $M \ge N$ and $r \ge 1$,

$$\|Wu - \mathscr{I}_M(WP_N u)\| \le cN^{1/3-r/2}(\|A^r(Wu)\| + \|A^r u\|)\,.$$

It remains to look at the second term in (3.8), for which we use the fact that the Gauss quadrature rule on Γ_M is exact for $M \ge N$:

$$\begin{aligned}\|\mathscr{I}_M(We_N^c)\|^2 &= \int_{\mathbb{R}} |\mathscr{I}_M(We_N^c)|^2\,dx = G_M\left(|\mathscr{I}_M(We_N^c)|^2\right) = G_M\left(|We_N^c|^2\right)\\ &\le C_W^2 G_M\left(|e_N^c|^2\right) = C_W^2\|e_N^c\|^2\,, &(3.10)\end{aligned}$$

with the upper bound C_W for the potential W.
The two terms give then for the collocation error:

$$\frac{d}{dt}\|e_N^c(t)\|^2 \le cN^{1/3-r/2}(\|A^r(Wu(t))\| + \|A^r u(t)\|)\,\|e_N^c(t)\| + C_W\|e_N^c(t)\|^2\,,$$

that brings us to the whished inequality using Lemma 2.1. ■

THEOREM 3.1 Let $u(t)$ be a solution of (1.1) with potential $V(x) = \frac{1}{2}x^2 + W(x)$ and $\varepsilon = m = 1$. Let $u_N^c(t)$ be the solution of the collocation problem (3.4) with $M \ge N$.

Assume that for $r \geq 1$, the function $t \mapsto A^r u(t)$ is continuous from $\mathbb{R}$ to L^2, $\|A^r(Wu)\| \in L^1(0,t)$ and $\|A^r u\| \in L^1(0,t)$ for all $t \geq 0$. Then the following bound for the error in the pseudo-spectral Hermite method for the simplified Schrödinger equation holds

$$\begin{aligned}\|u(t) - u_N^c(t)\| \quad \leq \quad & cN^{1/3-r/2}\left(N^{-1/3}\|A^r u(t)\| + e^{C_W t}\|A^r u(0)\|\right) + \\ & cN^{1/3-r/2}\int_0^t e^{C_W(t-s)}\left(\|A^r(Wu(s))\| + \|A^r u(s)\|\right) ds,\end{aligned}$$

for a bounded W with $C_W = \|W\|_{L^\infty}$ and $N \geq r-1$.

Proof. The Gronwall lemma and integration by parts gives then the upper bound for the collocation error at the time t:

$$\|e_N^c(t)\| \leq e^{C_W t}\|e_N^c(0)\| + cN^{1/3-r/2}\int_0^t e^{C_W(t-s)}\left(\|A^r(Wu(s))\| + \|A^r u(s)\|\right) ds.$$

We bound the first term using (3.2) with $\mu = 0$ and we find for $r \geq 1$,

$$\|e_N^c(0)\| \leq \|P_N u(0) - P_N \mathscr{I}_M u(0)\| \leq \|u(0) - \mathscr{I}_M u(0)\| \leq cM^{1/3-r/2}\|A^r u(0)\|.$$

The conclusion follows from the triangle inequality and Lemma 2.2. ■

3.2 Gauss-Hermite Collocation in the general case

We consider now the case of Gauss-Hermite wave-packets described in Section 2.2. The space approximation space is now made of the functions (2.13). We use the set of points $\tilde{\Gamma}_M = q + \frac{1}{\zeta}\Gamma_M$, that are the zeros of the Hermite polynomial $H_{M+1}(\zeta(x-q))$. We then define the corresponding interpolation operator

$$\tilde{\mathscr{I}}_M = T^{-1}\mathscr{I}_M T$$

where T is defined in (2.15) and $\mathscr{I}_M$ the interpolation operator of the previous section. We clearly have

$$\left\|w - \tilde{\mathscr{I}}_M w\right\| = \|Tw - \mathscr{I}_M Tw\|.$$

The inequality (3.2) and the relation (2.20) give then the interpolation error:

$$\left\|w - \tilde{\mathscr{I}}_M w\right\| \leq cM^{1/3-r/2}\|A^r Tw\| = cM^{1/3-r/2}|w|_r. \tag{3.11}$$

We define the bilinear form

$$\langle f,g\rangle_M := (Tf,Tg)_M = \sum_{\gamma\in\Gamma_M}(Tf)(\gamma)\overline{Tg}(\gamma)\rho_\gamma = \sum_{\gamma\in\Gamma_M}\frac{1}{\zeta}f(\tilde{\gamma})\bar{g}(\tilde{\gamma})\rho_\gamma, \tag{3.12}$$

with $\tilde{\gamma} = q + \frac{1}{\zeta}\gamma$. As in Section 2.2, we split the Schrödinger operator as $H = K + V$ with the potential function V and $K = -\frac{1}{2m}\varepsilon^2\Delta$. Analogously to the previous section, we consider the problem:

$$\begin{array}{l}\text{find } u_N^c(t) \in \tilde{\mathscr{V}}_N \text{ such that} \\ i\dfrac{d}{dt}\langle u_N^c(t), v_N\rangle_M = \langle Ku_N^c(t), v_N\rangle_M + \langle Vu_N^c(t), v_N\rangle_M \text{ for all } v_N \in \tilde{\mathscr{V}}_N, \\ u_N^c(0) = \tilde{P}_N\tilde{\mathscr{I}}_M u(0),\end{array} \tag{3.13}$$

where $\tilde{P}_N = T^{-1}P_N T$ is the orthogonal projection operator associated with the space $\tilde{\mathscr{V}}_N$, $\langle\cdot,\cdot\rangle_M$ is the bilinear form defined in (3.12), and $u(0)$ is the initial value of an exact solution $u(t)$ of (1.1).

We investigate now in which conditions the sums are exact quadrature rules.

LEMMA 3.2 If $M \geq N+1$, the problem (3.13) is equivalent to the problem

$$\begin{array}{l} \text{find } u_N^c(t) \in \tilde{\mathscr{V}}_N \text{ such that} \\ i\varepsilon \dfrac{d}{dt}\langle u_N^c(t), v_N\rangle = \langle Ku_N^c(t), v_N\rangle + \left\langle \tilde{\mathscr{I}}_M(Vu_N^c(t)), v_N\right\rangle \text{ for all } v_N \in \tilde{\mathscr{V}}_N\,, \\ u_N^c(0) = \tilde{P}_N \tilde{\mathscr{I}}_M u(0)\,. \end{array} \tag{3.14}$$

Proof. As the Gauss quadrature rule is exact on $\tilde{\mathscr{V}}_N$, it holds

$$\langle u_N^c(t), v_N\rangle_M = \langle u_N^c(t), v_N\rangle\,.$$

Owing to Lemma 2.3, we know that the operator $K = -\frac{\varepsilon^2}{2m}\Delta$ yields linear and quadratical terms:

$$\begin{aligned} Ku_N^c(x) &= K\left(\sum_{n=0}^{N} \tilde{u}_n \varphi_n(x)\right) \\ &= \sum_{n=0}^{N} \tilde{u}_n \left(\frac{1}{2m}\left[2\overline{a}(x-q)+p\right]^2 \varphi_n(x) + \mathscr{L}(\varphi_n, \varphi_{n+1}, \varphi_{n+2})\right)\,. \end{aligned}$$

Written in the variable y, the last expression is a polynomial of degree $N+2$ times the exponential weight. This makes the difference between the pseudo-spectral Gauss-Hermite method and the previous case. We are forced hence to require the condition $M \geq N+1$:

$$\begin{aligned} \langle Ku_N^c(t), v_N\rangle_M &= \sum_{\tilde{\gamma}\in\tilde{\Gamma}_M} \frac{1}{\zeta} Ku_N^c(t,\tilde{\gamma})\overline{v_N}(\tilde{\gamma})\rho_\gamma = \sum_{\gamma\in\Gamma_M} T(Ku_N^c)(\gamma)\overline{Tv_N}(\gamma)\rho_\gamma \\ &= \int_{\mathbb{R}} T(Ku_N^c)(y)\overline{Tv_N}(y)dy = \langle T(Ku_N^c), Tv_N\rangle = \langle Ku_N^c, v_N\rangle\,. \end{aligned}$$

As the potential part concerns, we have:

$$\begin{aligned} \langle Vu_N^c(t), v_N\rangle_M &= \sum_{\tilde{\gamma}\in\tilde{\Gamma}_M} \frac{1}{\zeta} V(\tilde{\gamma})u_N^c(t,\tilde{\gamma})\overline{v_N}(\tilde{\gamma})\rho_\gamma = \sum_{\gamma\in\Gamma_M} T(Vu_N^c)(\gamma)\overline{Tv_N}(\gamma)\rho_\gamma \\ &= \int_{\mathbb{R}} \mathscr{I}_M[T(Vu_N^c)](y)\overline{Tv_n}(y)dy = \left\langle T^{-1}\mathscr{I}_M[T(Vu_N^c)], v_N\right\rangle = \left\langle \tilde{\mathscr{I}}_M(Vu_N^c), v_N\right\rangle\,, \end{aligned}$$

and this yields the result. ∎

We proceed analogously to the previous case (Hermite spectral decomposition) with the only difference that we keep $M \geq N+1$. For the error $e_N^c = \tilde{P}_N u - u_N^c$, it holds

$$\varepsilon\,\|e_N^c\|\,\frac{d}{dt}\|e_N^c\| \leq \left\|Vu - \tilde{\mathscr{I}}_M(Vu_N^c)\right\| \cdot \|e_N^c\| + \left|\left\langle K\tilde{R}_N u, e_N^c\right\rangle\right|\,. \tag{3.15}$$

We bound the last term using (2.24):

$$\left|\left\langle K\tilde{R}_N u, e_N^c\right\rangle\right| \leq cN^{-r/2}\sqrt{\frac{|s_1|^2}{N} + |s_2|^2}\cdot |u|_{2+r}\,\|e_N^c\|\,.$$

LEMMA 3.3 The potential term $\left\|Vu-\tilde{\mathscr{I}}_M(Vu_N^c)\right\|$ is bounded from above by

$$C_V\left\|e_N^c\right\|+c\left(M^{1/3-r/2}|Vu|_r+N^{-r/2}|u|_r+M^{-1/6}N^{1/2-r/2}|u|_r\right),$$

where $C_V=\|V\|_{L^\infty}$, and where c is a constant depending on $\|V\|_{L^\infty}$ and $\|\nabla V\|_{L^\infty}$.

Proof. We concentrate now on the evaluation of the potential term:

$$\begin{aligned}\left\|Vu-\tilde{\mathscr{I}}_M(Vu_N^c)\right\| &= \|T(Vu)-\mathscr{I}_M[T(Vu_N^c)]\| \\ &\le \|T(Vu)-\mathscr{I}_M[T(Vu)]\|+\|\mathscr{I}_M[T(Ve_N^c)]\|+\left\|\mathscr{I}_M[T(V\tilde{R}_Nu)]\right\|.\end{aligned}$$

The first term is related to the interpolation error:

$$\|T(Vu)-\mathscr{I}_M[T(Vu)]\|\le cM^{1/3-r/2}\left\|A^rT(Vu)\right\|\le cM^{1/3-r/2}|Vu|_r.$$

The second term is bounded like in (3.10):

$$\|\mathscr{I}_M[T(Ve_N^c)]\|^2=\sum_{\gamma\in\Gamma_M}\frac{1}{\zeta}|V(\tilde{\gamma})e_N^c(\tilde{\gamma})|^2\rho_\gamma\le C_V^2\left\|Te_N^c\right\|^2=C_V^2\left\|e_N^c\right\|^2.$$

For the third term, we first notice that for two functions f and g, we have

$$T(fg)(y)=f(q+\frac{1}{\zeta}y)\cdot(Tg)(y).$$

Now we use (2.17) and (3.3) in order to obtain

$$\begin{aligned}\left\|\mathscr{I}_M[T(V\tilde{R}_Nu)]\right\| &= \left\|\mathscr{I}_M[V(q+\frac{1}{\zeta}\cdot)R_N(Tu)]\right\|=\left\|V(q+\frac{1}{\zeta}\cdot)R_N(Tu)\right\|_M \\ &\le c\left(\left\|V(q+\frac{1}{\zeta}\cdot)R_N(Tu)\right\|+M^{-1/6}\left|V(q+\frac{1}{\zeta}\cdot)R_N(Tu)\right|_{H^1}\right).\end{aligned}$$

The L^2 and the H^1-error estimates (2.18) and (3.9) yield

$$\left\|\mathscr{I}_M[T(V\tilde{R}_Nu)]\right\|\le cN^{-r/2}|u|_r+cM^{-1/6}N^{1/2-r/2}|u|_r,$$

where c depends on $\|V\|_{L^\infty}$ and $\|\nabla V\|_{L^\infty}$. Altogether, we obtain the upper bound for the potential term. ∎

Now, we turn back to the inequality (3.15). The previous Lemma with $r+2$ yields

$$\begin{aligned}\varepsilon\frac{d}{dt}\left\|e_N^c(t)\right\|^2 &\le C_V\left\|e_N^c(t)\right\|^2+c\left(M^{-2/3-r/2}|Vu|_{r+2}+M^{-1/6}N^{-1/2-r/2}|u|_{r+2}\right)\left\|e_N^c(t)\right\| \\ &\quad +cN^{-r/2}\left(\frac{1}{N}+\sqrt{\frac{|s_1|^2}{N}+|s_2|^2}\right)\cdot|u|_{2+r}\left\|e_N^c(t)\right\|.\end{aligned}$$

Combining Lemma 2.1 and the Gronwall Lemma, we obtain the following upper bound

for the collocation error:

$$\begin{aligned}\|e_N^c(t)\| &\leq e^{\frac{C_V}{\varepsilon}t}\|e_N^c(0)\| + cM^{-2/3-r/2}\int_0^t e^{\frac{C_V}{\varepsilon}(t-s)}\frac{1}{\varepsilon}|Vu(s)|_{r+2}ds + \\ &\quad c\frac{1}{\varepsilon}M^{-1/6}N^{-1/2-r/2}\int_0^t e^{\frac{C_V}{\varepsilon}(t-s)}|u(s)|_{r+2}ds + \\ &\quad cN^{-r/2}\int_0^t e^{\frac{C_V}{\varepsilon}(t-s)}\left(\frac{1}{N\varepsilon}+\frac{|a|}{2m}\sqrt{\frac{2}{N\varepsilon}\frac{p^2}{\beta}+\frac{1}{\beta^2}}\right)|u(s)|_{r+2}ds\,.\end{aligned}$$

Denoting

$$f_1(t)=\int_0^t e^{\frac{C_V}{\varepsilon}(t-s)}\frac{1}{\varepsilon}|Vu(s)|_{r+2}ds \quad \text{and} \quad f_2(t)=\int_0^t e^{\frac{C_V}{\varepsilon}(t-s)}|u(s)|_{r+2}ds, \quad (3.16)$$

we may rewrite the previous expression as

$$\begin{aligned}\|e_N^c(t)\| &\leq e^{\frac{C_V}{\varepsilon}t}\|e_N^c(0)\| + cM^{-2/3-r/2}f_1(t) + \\ &\quad cN^{-r/2}\left(\frac{1}{\varepsilon}M^{-1/6}N^{-1/2}+\frac{1}{N\varepsilon}+\frac{|a|}{2m}\sqrt{\frac{2}{N\varepsilon}\frac{p^2}{\beta}+\frac{1}{\beta^2}}\right)f_2(t)\,.\end{aligned}$$

Using (3.11) to bound the term $\|e_N^c(0)\|$ we finally obtain:

THEOREM 3.2 Let $u(t)$ be a solution of (1.1) and let $u_N^c(t)$ be the solution of the problem (3.13) with $M \geq N+1$ associated with the Gauss-Hermite basis of parameters $a=\alpha+i\beta$, p and q. Assume that for $r \geq 1$, $|Vu|_{r+2} \in L^1(0,t)$ for all $t \geq 0$ and that the application $t \mapsto |u(t)|_{r+2}$ is continuous on $\mathbb{R}$, so that in particular, the functions $f_1(t)$ and $f_2(t)$ in (3.16) are continuous. Then the following bound for the error in the pseudo-spectral Gauss-Hermite method holds:

$$\begin{aligned}\|u(t)-u_N^c(t)\| &\leq ce^{\frac{C_V}{\varepsilon}t}M^{-2/3-r/2}|u(0)|_{r+2} + cM^{-2/3-r/2}f_1(t) \\ &\quad + cN^{-r/2}\left(\frac{1}{\varepsilon}M^{-1/6}N^{-1/2}+\frac{1}{N\varepsilon}+\frac{|a|}{2m}\sqrt{\frac{2}{N\varepsilon}\frac{p^2}{\beta}+\frac{1}{\beta^2}}\right)f_2(t) \\ &\quad + cN^{-1-r/2}|u(t)|_{r+2}\,,\end{aligned}$$

where $C_V = \|V\|_{L^\infty}$, $f_1(t)$ and $f_2(t)$ are given by (3.16), and where the constant c depend on L^∞ bounds on V and ∇V.

REMARK 3.1 For $M = N+1$ we have the convergence rate $(N+1)^{1/3-r/2}$.

3.3 Practical Approach

In the previous section, we started from the collocation on $\tilde{\Gamma}_M$ and we reformulated the problem into the variational form. During this process, we remarked that we need at least $M+1 = N+2$ collocation points. From the algorithmical point of view, it is most advantageous to have the same number of quadrature points as basis functions. In this

case, the Christoffel-Darboux formula gives an elegant and quick method to transform from function values to Gauss-Hermite coefficients and back, see Tang (1993). This motivates us to use directly the variational formulation of the continuous problem and to discretise it by a Galerkin method and Gauss-Hermite quadrature:

$$\begin{aligned} &\text{find } u_N(t,\cdot) \in \tilde{\mathscr{V}}_N \text{ such that} \\ &i\varepsilon \frac{d}{dt}\langle u_N(t), v_N\rangle = \langle Ku_N, v_N\rangle + \left\langle \tilde{\mathscr{I}}_N(Vu_N), v_N\right\rangle \text{ for all } v_N \in \tilde{\mathscr{V}}_N\,, \\ &u_N(0,\cdot) = \tilde{\mathscr{I}}_N u^0(\cdot)\,. \end{aligned} \tag{3.17}$$

This is exactly the formulation (3.14) with the only difference that we now interpolate on exactly $N+1$ points ($M=N$ instead of $M=N+1$). Hence, the same estimate of the error holds as in the collocation case with $M=N$ in the last Theorem. However, the formulation (3.17) is not equivalent to any collocation formulation. We work now with $N+1$ basis functions and we use the special form of $\langle Ku_N^c, v_N\rangle$ and the formulas for the Gaussian integrals (2.22) and (2.23). The moment is come to reveal the linear combination term in the Lemma 2.3:

$$\begin{aligned} \mathscr{L}(\varphi_n,\varphi_{n+1},\varphi_{n+2}) &= \varphi_n\left(\frac{2\alpha}{\varepsilon}i - \frac{4\alpha}{\varepsilon}i(n+1) - (2n+1)\right) \\ &\quad -\varphi_{n+1}\frac{2p\zeta}{\varepsilon}i\sqrt{2(n+1)} - \varphi_{n+2}\frac{4\alpha}{\varepsilon}i\sqrt{(n+1)(n+2)}. \end{aligned} \tag{3.18}$$

Consider $u_N(x) = \sum_{m=0}^{N} u_m^G \varphi_m(x)$ and test with all basis functions $v_N := \varphi_n$:

$$\begin{aligned} \langle Ku_N, \varphi_n\rangle &= \frac{p^2}{2m}u_n^G + \frac{2ap}{m}\frac{1}{\zeta}\left(\sqrt{\frac{n}{2}}u_n^G + \sqrt{\frac{n+2}{2}}u_{n+2}^G\right) + \\ &\quad \frac{2a^2}{m}\frac{1}{2\zeta^2}\left((2n+1)u_n^G + \sqrt{(n-1)n}u_{n-2}^G + \sqrt{(n+1)(n+2)}u_{n+2}^G\right) \\ &\quad + \left(-\frac{2\alpha}{\varepsilon} + \frac{4\alpha}{\varepsilon}(n+1) - (2n+1)\right)u_n^G + \frac{2p\zeta}{\varepsilon}\sqrt{2(n+1)}u_{n+1}^G + \\ &\quad \frac{4\alpha}{\varepsilon}\sqrt{(n+1)(n+2)}u_{n+2}^G\,. \end{aligned}$$

Hence, the kinetic energy operator may be discretised by a very sparse Hermite matrix. The potential energy operator is then obtained using quadrature on $\tilde{\Gamma}_N$:

$$\mathtt{P} * \mathrm{diag}(\omega .* \mathtt{V}(\gamma)) * \mathtt{P}^{\mathtt{T}}\,,$$

where γ and ω are vectors of length $N+1$ containing the points and the weights of the Gauss quadrature, P is the $(N+1)\times(N+1)$-matrix of the Hermite polynomials evaluated at the the quadrature points and $.*$ denotes pointwise multiplication. We obtain a small linear system of ordinary differential equations.

4 Numerical examples

In order to illustrate the previous results, we consider the approximation of (1.1) in the case where $m=1$ and where the potential function is given by $V(x) = (1-\cos(x))/2$.

We consider the space spanned by the functions $\varphi_n(x)$, $n = 0,\dots,N$, given by (2.14) associated with the parameters $a = i/2$, $q = 0$ and $p = 0$ in Eqn. (2.12), i.e. the Gauss-Hermite functions associated with the Gaussian $\exp(-x^2/(2\varepsilon))$.
The initial value is

$$v_0(x) = \left(\frac{2\beta_0}{\varepsilon\pi}\right)^{1/4} \exp\left(-\frac{\beta_0}{\varepsilon}(x-q_0)^2\right)$$

where $\beta_0 > 0$ and q_0 are real parameters. Note that in all case, we have $\|v_0\| = 1$.

4.1 Fixed basis in time

We consider the solution of (3.17) at time $T = 1$, i.e. the exact solution of the Pseudo-spectral Gauss-Hermite problem with $N+1$ interpolation points, which means that $M = N$ as in the previous section. In this case, the system is a linear system of ODE's, and its solution is calculated using an approximation of the matrix exponential.

For each N, we compare these solutions with the numerical solutions given by the Strang-splitting scheme in time with stepsize $\delta t = 10^{-4}$, combined with fast Fourier transform with $2^{16} = 65536$ points on the interval $[-\pi,\pi]$. This provides a very good approximation of the exact solution, see Jahnke & Lubich (2000), and we take it for the exact solution in our comparisons.

In Figure 1, we consider the case where $\beta_0 = 0.5$ and $q_0 = 0.1$. We plot the relative error and observe the convergence of the approximation with N. Note that the convergence is relatively robust with ε.

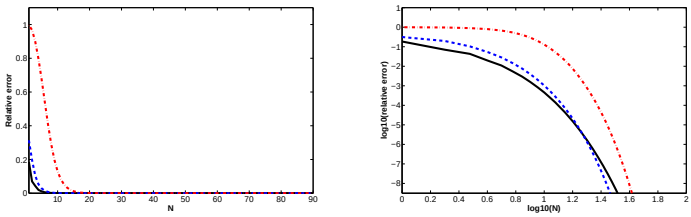

Figure 1: Relative approximation error with N at $T = 1$ for $\varepsilon = 0.1$ (line), $\varepsilon = 0.01$ (dashed) and $\varepsilon = 0.001$ (dash-dotted). $q_0 = 0.1$. Fixed approximation basis in time.

In Figure 2, we focus on the case $q_0 = 0.3$. We note that the convergence is slower than in the previous case. In particular, it deteriorates with smaller ε. This is due to the fact that the definition of the basis $\{\varphi_n(x)\,|\,n = 0,\dots,N\}$, which is constructed from Gaussian function centered at $q = 0$, requires to take large N to approximate a Gaussian-shaped function centered around $q = q_0 \neq 0$, particularly when $\varepsilon \to 0$.

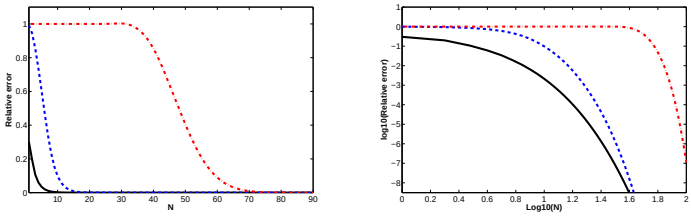

Figure 2: Relative approximation error at $T = 1$ for $\varepsilon = 0.1$ (line), $\varepsilon = 0.01$ (dashed) and $\varepsilon = 0.001$ (dash-dotted). $q_0 = 0.3$. Fixed approximation basis in time.

In Figure 3, we turn to the case $q_0 = 0.7$, and we oberve that the results are worse (in particular, the convergence for $\varepsilon = 10^{-3}$ requires at least $N > 100$).

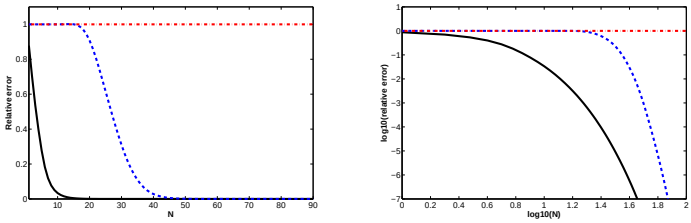

Figure 3: Relative approximation error at $T = 1$ for $\varepsilon = 0.1$ (line), 0.01 (dashed) and 0.001 (dash-dotted). $q_0 = 0.7$. Fixed approximation basis in time.

In Figure 4, we plot the evolution of the error with the time, in the case where $N = M = 10$ is fixed, and $\varepsilon = 0.01$. We display the results for $q_0 = 0.1$ (left) and $q_0 = 0.25$ (right), both in L^∞ and L^2 norm. As before, we observe a significant difference when q_0 is away from $q = 0$ or not.

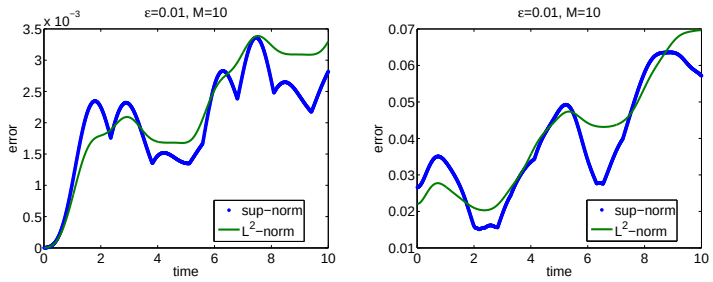

Figure 4: Evolution of the error with time. $q_0 = 0.1$ (left) and $q_0 = 0.25$ (right).

4.2 Gauss-Hermite wave packets dynamics examples

We have seen in the previous section that the quality of the Gauss-Hermite approximation of (1.1) with fixed parameters in time heavily depends on the choice of these parameters with respect to the behaviour of the exact solution.

In Faou *et al.* (2007), we introduce an algorithm to approximate (1.1) by functions of the form $\sum_{k=0}^{N} c_k \varphi_k(x)$ where the $\varphi_k(x)$ are functions of the form (2.14) but where *all* the parameters a, p, q and c_k ($k = 0, \ldots, N$) evolve with time. The algorithm can be quickly described as follows: Given the parameters a^n, p^n and q^n and c_k^n ($k = 0, \ldots, N$) associated with an approximate solution at the time $t_n = n\Delta t$, we determine the parameters at the time t_{n+1} using a symmetric combination of the following three pieces:

1. Free Schrödinger equation: The exact solution of the equation (1.1) without potential, with an initial value given as a Gauss-Hermite wave packet can be calculate explicitly for any time.

2. Quadratic potential part: We split the potential $V(x)$ into its quadratic Taylor expansion around q_0 and the corresponding remainder term: We define the potentials

$$Q^n(x) = V(q^n) + \nabla V(q^n)\,(x - q^n) + \frac{1}{2}\nabla^2 V(q^n)(x - q^n)^2$$

   as the local quadratic approximation to $V(x)$. In this case, we can again calculate explicitly the exact solution of the equation $i\varepsilon\psi = Q^n\psi$, for an initial value given as a Gauss-Hermite wave packet.

3. Cubic potential part: With the previous notation, we define

$$W^n(x) = V(x) - Q^n(x).$$

   The solution of the equation $i\varepsilon\psi = W^n\psi$ is then approximated by solving the corresponding Galerkin problem over Gauss-Hermite functions with fixed parameters a^n, p^n and q^n.

We can show that in this algorithm, the numerical trajectory corresponding to the parameters p and q correspond to the Verlet algorithm applied to the Hamiltonian system with potential V. Moreover, when $N \to \infty$, if converges towards the (abstract) Strang splitting between the kinetic and potential energy.

In Figure 5, we show the convergence of this algorithm applied to the same case as in the previous subsection. We see that we need much less numbers N to obtain correct approximation results. Note that we compute the error between the moduli of the solutions (in this case the error is $\mathcal{O}(\Delta t^2)$ while it is of order $\mathcal{O}(\Delta t^2/\varepsilon)$ for the phase error, see Faou *et al.* (2006) for the case where $N = 1$).

The step size used to calculate the solution associated with the algorithm described above is $\Delta t = 0.01$, while N ranges from 1 to 10.

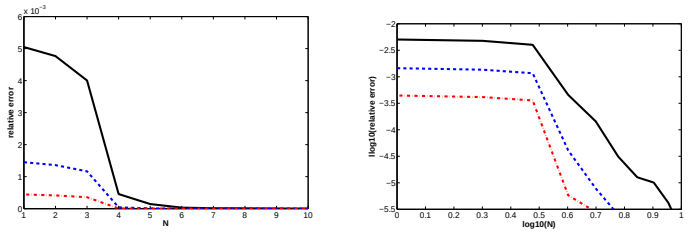

Figure 5: Relative approximation error at $T = 0.5$ for $\varepsilon = 0.1$ (line), $\varepsilon = 0.01$ (dashed) and $\varepsilon = 0.001$ (dash-dotted); $q_0 = 0.3$. Adaptative parameters.

Note that for small epsilon, the convergence is better. This is due to the compatibility of the algorithm with the semi-classical limit (see Faou *et al.* (2006, 2007) for further details).

Finally, we consider in Figure 6 the same situation as for the Figure 4, where ε is fixed to 0.01, $\beta_0 = 0.5$, $q_0 = 0.1$ and $q_0 = 0.25$. We take $N = 5$ and $\Delta t = 0.1$ in the adaptative Gauss-Hermite algorithm. We see that the behaviour is the same in both cases, as opposed to the situation of the Fig. 4.

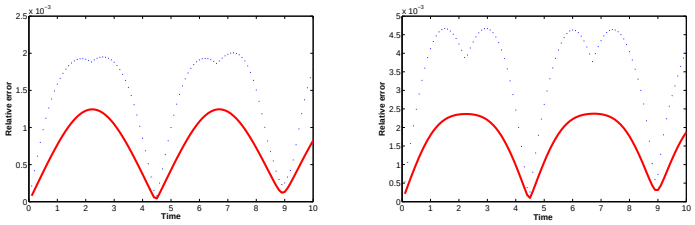

Figure 6: Time evolution of the error for the adaptative algorithm in L^∞ (points) and L^2 norms (lines); $q_0 = 0.1$ (left) and $q_0 = 0.25$ (right).

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