*Advances in Computational Mathematics* **19:** 35–55, 2003.


# Spectral and pseudospectral approximations using Hermite functions: application to the Dirac equation

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Received 4 August 2001; accepted 19 September 2002
Communicated by C.A. Micchelli

We consider in this paper spectral and pseudospectral approximations using Hermite functions for PDEs on the whole line. We first develop some basic approximation results associated with the projections and interpolations in the spaces spanned by Hermite functions. These results play important roles in the analysis of the related spectral and pseudospectral methods. We then consider, as an example of applications, spectral and pseudospectral approximations of the Dirac equation using Hermite functions. In particular, these schemes preserve the essential conservation property of the Dirac equation. We also present some numerical results which illustrate the effectiveness of these methods.

**Keywords:** Hermite approximation, Dirac equation, spectral and pseudospectral

**AMS subject classification:** 33A65, 41A10, 65M60, 65M70, 81C05

## 1. Introduction

Many problems in science and engineering lead to partial differential equations in unbounded domains, e.g., fluid flows in exterior domains, nonlinear wave equations in quantum mechanics, electro-magnetic fields, plasma physics, biology and mathematical economics. An effective mean for solving them numerically is to use spectral approximations associated with a set of basis functions which are mutually orthogonal in unbounded domains, see, for example, [6,10, and the references therein].

* The work of this author is supported by the special funds for Major State Basic Research Projects of China No. G1999032804 and Shanghai natural science foundation No. OOJC14057, and the Special Funds for Major Specialities of Shanghai Education Committee.
** The work of this author is partially supported by NFS grants DMS-0074283.

If the underlying domain is the whole line, it is natural to use Hermite polynomials/functions. Hill [14], Boyd [4,5], and Boyd and Moore [7] investigated various Hermite approximations and their applications. Funaro and Kavian [9] used the generalized Hermite functions which form a mutually orthogonal system on the whole line with the weight function $\mathrm{e}^{x^2/4a^2}$, and proved the convergences of the associated schemes for linear parabolic problems. Guo [11] considered the Hermite polynomials as the basis functions which are mutually orthogonal with the weight function $\mathrm{e}^{-x^2}$, and proved the convergences of the associated schemes for some nonlinear problems. Guo and Xu [13] developed the Hermite interpolation approximation and its applications to numerical solutions of certain nonlinear partial differential equations. Weideman [22] presented some interesting results on the practical implementations of the Hermite approximation. On the other hand, if the underlying domain is half line, then Laguerre polynomials/functions should be used. For instance, Maday et al. [16], Guo and Shen [12], and Xu and Guo [23] considered various aspects of approximations using Laguerre polynomials.

Most of the work mentioned above involve non-uniform weights which are not natural for the underlying physical problems and may lead to complications in analysis and implementation. In particular, the numerical schemes associated with non-uniform weights usually do not preserve conservation properties of the underlying physical problems. Generally speaking, it is not difficult to derive error estimates of the standard spectral methods for elliptic problems and parabolic systems in unbounded domains. But for partial differential equations in which conservation properties are essential, such as the Korteweg de Vries equation, the Schrödinger equation, the Dirac equation and hyperbolic conservations laws, spectral and pseudospectral methods for these problems may be unstable and are extremely complicated to analyze due to the non-uniform weights. In order to simplify the analysis and implementation, and to stabilize the numerical procedure, Shen [19] considered approximations using Laguerre functions which are mutually orthogonal in $L^2(0,\infty)$. The theoretical and numerical results in [19] demonstrated the effectiveness of this approach. A similar technique was used for the Hermite approximation on the whole line in [21]. We note that for spectral methods on finite intervals, there were also efforts to avoid using non-uniform weights. For example, Don and Gottlieb [8] proposed the Chebyshev–Legendre approximation using the Chebyshev interpolation nodes with a Legendre formulation.

In this paper, we investigate the spectral and pseudospectral approximations using Hermite functions on the whole line. In the next section, we derive some basic approximation results and inverse inequalities related to Hermite spectral approximations. In section 3, we derive corresponding results for pseudospectral (Hermite–Gauss interpolation) approximations which are more convenient in actual computations. The results in these two sections play important roles in the analysis of the associated spectral and pseudospectral methods. In sections 4 and 5, we show how to construct Hermite spectral and pseudospectral schemes to approximate, as an example, the Dirac equation.

## 2. Spectral approximations using Hermite functions

Let us first introduce some notations. We set $\Lambda = \{x \mid -\infty < x < \infty\}$ and denote by $L^2(\Lambda)$, $L^P(\Lambda)$, $L^\infty(\Lambda)$ and $H^r(\Lambda)$ the usual Sobolev spaces and by $\|v\|$, $\|v\|_{L^p}$, $\|v\|_\infty$, and $\|v\|_r$ their corresponding norms. The inner product of $L^2(\Lambda)$ and $H^m(\Lambda)$ are denoted by $(u, v)$ and $(u, v)_m$, and $|v|_r$ denotes the semi-norm of $H^r(\Lambda)$.

We shall use $c$ to denote a generic positive constant independent of any functions and the parameter $N$. For any two sequences of $\{a_l\}$ and $\{b_l\}$ of non-negative numbers, we write $a_l \preceq b_l$, if there exists a positive constant $d$ independent of $l$, such that $a_l \leqslant d b_l$ for all $l$. If $a_l \preceq b_l$ and $b_l \preceq a_l$, then we write $a_l \sim b_l$.

Let $H_l(x)$ be the Hermite polynomial of degree $l$. We recall that $H_l(x)$ are the eigenfunctions of the following singular Strum–Liouville problem,

$$\partial_x\big(\mathrm{e}^{-x^2}\partial_x H_l(x)\big) + \lambda_l \mathrm{e}^{-x^2} H_l(x) = 0, \quad \lambda_l = 2l,\ l = 0, 1, 2, \ldots. \tag{2.1}$$

They satisfy the recurrence relations

$$H_{l+1}(x) - 2xH_l(x) + 2lH_{l-1}(x) = 0, \quad l \geqslant 1, \tag{2.2}$$

$$\partial_x H_l(x) = 2lH_{l-1}(x), \quad l \geqslant 1. \tag{2.3}$$

The set $\{H_l(x)\}$ is mutually orthogonal in a weighted Sobolev space, namely,

$$\int_\Lambda H_l(x)H_m(x)\mathrm{e}^{-x^2}\,\mathrm{d}x = c_l\delta_{l,m}, \quad c_l = 2^l l!\sqrt{\pi}. \tag{2.4}$$

By virtue of (2.1) and (2.4), we also have

$$\int_\Lambda \partial_x H_l(x)\partial_x H_m(x)\mathrm{e}^{-x^2}\,\mathrm{d}x = d_l\delta_{l,m}, \quad d_l = 2lc_l. \tag{2.5}$$

The Hermite functions of degree $l$ are defined by

$$\widehat{H}_l(x) = \mathrm{e}^{-x^2/2}H_l(x), \quad l = 0, 1, 2 \ldots.$$

Due to (2.1), they are the eigenfunctions of the following singular Strum–Liouville problem,

$$\mathrm{e}^{-x^2/2}\partial_x\big(\mathrm{e}^{-x^2/2}\partial_x\widehat{H}_l(x) + x\mathrm{e}^{-x^2/2}\widehat{H}_l(x)\big) + \lambda_l\widehat{H}_l(x), \quad l = 0, 1, 2, \ldots. \tag{2.6}$$

By (2.2),

$$\widehat{H}_{l+1} + 2x\widehat{H}_l(x) + 2l\widehat{H}_{l-1}(x) = 0, \quad l \geqslant 1. \tag{2.7}$$

By (2.3) and (2.7), we have

$$\partial_x\widehat{H}_l(x) = 2l\widehat{H}_{l-1}(x) - x\widehat{H}_l(x) = l\widehat{H}_{l-1}(x) - \frac{1}{2}\widehat{H}_{l+1}(x), \quad l \geqslant 1. \tag{2.8}$$

The functions $\{\widehat{H}_l(x)\}$ are mutually-orthogonal in $L^2(\Lambda)$, i.e.,

$$\int_\Lambda \widehat{H}_l(x)\widehat{H}_m(x)\,\mathrm{d}x = c_l\delta_{l,m}. \tag{2.9}$$

Moreover, (2.8) and (2.9) imply that

$$\int_\Lambda \partial_x \widehat{H}_l(x)\partial_x \widehat{H}_m(x)\,\mathrm{d}x = \begin{cases} -\frac{l}{2}c_{l-1}, & m = l-2, \\ l^2 c_{l-1} + \frac{1}{4}c_{l+1}, & m = l, \\ -\frac{1}{2}(l+2)c_{l+1}, & m = l+2, \\ 0 & \text{otherwise.} \end{cases} \tag{2.10}$$

For any $v \in L^2(\Lambda)$, we may write $v(x) = \sum_{l=0}^{\infty} \hat{v}\widehat{H}_l(x)$, where

$$\hat{v}_l = c_l^{-1}\int_\Lambda v(x)\widehat{H}_l(x)\,\mathrm{d}x, \quad l = 0, 1, 2, \ldots,$$

$\hat{v}_i$ are the Hermite coefficients.

Let $N$ be any positive integer, $\mathcal{P}_N$ be the set of all polynomials of degree at most $N$, and

$$\mathcal{H}_N = \mathrm{span}\{\widehat{H}_0(x), \widehat{H}_1(x), \ldots, \widehat{H}_N(x)\},$$

We first derive two inverse inequalities which will be used in the sequel.

**Theorem 2.1.** For any $\phi \in \mathcal{H}_N$ and $1 \leqslant p \leqslant q \leqslant \infty$,

$$\|\phi \mathrm{e}^{(1/2-1/q)x^2}\|_{L^q} \leqslant cN^{(5/6)(1/p-1/q)}\|\phi \mathrm{e}^{(1/2-1/p)x^2}\|_{L^p}.$$

*Proof.* For any $\phi \in \mathcal{H}_N$, there exists $\psi \in \mathcal{P}_N$ such that $\psi(x) = \mathrm{e}^{x^2}\phi(x)$. Hence, the inverse inequality (see [18] or [10, theorem 2.23])

$$\left(\int_\Lambda |\psi(x)|^q \mathrm{e}^{-x^2}\,\mathrm{d}x\right)^{1/q} \leqslant cN^{(5/6)(1/p-1/q)}\left(\int_\Lambda |\psi(x)|^p \mathrm{e}^{-x^2}\,\mathrm{d}x\right)^{1/p}$$

leads to the desired result. □

*Remark 2.1.* By theorem 2.1, for any $\phi \in \mathcal{H}_N$ and $q \geqslant 1$,

$$\|\phi\|_{L^{2q}} \leqslant \|\phi \mathrm{e}^{(1/2)(1-1/q)x^2}\|_{L^{2q}} \leqslant cN^{(5/12)(1-1/q)}\|\phi\|.$$

In particular,

$$\|\phi\|_\infty \leqslant \|\phi \mathrm{e}^{x^2/2}\|_\infty \leqslant cN^{5/12}\|\phi\|.$$

**Theorem 2.2.** For any $\phi \in \mathcal{H}_N$ and non-negative integer $m$,

$$\|\partial_x^m \phi\| \leqslant (2N+1)^{m/2}\|\phi\|.$$

*Proof.* For any $\phi \in \mathcal{H}_N$, we write $\phi(x) = \sum_{l=0}^{N} \hat{\phi}_l \widehat{H}_l(x)$. Using (2.8), we find

$$\partial_x \phi(x) = \sum_{l=0}^{N-1} (l+1)\hat{\phi}_{l+1} \widehat{H}_l(x) - \frac{1}{2} \sum_{l=1}^{N+1} \hat{\phi}_{l-1} \widehat{H}_l(x).$$

Therefore,

$$\begin{aligned} \|\partial_x \phi\|^2 &\leqslant 2 \sum_{l=0}^{N-1} (l+1)^2 \hat{\phi}_{l+1}^2 c_l + \frac{1}{2} \sum_{l=1}^{N+1} \hat{\phi}_{l-1}^2 c_l \\ &\leqslant \frac{1}{2} \|\phi^2\| \left( 4 \max_{0 \leqslant l \leqslant N-1} \frac{(l+1)^2 c_l}{c_{l+1}} + \max_{1 \leqslant l \leqslant N+1} \frac{c_l}{c_{l-1}} \right) \\ &\leqslant (2N+1) \|\phi\|^2. \end{aligned}$$

Repeating the above procedure, we reach the desired result. □

*Remark 2.2.* The above result can be extended to non-integer cases. Indeed, for any $\phi \in \mathcal{H}_N$ and $r \geqslant 0$, we have by space interpolation,

$$\|\phi\|_r \leqslant c N^{r/2} \|\phi\|.$$

We are now in position to study several orthogonal projection operators. The $L^2(\Lambda)$-orthogonal projection $P_N : L^2(\Lambda) \to \mathcal{H}_N$ is a mapping such that for any $v \in L^2(\Lambda)$,

$$(P_N v - v, \phi) = 0, \quad \forall \phi \in \mathcal{H}_N,$$

or equivalently,

$$P_N v(x) = \sum_{l=0}^{N} \hat{v}_l \widehat{H}_l(x).$$

The $H^1(\Lambda)$-orthogonal projection $P_N^1 : H^1(\Lambda) \to \mathcal{H}_N$ is a mapping such that for any $v \in H^1(\Lambda)$,

$$\left( \left( P_N^1 v - v \right)', \phi' \right) = 0, \quad \forall \phi \in \mathcal{H}_N.$$

We define also

$$A v(x) = \partial_x v(x) + x v(x).$$

For technical reasons, we introduce the space $H_A^r(\Lambda)$ defined by

$$H_A^r(\Lambda) = \left\{ v \mid v \text{ is measurable on } \Lambda \text{ and } \|v\|_{r,A} < \infty \right\},$$

and equipped with the norm $\|v\|_{r,A} = \|A^r v\|$. For any $r > 0$, the space $H_A^r(\Lambda)$ and its norm are defined by space interpolation. By induction, for any non-negative integer $r$,

$$A^r v(x) = \sum_{k=0}^{r} \left( x^2 + 1 \right)^{(r-k)/2} p_k(x) \partial_x^k v(x),$$

where $p_k(x)$ are certain rational functions which are bounded uniformly on $\Lambda$. Thus,

$$\|v\|_{r,A} \leqslant c\left(\sum_{k=0}^{r} \left\|\left(x^2+1\right)^{(r-k)/2}\partial_x^k v\right\|^2\right)^{1/2}.$$

**Lemma 2.1.** For any $v \in H_A^r(\Lambda)$ and $r \geqslant 0$,

$$\|P_N v - v\| \leqslant cN^{-r/2}\|v\|_{r,A}.$$

*Proof.* Let $m$ be any non-negative integer. By (2.6), (2.8) and integration by parts,

$$\begin{aligned}
c_l\hat{v}_l &= \int_\Lambda v(x)\widehat{H}_l(x)\,\mathrm{d}x = -\frac{1}{2l}\int_\Lambda \mathrm{e}^{x^2/2}v(x)\partial_x\left(\mathrm{e}^{-x^2/2}\partial_x\widehat{H}_l(x) + x\mathrm{e}^{-x^2/2}\widehat{H}_l(x)\right)\mathrm{d}x \\
&= \frac{1}{2l}\int_\Lambda \left(\partial_x v(x) + xv(x)\right)\left(\partial_x\widehat{H}_l(x) + x\widehat{H}_l(x)\right)\mathrm{d}x \\
&= \int_\Lambda Av(x)\widehat{H}_{l-1}(x)\,\mathrm{d}x = \cdots = \int_\Lambda A^m v(x)\widehat{H}_{l-m}(x)\,\mathrm{d}x.
\end{aligned}$$

Consequently,

$$\begin{aligned}
\|P_N v - v\|^2 &= \sum_{l=N+1}^{\infty} c_l\hat{v}_l^2 = \sum_{l=N+1}^{\infty} c_l^{-1}c_{l-m}^2\left(c_{l-m}^{-1}\int_\Lambda A^m v(x)\widehat{H}_{l-m}(x)\,\mathrm{d}x\right)^2 \\
&\leqslant \max_{l\geqslant N+1}\frac{c_{l-m}}{c_l}\left\|A^m v\right\|^2.
\end{aligned}$$

Since $c_l^{-1}c_{l-m} \leqslant cl^{-m}$, we assert that

$$\|P_N v - v\| \leqslant cN^{-m/2}\|v\|_{m,A}.$$

Using the space interpolation technique on the above result leads to the desired result for $r \geqslant 0$. □

Generally, $\partial_x P_N v(x) \neq P_N\partial_x v(x)$. But we have the following result.

**Lemma 2.2.** For any $v \in H_A^r(\Lambda)$ and $r \geqslant 1$,

$$\|P_N\partial_x v - \partial_x P_N v\| \leqslant cN^{(1-r)/2}\|v\|_{r,A}.$$

*Proof.* By (2.8),

$$\partial_x P_N v(x) = \sum_{l=0}^{N-1}(l+1)\hat{v}_{l+1}\widehat{H}_l(x) - \frac{1}{2}\sum_{l=1}^{N+1}\hat{v}_{l-1}\widehat{H}_l(x).$$

Similarly

$$P_N\partial_x v(x) = \sum_{l=0}^{N}(l+1)\hat{v}_{l+1}\widehat{H}_l(x) - \frac{1}{2}\sum_{l=1}^{N}\hat{v}_{l-1}\widehat{H}_l(x).$$

Thus

$$P_N \partial_x v(x) - \partial_x P_N v(x) = (N+1)\hat{v}_{N+1} \widehat{H}_N(x) + \frac{1}{2}\hat{v}_N \widehat{H}_{N+1}(x).$$

By (2.9),

$$\begin{aligned}\|P_N \partial_x v - \partial_x P_N v\|^2 &\leqslant 2(N+1)^2 \hat{v}_{N+1}^2 c_N + \frac{1}{2}\hat{v}_N^2 c_{N+1} \\ &\leqslant (N+1)\big(\hat{v}_{N+1}^2 c_{N+1} + \hat{v}_N^2 c_N\big).\end{aligned} \tag{2.11}$$

Furthermore, by virtue of lemma 2.1,

$$c_{N+1}\hat{v}_{N+1}^2 \leqslant \|P_N v - v\|^2 \leqslant cN^{-r}\|v\|_{r,A}^2.$$

Similarly

$$c_N \hat{v}_N^2 \leqslant \|P_{N-1} v - v\|^2 \leqslant cN^{-r}\|v\|_{r,A}^2.$$

The result follows from the combination of the above two estimates and (2.11). □

**Corollary 2.1.** For any $v \in H_A^r(\Lambda)$ and $r \geqslant 0$,

$$\big\|\partial_x\big(P_N^1 v - v\big)\big\| \leqslant cN^{(1-r)/2}\|v\|_{r,A}.$$

*Proof.* Using lemmas 2.1, 2.2 and the fact that $\|\partial_x v\|_{r-1,A} \leqslant c\|v\|_{r,A}$, we have

$$\begin{aligned}\big\|\partial_x\big(P_N^1 v - v\big)\big\| &= \inf_{v_N \in \mathcal{H}_\mathcal{N}} \|\partial_x v_N - \partial_x v\| \leqslant \big\|\partial_x(P_N v) - \partial_x v\big\| \\ &\leqslant \|\partial_x v - P_N \partial_x v\| + \big\|P_N \partial_x v - \partial_x(P_N v)\big\| \\ &\leqslant c\big(N^{(1-r)/2}\|\partial_x v\|_{r-1,A} + N^{(1-r)/2}\|v\|_{r,A}\big) \leqslant cN^{(1-r)/2}\|v\|_{r,A}.\end{aligned}$$ □

**Theorem 2.3.** For any $v \in H_A^r(\Lambda)$ and $0 \leqslant \mu \leqslant r$,

$$\|P_N v - v\|_\mu \leqslant cN^{(\mu-r)/2}\|v\|_{r,A}.$$

*Proof.* We only need to consider non-negative integer $\mu$. The general case follows from space interpolation.

We proceed by induction. Clearly, lemma 2.1 implies the result for $\mu = 0$. Now assume that

$$\|P_N v - v\|_m \leqslant cN^{(m-r)/2}\|v\|_{r,A}, \quad m \leqslant \mu - 1. \tag{2.12}$$

Then, by lemmas 2.1, 2.2, theorem 2.2 and (2.12),

$$\begin{aligned}\|P_N v - v\|_\mu &\leqslant \|\partial_x v - P_N \partial_x v\|_{\mu-1} + \|P_N \partial_x v - \partial_x P_N v\|_{\mu-1} + \|P_N v - v\| \\ &\leqslant cN^{(\mu-r)/2}\|\partial_x v\|_{r-1,A} + cN^{(\mu-1)/2}\|P_N \partial_x v - \partial_x P_N v\| + cN^{(\mu-r)/2}\|v\|_{r,A} \\ &\leqslant cN^{(\mu-r)/2}\|v\|_{r,A}.\end{aligned}$$

This completes the proof. □

We end this section with an estimate on $L^\infty(\Lambda)$-norm of $P_N v$.

**Theorem 2.4.** For any $v \in H_A^d(\Lambda)$ and $d > 1/2$,

$$\|P_N v\|_\infty \leqslant c\|v\|_{d,A}.$$

*Proof.* We derive from the Sobolev imbedding theory and theorem 2.3 that

$$\begin{aligned}\|P_N v\|_\infty &\leqslant \|v\|_\infty + \|P_N v - v\|_\infty \\ &\leqslant \|v\|_d + \|P_N v - v\|_d \leqslant \|v\|_d + c\|v\|_{d,A}.\end{aligned}$$ □

## 3. Hermite–Gauss interpolation

Let us denote by $\sigma_{N,j}$ $(0 \leqslant j \leqslant N)$ the zeros of $H_{N+1}(x)$, and arrange them as

$$\sigma_{N,N} < \sigma_{N,N-1} < \cdots < \sigma_{N,0}.$$

Let $\omega_{N,j}$ be the corresponding Hermite–Gauss weights, namely

$$\omega_{N,j} = \frac{2^N N!\sqrt{\pi}}{(N+1)\widehat{H}_N^2(\sigma_{N,j})} = \rho_{N,j}\mathrm{e}^{\sigma_{N,j}^2}, \tag{3.1}$$

where $\rho_{N,j}$ are the Christoffel numbers of the standard Hermite–Gauss interpolation (see, for instance, [13]). Let $a_N = \sqrt{2N}$ be the $N$th Mhaskar–Rahmanov–Saff number. According to (2.7) of [13],

$$\rho_{N,j} \sim \frac{1}{\sqrt{N}}\mathrm{e}^{-\sigma_{N,j}^2}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2}.$$

The above and (3.1) lead to

$$\omega_{N,j} \sim \frac{1}{\sqrt{N}}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2}. \tag{3.2}$$

We now define the discrete inner product and the discrete norm by

$$(u, v)_N = \sum_{j=0}^{N} u(\sigma_{N,j})v(\sigma_{N,j})\omega_{N,j}, \quad \|v\|_N = (v, v)_N^{1/2}.$$

As is well known, for any $q \in \mathcal{P}_{2N+1}$ (see [20]),

$$\int_\Lambda q(x)\,\mathrm{e}^{-x^2}\,\mathrm{d}x = \sum_{j=0}^{N} q(\sigma_{N,j})\rho_{N,j}. \tag{3.3}$$

For any $\phi \in \mathcal{H}_m$ and $\psi \in \mathcal{H}_{2N+1-m}$ and any non-negative integer $m \leqslant 2N+1$, there exist $q_m \in \mathcal{P}_m$ and $q_{2N+1-m} \in \mathcal{P}_{2N+1-m}$ such that

$$\phi(x) = \mathrm{e}^{-x^2/2}q_m(x), \qquad \psi(x) = \mathrm{e}^{-x^2/2}q_{2N+1-m}(x).$$

Thus by virtue of (3.1) and (3.3), for any $\phi \in \mathcal{H}_m$ and $\psi \in \mathcal{H}_{2N+1-m}$,

$$\begin{aligned}\int_\Lambda \phi(x)\psi(x)\,\mathrm{d}x &= \int_\Lambda q_m(x)q_{2N+1-m}(x)\mathrm{e}^{-x^2}\,\mathrm{d}x \\ &= \sum_{j=0}^{N} q_m(\sigma_{N,j})q_{2N+1-m}(\sigma_{N,j})\rho_{N,j} \\ &= \sum_{j=0}^{N} \phi(\sigma_{N,j})\psi(\sigma_{N,j})\omega_{N,j} = (\phi,\psi)_N. \qquad (3.4)\end{aligned}$$

In particular,

$$\|\phi\| = \|\phi\|_N, \quad \forall \phi \in \mathcal{H}_N. \qquad (3.5)$$

For any $v \in C(\Lambda)$, the Hermite–Gauss interpolant $I_N v \in \mathcal{H}_N$ is determined by

$$I_N v(\sigma_{N,j}) = v(\sigma_{N,j}), \quad 0 \leqslant j \leqslant N,$$

or equivalently,

$$(I_N v - v, \phi)_N = 0, \quad \forall \phi \in \mathcal{H}_N.$$

The following lemma is related to the stability of the interpolation.

**Lemma 3.1.** For any $v \in H^1(\Lambda)$,

$$\|v\|_N \leqslant c\big(\|v\| + cN^{-1/6}|v|_1\big).$$

*Proof.* It is shown in [3] that for any $a < b$,

$$\sup_{x\in[a,b]} \big|v(x)\big|^2 \leqslant \frac{c}{b-a}\|v\|^2_{L^2(a,b)} + c(b-a)|v|^2_{H^1(a,b)}. \qquad (3.6)$$

Let $\Lambda_{N,j} = (\sigma_{N,j+1}, \sigma_{N,j-1})$ and $\Delta_{N,j} = \sigma_{N,j-1} - \sigma_{N,j+1}$. It is proved by Levin and Lubinsky [15] that

$$-a_{N+1}\big(1 - N^{-2/3}\big) \preceq \sigma_N, \qquad \sigma_0 \preceq a_{N+1}\big(1 - N^{-2/3}\big), \qquad (3.7)$$

and for $1 \leqslant j \leqslant N-1$,

$$\Delta_{N,j} \sim \frac{1}{\sqrt{N+1}}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2}. \qquad (3.8)$$

By (3.6), for $1 \leqslant j \leqslant N-1$,

$$v^2(\sigma_{N,j}) \leqslant \frac{c}{\Delta_{N,j}}\|v\|^2_{L^2(\Lambda_{N,j})} + c\Delta_{N,j}|v|^2_{H^1(\Lambda_{N,j})}. \qquad (3.9)$$

By (3.7), for $j = 0, N$,

$$v^2(\sigma_{N,j})\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2} \leqslant cN^{1/3}\|v\|_\infty^2 \leqslant cN^{1/3}\|v\|\|v\|_1. \tag{3.10}$$

The combination of (3.2), (3.5), (3.9) and (3.10) leads to

$$\begin{aligned}\|v\|_N^2 &\leqslant cN^{-1/2}\sum_{j=0}^{N} v^2(\sigma_{N,j})\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2} \\ &\leqslant cN^{-1/6}\|v\|\,\|v\|_1 + cN^{-1/2}\sum_{j=1}^{N-1}\Delta_{N,j}^{-1}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2}\|v\|_{L^2(\Lambda_{N,j})}^2 \\ &\quad + cN^{-1/2}\sum_{j=1}^{N-1}\Delta_{N,j}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2}|v|_1^2.\end{aligned} \tag{3.11}$$

Furthermore, (3.8) implies that

$$N^{-1/2}\Delta_{N,j}^{-1}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2} \leqslant c. \tag{3.12}$$

On the other hand, (3.7) implies that

$$\left|1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right| \geqslant \left|1 - \frac{\sigma_{N,0}}{a_{N+1}}\right| \geqslant cN^{-2/3}.$$

Thus using (3.8) again yields

$$N^{-1/2}\Delta_{N,j}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1/2} \leqslant cN^{-1}\left(1 - \frac{|\sigma_{N,j}|}{a_{N+1}}\right)^{-1} \leqslant cN^{-1/3}. \tag{3.13}$$

Substituting (3.12) and (3.13) into (3.11), we derive

$$\begin{aligned}\|v\|_N^2 &\leqslant c\big(N^{-1/6}\|v\|\|v\|_1 + \|v\|^2 + N^{-1/3}|v|_1^2\big) \\ &\leqslant c\big(\|v\|^2 + N^{-1/3}|v|_1^2\big).\end{aligned}$$

The proof is complete. □

We now state the main result of this section.

**Theorem 3.1.** For any $v \in H_A^r(\Lambda)$, $r \geqslant 1$ and $0 \leqslant \mu \leqslant r$,

$$\|I_N v - v\|_\mu \leqslant cN^{1/3+(\mu-r)/2}\|v\|_{r,A}.$$

*Proof.* By theorems 2.2, 2.3, lemma 3.1, and the fact that $I_N P_N v = P_N v$,

$$\begin{aligned}\|I_N v - P_N v\|_\mu &\leqslant cN^{\mu/2}\big\|I_N(P_N v - v)\big\| \\ &\leqslant cN^{\mu/2}\|P_N v - v\| + cN^{\mu/2-1/6}|P_N v - v|_1 \\ &\leqslant cN^{1/3+(\mu-r)/2}\|v\|_{r,A}.\end{aligned}$$

Using theorem 2.3 again yields

$$\|I_N v - v\|_\mu \leqslant \|P_N v - v\|_\mu + \|I_N v - P_N v\|_\mu \leqslant cN^{1/3+(\mu-r)/2}\|v\|_{r,A}. \qquad \square$$

We note that by (3.4) and theorem 3.1, we have

$$\begin{aligned}\big|(v,\phi)-(v,\phi)_N\big| &= \big|(v-I_N v,\phi)\big| \leqslant c\|v-I_N v\|\|\phi\| \\ &\leqslant cN^{1/3-r/2}\|v\|_{r,A}\,\|\phi\|.\end{aligned}$$

## 4. Hermite spectral method for the Dirac equation

We take the Dirac equation as an example to demonstrate how approximations using Hermite functions works well for this type of nonlinear partial differential equations, and why it is difficult to deal with them by using the Hermite polynomials which involve a non-uniform weight.

The Dirac equation plays an important role in quantum mechanics. It describes the quantum electro-dynamical law which applies to spin-(1/2) particles and is the relativistic generalization of the Schödinger equation (see [24]). Let $\mathrm{i} = \sqrt{-1}$. We denote $\Psi(x,t) = (\psi_1(x,t), \psi_2(x,t))$, $f(x,t) = (f_1(x,t), f_2(x,t))$ and

$$\begin{aligned} Q_1\big(\Psi(x,t)\big) &= \mathrm{i}\big(\big|\psi_2(x,t)\big|^2 - \big|\psi_1(x,t)\big|^2\big)\psi_1(x,t), \\ Q_2\big(\Psi(x,t)\big) &= \mathrm{i}\big(\big|\psi_1(x,t)\big|^2 - \big|\psi_2(x,t)\big|^2\big)\psi_2(x,t). \end{aligned}$$

Then, the initial value problems of the Dirac equation in 1 + 1 dimensions is: Find $\psi_1$ and $\psi_2$ such that

$$\begin{cases} \partial_t\psi_1(x,t) + \partial_x\psi_2(x,t) + \mathrm{i}m\psi_1(x,t) + 2\lambda Q_1\big(\Psi(x,t)\big) = f_1(x,t), \\ \quad x\in\Lambda,\ 0<t\leqslant T, \\ \partial_t\psi_2(x,t) + \partial_x\psi_1(x,t) + \mathrm{i}m\psi_2(x,t) + 2\lambda Q_2\big(\Psi(x,t)\big) = f_2(x,t), \\ \quad x\in\Lambda,\ 0<t\leqslant T, \\ \lim\limits_{|x|\to\infty}\Psi(x,t) = 0, \qquad 0<t\leqslant T, \\ \Psi(x,0) = \Psi^{(0)}(x), \quad x\in\Lambda, \end{cases} \tag{4.1}$$

where $m$, $\lambda$ are given real numbers.

Let $v(x)$ be a complex-valued function,

$$v(x) = v_{\mathrm{R}}(x) + \mathrm{i}v_{\mathrm{I}}(x),$$

where $v_{\mathrm{R}}(x)$ and $v_{\mathrm{I}}(x)$ are the real part and the imaginary part, respectively. Define

$$\big|v(x)\big| = \big(\big|v_{\mathrm{R}}(x)\big|^2 + \big|v_{\mathrm{I}}(x)\big|^2\big)^{1/2}.$$

Let $\bar{v}$ be the complex conjugate of $v$, and

$$(u,v) = \int_\Lambda u(x)\overline{v(x)}\,\mathrm{d}x, \qquad \|v\| = (v,v)^{1/2}.$$

If $v_{\mathrm{R}}, v_{\mathrm{I}} \in H^r(\Lambda)$, we say that $v \in H^r(\Lambda)$, with the following semi-norm and norm,

$$|v|_r = \big(|v_{\mathrm{R}}|_r^2 + |v_{\mathrm{I}}|_r^2\big)^{1/2}, \qquad \|v\|_r = \big(\|v_{\mathrm{R}}\|_r^2 + \|v_{\mathrm{I}}\|_r^2\big)^{1/2}.$$

We define the space $H_A^r(\Lambda)$ and its norm $\|v\|_{r,A}$ accordingly. To simplify the notation, we shall use the same notations to denote the spaces of complex-valued vector functions.

A weak formulation of (4.1) is: find $\psi_1$ and $\psi_2$ in $L^2(0,T;H^1(\Lambda)) \cap L^\infty(0,T; L^2(\Lambda))$ such that

$$\begin{cases} \big(\partial_t\psi_1(t) + \partial_x\psi_2(t) + \mathrm{i}m\psi_1(t) + 2\lambda Q_1\big(\Psi(t)\big), v\big) = \big(f_1(t), v\big), \\ \quad \forall v \in H^1(\Lambda),\ 0 < t \leqslant T, \\ \big(\partial_t\psi_2(t) + \partial_x\psi_1(t) - \mathrm{i}m\psi_2(t) + 2\lambda Q_2\big(\Psi(t)\big), v\big) = \big(f_2(t), v\big), \\ \quad \forall v \in H^1(\Lambda),\ 0 < t \leqslant T, \\ \Psi(0) = \Psi^{(0)}. \end{cases} \tag{4.2}$$

The Dirac equation possesses an essential conservation property which we shall derive below.

We note that for any complex-valued functions $u, v \in H^1(\Lambda)$,

$$(\partial_x u, v) + \overline{(\partial_x u, v)} + (u, \partial_x v) + \overline{(u, \partial_x v)} = 0. \tag{4.3}$$

Next, for any complex-valued vector functions $U = (u_1, u_2)^{\mathrm{T}} \in L^4(\Lambda)$ and $V = (v_1, v_2)^{\mathrm{T}} \in L^4(\Lambda)$,

$$\big(Q_1(U), u_1\big) + \overline{(Q_1(U), u_1)} = 0, \tag{4.4}$$

$$\big(Q_2(U), u_2\big) + \overline{(Q_2(U), u_2)} = 0. \tag{4.5}$$

Furthermore, for any complex-valued function $v \in H^1(0,T;L^2(\Lambda))$,

$$\big(\partial_t v(t), v(t)\big) + \overline{\big(\partial_t v(t), v(t)\big)} = \partial_t \big\|v(t)\big\|^2. \tag{4.6}$$

Now, we take $v = \psi_1$ in the first formula of (4.2) and $v = \psi_2$ in the second one, respectively. Then, we take the complex conjugates of these two resulting equations. Putting the four relations together and using (4.3)–(4.6), we find that in the case $f_1 = f_2 \equiv 0$, we have

$$\partial_t \big\|\Psi(t)\big\|^2 = 0, \quad 0 < t \leqslant T.$$

Thus the solution of (4.2) possesses the following conservation

$$\big\|\Psi(t)\big\| = \big\|\Psi^{(0)}\big\| \quad (\text{if } f_1 = f_2 \equiv 0). \tag{4.7}$$

Several authors have developed numerical approximations of (4.1) to study the dynamics of soliton interactions, see, e.g., [17, and the references therein]. Alvarez and Carreras [1] first provided a finite difference scheme which preserve a reasonable analogy of (4.7). Alvarez et al. [2] proved the stability and the convergence of this scheme.

However, since the domain is infinite, certain artificial boundary conditions are imposed in actual computations. This treatment introduces additional error which might pollute the accuracy in long-time calculations. On the other hand, no artificial boundary conditions are needed if we employ the spectral and pseudospectral methods using Hermite polynomials as in [11,13] to solve (4.1) directly. However, the associated variational formulation with the weight function $e^{-x^2}$ does not preserve the conservation (4.7). Thus, it is clear that a spectral method using Hermite functions is suitable for this problem.

Let $\phi = \phi_R + i\phi_I$. If $\phi_R, \phi_I \in \mathcal{H}_N$, then we write $\phi \in \mathcal{H}_N$. For any vector function $\Phi = (\phi_1, \phi_2)$, if $\phi_1 \in \mathcal{H}_N$ and $\phi_2 \in \mathcal{H}_N$, then we write $\Phi \in \mathcal{H}_N$.

The Hermite-spectral scheme for (4.2) is to find $\Psi_N(x,t) \in \mathcal{H}_N$ for all $0 \leqslant t \leqslant T$ such that

$$\begin{cases} \big(\partial_t \psi_{1,N}(t) + \partial_x \psi_{2,N}(t) + \mathrm{i}m\psi_{1,N}(t) + 2\lambda Q_1\big(\Psi_N(t)\big), \phi\big) = \big(f_1(t), \phi\big), \\ \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \big(\partial_t \psi_{2,N}(t) + \partial_x \psi_{1,N}(t) - \mathrm{i}m\psi_{2,N}(t) + 2\lambda Q_2\big(\Psi_N(t)\big), \phi\big) = \big(f_2(t), \phi\big), \\ \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \Psi_N(0) = P_N\Psi^{(0)} = \big(P_N\psi_1^{(0)}, P_N\psi_2^{(0)}\big)^{\mathrm{T}}. \end{cases} \tag{4.8}$$

Following the same procedure as in the derivation of (4.7), we can derive that

$$\|\Psi_N(t)\| = \|\Psi_N^{(0)}\| \quad (\text{if } f_1 = f_2 \equiv 0). \tag{4.9}$$

So the numerical solution possesses the same conservation property as the exact solution $\Psi$.

We now study the convergence property of (4.8). To this end, we set $\Psi_N^* = (\psi_{1,N}^*, \psi_{2,N}^*) = (P_N\psi_1, P_N\psi_2)^{\mathrm{T}}$ and

$$\begin{aligned} E_1(t) &= \big(\partial_x\psi_2(t) - \partial_x\psi_{2,N}^*\big), \\ E_2(t) &= \big(\partial_x\psi_1(t) - \partial_x\psi_{1,N}^*\big), \\ F_j(t) &= Q_j\big(\Psi(t)\big) - Q_j\big(\Psi_N^*(t)\big), \quad j = 1, 2. \end{aligned}$$

Then, we derive from (4.2) that

$$\begin{cases} \big(\partial_t \psi_{1,N}^*(t) + \partial_x \psi_{2,N}^*(t) + \mathrm{i}m\psi_{1,N}^*(t) + 2\lambda Q_1\big(\Psi_N^*(t)\big) + E_1(t) + 2\lambda F_1(t), \phi\big) \\ \quad = \big(f_1(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \big(\partial_t \psi_{2,N}^*(t) + \partial_x \psi_{1,N}^*(t) - \mathrm{i}m\psi_{2,N}^*(t) + 2\lambda Q_2\big(\Psi_N^*(t)\big) + E_2(t) + 2\lambda F_2(t), \phi\big) \\ \quad = \big(f_2(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \Psi_N^*(0) = P_N\Psi^{(0)}. \end{cases} \tag{4.10}$$

Next, let obtain $\widetilde{\Psi}_N = (\tilde{\psi}_{1,N}, \tilde{\psi}_{2,N})^{\mathrm{T}} = (\psi_{1,N} - \psi^*_{1,N}, \psi_{2,N} - \psi^*_{2,N})^{\mathrm{T}}$. Subtracting (4.10) from (4.8), we obtain

$$\begin{cases} \big(\partial_t \tilde{\psi}_{1,N}(t) + \partial_x \tilde{\psi}_{2,N}(t) + \mathrm{i}m\tilde{\psi}_{1,N}(t) + 2\lambda Q_1\big(\widetilde{\Psi}_N(t)\big), \phi\big) \\ \quad = \big(E_1(t) + 2\lambda F_1(t) + G_1(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \big(\partial_t \tilde{\psi}_{2,N}(t) + \partial_x \tilde{\psi}_{1,N}(t) + \mathrm{i}m\tilde{\psi}_{2,N}(t) + 2\lambda Q_2\big(\widetilde{\Psi}_N, (t)\big), \phi\big) \\ \quad = \big(E_2(t) + 2\lambda F_2(t) + G_2(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \widetilde{\Psi}_N(0) = (0), \end{cases} \tag{4.11}$$

where

$$G_j(t) = -Q_j\big(\Psi^*_N(t) + \widetilde{\Psi}_N(t)\big) + Q_j\big(\Psi^*_N(t)\big) + Q_j\big(\widetilde{\Psi}_N(t)\big), \quad j = 1, 2.$$

We take $\phi = \tilde{\psi}_{j,N}$ ($j = 1, 2$) in the $j$th equation of (4.11), and then take the complex conjugates of those two resulting equations. Putting the four relations together, and using (4.3)–(4.6), we arrive at

$$\frac{\mathrm{d}}{\mathrm{d}t}\big\|\widetilde{\Psi}_N(t)\big\|^2 \leqslant c\big\|\widetilde{\Psi}_N(t)\big\|^2 + c\sum_{j=1}^{3}\big(\big\|E_j(t)\big\|^2 + \big\|F_j(t)\big\|^2 + \big\|G_j(t)\big\|^2\big). \tag{4.12}$$

Hence, it remains to estimate the upper-bounds of the last term in (4.12).

We derive from theorem 2.3 that

$$\big\|E_j(t)\big\|^2 \leqslant cN^{1-r}\big\|\Psi(t)\big\|^2_{r,A}, \quad j = 1, 2. \tag{4.13}$$

Thanks to theorems 2.3 and 2.4,

$$\begin{aligned} \big\|F_j(t)\big\|^2 &\leqslant c\sum_{k=0}^{2}\sum_{j=1}^{2}\big\|\psi_j(t)\big\|_\infty^{4-2k}\big\|\psi^*_{j,N}(t)\big\|_\infty^{2k}\big\|\psi_j(t) - \psi^*_{j,N}(t)\big\|^2_\infty \\ &\leqslant c^*(\Psi)N^{-r}\big\|\Psi(t)\big\|^2_{r,A}, \quad j = 1, 2, \end{aligned} \tag{4.14}$$

where $c^*(\Psi)$ is a positive constant depending only on $\|\Psi\|_{L^\infty(0,T;L^\infty(\Lambda)\cap H^1_A(\Lambda))}$. Finally, we derive from theorem 2.1 that

$$\big\|G_j(t)\big\|^2 \leqslant c\sum_{k=1}^{2}\sum_{j=1}^{2}\big\|\psi^*_{j,N}(t)\big\|_\infty^{6-2k}\big\|\tilde{\psi}_{j,N}(t)\big\|^{2k}_{L^{2k}} \leqslant c^*(\Psi)\sum_{k=1}^{2}N^{5/6(k-1)}\big\|\widetilde{\Psi}_N(t)\big\|^{2k}. \tag{4.15}$$

Substituting (4.13)–(4.15) into (4.12) and integrating the resulting inequality with respect to $t$, we obtain that

$$\big\|\widetilde{\Psi}_N(t)\big\|^2 \leqslant c^*(\Psi)\int_0^t\sum_{k=1}^{2}N^{5/6(k-1)}\big\|\widetilde{\Psi}_N(s)\big\|^{2k}\,\mathrm{d}s + c^*(\Psi)N^{1-r}\|\Psi\|^2_{L^2(0,T;H^r_A(\Lambda))}. \tag{4.16}$$

The following Gronwall-type lemma is needed for the convergence analysis.

**Lemma 4.1.** Assume that

(i) $a$ and $a_k$ are non-negative constants,

(ii) $E(t)$ is a non-negative function of $t$,

(iii) $\rho \geqslant 0$ and for all $0 \leqslant t \leqslant t_1$,

$$E(t) \leqslant \rho + a \int_0^t \left( E(s) + \sum_{k=2}^{n} N^{a_k} E^k(s) \right) \mathrm{d}s,$$

(iv) for certain $t_1 > 0$, $\rho \mathrm{e}^{ant_1} \leqslant \min_{2 \leqslant k \leqslant n} N^{-a_k/(k-1)}$.

Then for all $0 \leqslant t \leqslant t_1$,

$$E(t) \leqslant \rho \mathrm{e}^{ant}.$$

*Proof.* Consider the function $Y(t)$ satisfying

$$Y(t) = \rho + an \int_0^t Y(s)\, \mathrm{d}s.$$

Clearly $Y(t) = \rho \mathrm{e}^{ant}$. Thus for all $t \leqslant t_1$,

$$E(t) \leqslant Y(t) \leqslant \rho \mathrm{e}^{ant}. \qquad \square$$

Applying lemma 4.1 to (4.16) and using theorem 2.3 again, we obtain the following result.

**Theorem 4.1.** If for $r \geqslant 11/6$, $\Psi \in L^\infty(0.T; L^\infty(\Lambda) \cap H_A^1(\Lambda)) \cap L^2(0, T; H_A^r(\Lambda))$, then for all $0 \leqslant t \leqslant T$,

$$\left\| \Psi(t) - \Psi_N(t) \right\| \leqslant c^*(\Psi) N^{(1-r)/2} \|\Psi\|_{L^2(0,T;H_A^r(\Lambda))}.$$

## 5. Hermite-pseudospectral method for the Dirac equation

Although the Hermite-spectral method in the last section is theoretically attractive, its actual implementation is not very efficient due to the nonlinear terms involved. In this section, we investigate a Hermite-pseudospectral scheme which is much easier to implement in practice and much more computationally efficient.

Let $\Lambda_N = \{x = \sigma_{N,j},\ 0 \leqslant j \leqslant N\}$. We look for $\Psi_N(x, t) \in \mathcal{H}_N$ for all $0 \leqslant t \leqslant T$, such that

$$\begin{cases} \partial_t \psi_{1,N}(x, t) + \partial_x \psi_{2,N}(x, t) + \mathrm{i} m \psi_{1,N}(x, t) + 2\lambda Q_1\big(\Psi_N(x, t)\big) = f_1(x, t), \\ \quad x \in \Lambda_N,\ 0 < t \leqslant T, \\ \partial_t \psi_{2,N}(x, t) + \partial_x \psi_{1,N}(x, t) - \mathrm{i} m \psi_{2,N}(x, t) + 2\lambda Q_2\big(\Psi_N(x, t)\big) = f_2(x, t), \\ \quad x \in \Lambda_N,\ 0 < t \leqslant T, \\ \Psi_N(0) = I_N \Psi^{(0)} = \big(I_N \psi_{1,N}^{(0)}, I_N \psi_{2,N}^{(0)}\big)^{\mathrm{T}}. \end{cases} \tag{5.1}$$

Thanks to (3.4) and the fact that $\partial_x \psi_{j,N} \in \mathcal{H}_{N+1}$, (5.1) is equivalent to the system

$$\begin{cases} \big(\partial_t \psi_{1,N}(t) + \partial_x \psi_{2,N}(t) + \mathrm{i}m\psi_{1,N}(t) + 2\lambda I_N Q_1\big(\Psi_N(t)\big), \phi\big) = \big(I_N f_1(t), \phi\big), \\ \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \big(\partial_t \psi_{2,N}(t) + \partial_x \psi_{1,N}(t) - \mathrm{i}m\psi_{2,N}(t) + 2\lambda I_N Q_2\big(\Psi_N(t)\big), \phi\big) = \big(I_N f_2(t), \phi\big), \\ \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \Psi_N(0) = I_N \Psi^{(0)}. \end{cases} \tag{5.2}$$

It can be verified that for any vector function $U = (u_1, u_2)^{\mathrm{T}}$,

$$\big(I_N Q_j(U), u_j\big) + \overline{\big(I_N Q_j(U), u_j\big)} = 0, \quad j = 1, 2. \tag{5.3}$$

Thus, following an argument similar to the proof of (4.7), we derive that $\Psi_N$ satisfies the same conservation property as (4.7).

We next prove the convergence of scheme (5.2) under some conditions on the smoothness of $\Psi$. Let $\Psi_N^*$ and $\widetilde{\Psi}_N$ be the same as in the last section. By an argument similar to the derivation of (4.10) and (4.11), we derive from (4.2) and (5.2) that

$$\begin{cases} \big(\partial_t \tilde{\psi}_{1,N}(t) + \partial_x \tilde{\psi}_{2,N}(t) + \mathrm{i}m\tilde{\psi}_{1,N}(t) + 2\lambda I_N Q_1\big(\widetilde{\Psi}_N(t)\big), \phi\big) \\ \quad = \big(E_1(t) + 2\lambda \widetilde{F}_1(t), \phi\big) + \big(\widetilde{G}_1(t) + \widetilde{H}_1(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \big(\partial_t \tilde{\psi}_{2,N}(t) + \partial_x \tilde{\psi}_{1,N}(t) - \mathrm{i}m\tilde{\psi}_{2,N}(t) + 2\lambda I_N Q_2\big(\widetilde{\Psi}_N(t)\big), \phi\big) \\ \quad = \big(E_2(t) + 2\lambda \widetilde{F}_2(t), \phi\big) + \big(\widetilde{G}_2(t) + \widetilde{H}_2(t), \phi\big), \quad \forall \phi \in \mathcal{H}_N,\ 0 < t \leqslant T, \\ \widetilde{\Psi}_N(0) = I_N \Psi^{(0)} - P_N \Psi^{(0)}, \end{cases} \tag{5.4}$$

where $E_j(t)$ are the same as in (4.11), and

$$\begin{aligned} \widetilde{F}_j(t) &= Q_j\big(\Psi(t)\big) - I_N Q_j\big(\Psi_N^*(t)\big), && j = 1, 2, \\ \widetilde{G}_j(t) &= -I_N\big(Q_j\big(\Psi_N^*(t) + \widetilde{\Psi}_N(t)\big) - Q_j\big(\Psi_N^*(t)\big) - Q_j\big(\widetilde{\Psi}_N(t)\big)\big), && j = 1, 2, \\ \widetilde{H}_j(t) &= I_N f_j(t) - f_j(t), && j = 1, 2. \end{aligned}$$

In the same manner as in the derivation of (4.12), we can derive

$$\frac{\mathrm{d}}{\mathrm{d}t}\big\|\widetilde{\Psi}_N(t)\big\|^2 \leqslant c\big\|\widetilde{\Psi}_N(t)\big\|^2 + c\sum_{j=1}^{2}\big(\big\|E_j(t)\big\|^2 + \big\|\widetilde{F}_j(t)\big\|^2 + \big\|\widetilde{G}_j(t)\big\|^2\big). \tag{5.5}$$

We have already estimated $\|E_j(t)\|^2$ by (4.13). Next, we have

$$\big\|\widetilde{F}_j(t)\big\|^2 \leqslant 2\big\|Q_j\big(\Psi(t)\big) - I_N Q_j\big(\Psi(t)\big)\big\|^2 + 2\big\|I_N\big(Q_j\big(\Psi(t)\big) - Q_j\big(\Psi_N^*(t)\big)\big)\big\|^2. \tag{5.6}$$

By theorem 3.1,

$$\begin{aligned} \big\|Q_j\big(\Psi(t)\big) - I_N Q_j\big(\Psi(t)\big)\big\| &\leqslant cN^{2/3-r}\big\|Q_j\big(\Psi(t)\big)\big\|_{r,A}^2 \\ &\leqslant cN^{2/3-r}\big\|\Psi(t)\big\|_{W^{[r/2],\infty}}^4\big\|\Psi(t)\big\|_{r,A}^2. \end{aligned} \tag{5.7}$$

We derive by lemma 3.1 that

$$\begin{aligned}&\left\| I_N\big(Q_j\big(\Psi(t)\big) - \big(Q_j\big(\Psi_N^*(t)\big)\big)\right\|^2\\&\quad\leqslant c\Big(\left\| Q_j\big(\Psi(t)\big) - Q_j\big(\Psi_N^*(t)\big)\right\|^2 + n^{-1/3}\left| Q_j\big(\Psi(t)\big) - Q_j\big(\Psi_N^*(t)\big)\right|_1^2\Big).\end{aligned} \tag{5.8}$$

The first term at the right side of the above inequality has been also estimated by (4.14). Moreover by theorems 2.3 and 2.4,

$$\begin{aligned}&N^{-1/3}\left| Q_j\big(\Psi(t)\big) - Q_j\big(\Psi_N^*(t)\big)\right|_1^2\\&\quad\leqslant cN^{-1/3}\sum_{k=1}^{2}\sum_{j=1}^{2}\Big(\left\|\psi_j(t)\right\|_{W^{1,\infty}}^{4-2k}\left\|\psi_{j,N}^*\right\|_{W^{1,\infty}}^{2k}\left\|\psi_j(t) - \psi_{j,N}^*\right\|^2\\&\qquad + \left\|\psi_j(t)\right\|_{\infty}^{4-2k}\left\|\psi_{j,N}^*\right\|_{\infty}^{2k}\left|\psi_j(t) - \psi_{j,N}^*(t)\right|_1^2\Big)\\&\quad\leqslant c^{**}(\Psi)N^{2/3-r}\left\|\Psi(t)\right\|_{r,A}^2,\end{aligned} \tag{5.9}$$

where $c^{**}(\Psi)$ is a certain positive constant depending only on

$$\left\|\Psi^{(0)}\right\| \quad\text{and}\quad \|\Psi\|_{L^\infty(0,T;W^{[1/2],\infty}(\Lambda)\cap H_A^{1+d}(\Lambda))} \quad (d > 1/2).$$

The combination of (5.6)–(5.9) and (4.14) leads to

$$\left\|\widetilde{F}_j(t)\right\|^2 \leqslant c^{**}(\Psi)N^{2/3-r} + \left\|\Psi(t)\right\|_{r,A}^2. \tag{5.10}$$

Furthermore, using (3.5) and remark 2.1 yields

$$\begin{aligned}\left\|\widetilde{G}_j(t)\right\|^2 = \left\|\widetilde{G}_j(t)\right\|_N^2 &\leqslant c\Big(\left\|\Psi_N^*(t)\right\|_\infty^4\left\|\widetilde{\Psi}_N(t)\right\|_N^2 + \left\|\Psi_N^*(t)\right\|_\infty^2\left\||\widetilde{\Psi}_N(t)|^2\right\|_N^2\Big)\\&\leqslant c^{**}(\Psi)\Big(\left\|\widetilde{\Psi}_N(t)\right\|^2 + \left\|\widetilde{\Psi}_N(t)\right\|_\infty^2\left\|\widetilde{\Psi}_N(t)\right\|^2\Big)\\&\leqslant c^{**}(\Psi)\Big(\left\|\widetilde{\Psi}_N(t)\right\|^2 + N^{5/6}\left\|\widetilde{\Psi}_N(t)\right\|^4\Big),\end{aligned} \tag{5.11}$$

and

$$\left\|\widetilde{H}_j(t)\right\|^2 \leqslant cN^{2/3-r_1}\left\|f_i(t)\right\|_{r_1,A}^2. \tag{5.12}$$

Finally, by theorem 2.3 and 3.1,

$$\begin{aligned}\left\|\widetilde{\Psi}(0)\right\|^2 &\leqslant \left\|\Psi^{(0)} - P_N\Psi^{(0)}\right\|^2 + \left\|\Psi^{(0)} - I_N\Psi^{(0)}\right\|^2\\&\leqslant cN^{2/3-r_0}\left\|\Psi^{(0)}\right\|_{r_0,A}^2.\end{aligned} \tag{5.13}$$

Substituting (5.10)–(5.13) and (4.13) into (5.5) and integrating the resulting inequality with respect to $t$, we derive that

$$\left\|\widetilde{\Psi}_N(t)\right\|^2 \leqslant c^{**}(\Psi)\int_0^t\Big(\left\|\widetilde{\Psi}_N(s)\right\|^2 + N^{5/6}\left\|\widetilde{\Psi}_N(s)\right\|^4\Big)\,\mathrm{d}s + \rho(t) \tag{5.14}$$

with

$$\rho(t) = c^{**}(\Psi)N^{1-r}\|\Psi\|^2_{L^2(0,t;H^r_A(\Lambda))} + cN^{2/3-r_0}\big\|\Psi^{(0)}\big\|^2_{r_0,A} + cN^{2/3-r_1}\big\|f(t)\big\|^2_{L^2(0,T;H^{r_1}_A(\Lambda))}.$$

If $r > 11/6$ and $r_0, r_1 > 3/2$, then $\rho = \mathrm{o}(N^{-5/6})$. Hence, application of lemma 4.1 to (5.13) leads to following result:

**Theorem 5.1.** If for $r > 11/6$, $r_0, r_1 > 3/2$ and $d > 1/2$, $\Psi \in L^\infty(0,T; W^{[r/2],\infty} \cap H^{1+d}_A(\Lambda)) \cap L^2(0,T; H^r_A(\Lambda))$, $f \in L^2(0,T; H^{r_1}_A(\Lambda))$ and $\Psi^{(0)} \in H^{r_0}_A(\Lambda)$, then for all $0 \leqslant t \leqslant T$,

$$\big\|\Psi(t) - \Psi_N(t)\big\| \leqslant c^{**}(\Psi)\big(N^{(1-r)/2} + N^{1/3-r_0/2} + N^{1/3-r_1/2}\big).$$

*Remark 5.1.* The conditions on $\Psi$ in theorem 5.1 seems rather restrictive. However, such solutions do exist in physically relevant situations. For instance, the soliton solutions of (4.1) are in $C^\infty(0,T; C^\infty(\Lambda))$.

## 6. Numerical results

We consider first a model second-order linear equation: find $u \in H^1(\Lambda)$ such that

$$\alpha(u,v) + (\partial_x u, \partial_x v) = (f,v), \quad \forall v \in H^1(\Lambda). \tag{6.1}$$

We define a Hermite pseudospectral approximation for (6.1) as follows: find $u_N \in \mathcal{H}_N$ such that

$$\alpha(u_N, v_N) + (\partial_x u_N, \partial_x v_N) = (I_N f, v_N), \quad \forall v_N \in \mathcal{H}_N. \tag{6.2}$$

Using theorems 2.3 and 3.1, it is an easy matter to verify, assuming $\alpha > 0$, that the following error estimate holds (for $r, \mu \geqslant 1$):

$$\|u - u_N\|_1 \leqslant c\big(N^{(1-r)/2}\|u\|_{r,A} + N^{1/3-\mu/2}\|f\|_{\mu,A}\big). \tag{6.3}$$

Let us write

$$\begin{aligned} u_N &= \sum_{k=0}^{N} \tilde{u}_k \widehat{H}_k(x), & \bar{u} &= \big(\tilde{u}_0, \tilde{u}_1, \ldots, \tilde{u}_N\big)^{\mathrm{T}}, \\ \tilde{f}_k &= \big(I_N f, \widehat{H}_k\big), & \bar{f} &= \big(\tilde{f}_0, \tilde{f}_1, \ldots, \tilde{f}_N\big)^{\mathrm{T}}, \\ s_{kj} &= \big(\partial_x \widehat{H}_j, \partial_x \widehat{H}_k\big), & S &= (s_{kj})_{k,j=0,1,\ldots,N}, \\ m_{kj} &= \big(\widehat{H}_j, \widehat{H}_k\big), & M &= (m_{kj})_{k,j=0,1,\ldots,N}. \end{aligned}$$

Then, (6.3) becomes the matrix equation

$$(\alpha M + S)\bar{u} = \bar{f}. \tag{6.4}$$

Thanks to (2.9) and (2.10), $M$ is a diagonal matrix and $S$ is a symmetric positive definite matrix with three nonzero diagonals (which can be split-up into two tridiagonal matrices for odd and even entries). Hence, (6.4) can be efficiently inverted.

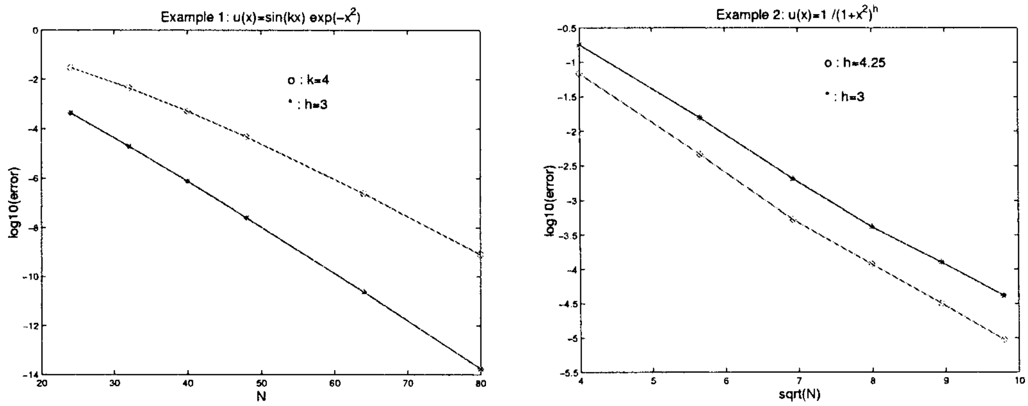
In order to examine numerically the convergence behaviors, we present some illustrative numerical results using the Hermite–Gauss pseudospectral method. We considered the following three exact solutions of (6.1):

**Example 1.** $u(x) = \sin kx \mathrm{e}^{-x^2}$ (exponential decay at infinity).

**Example 2.** $u(x) = 1/(1+x^2)^h$ (algebraic decay without essential singularity at infinities).

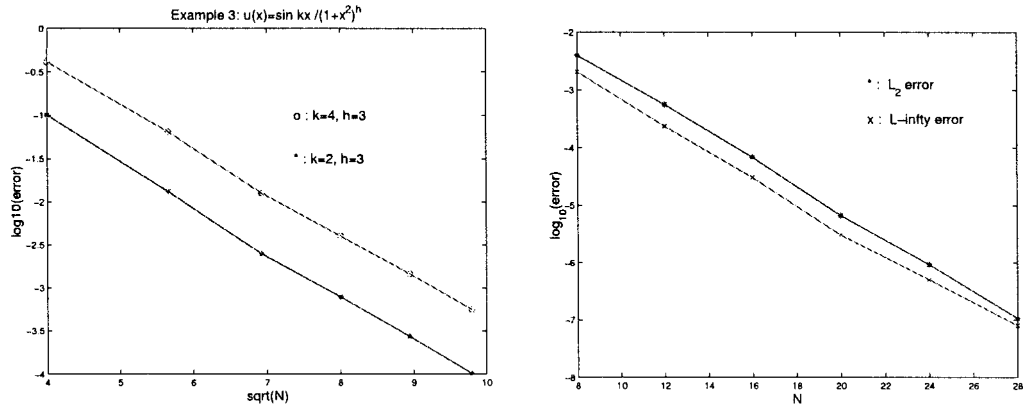
**Example 3.** $u(x) = \sin kx/(1+x^2)^h$ (algebraic decay with essential singularities at infinities).

In figures 1 and 2(a), we plot the convergence rates of the maximum error at the Hermite–Gauss points for the three examples. These plots indicate that for example 1, we have $\|u - u_N\| \sim \exp(-cN)$, while for examples 2 and 3, we have $\|u - u_N\| \sim \exp(-c\sqrt{N})$. According to (6.3), the geometric convergence is expected for example 1 but only algebraic convergence is predicted for examples 2 and 3. It is surprising that a subgeometric exponential convergence rate is observed even for example 3, which has essential singularities at infinities. It is still an open question whether (6.3) is optimal in the general cases and whether one can improve the error estimates for a special class of functions including those in examples 2 and 3.




(a) (b)

Figure 1. Convergence rates of the Hermit–Gauss pseudospectral approximation. (a) Example 1; (b) Example 2.




(a) (b)

Figure 2. Convergence rates of the Hermit–Gauss pseudospectral approximation, (a) Example 3; (b) Dirac equation.

Next, we consider the Hermite–Gauss pseudospectral approximation (5.1) for the Dirac equation. We take the exact solution of the Dirac equation to be

$$\psi_1(x,t) = \psi_2(x,t) = \mathrm{e}^{-x^2+t}.$$

We used the standard fourth-order Runge–Kutta method for the time discretization with a time step small enough so that the time discretization error can be ignored compared to the spacial discretization error. In figure 2(b), we plot the $L^2$-error and $L^\infty$-error for various $N$ at time $t = 1$. It is clear from the plot that both errors behave like $\exp(-cN)$.

In summary, although we have only performed analysis and implementations of the Hermite spectral and pseudospectral methods for a second-order model linear equation and a nonlinear Dirac equation, it is clear that these methods can be applied to more general linear and nonlinear PDEs. The excellent theoretical and numerical convergence rates presented in this paper indicate that the spectral and pseudospectral methods using Hermite functions are very effective tools for numerical solutions of PDEs on the whole line.

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