

# THE HERMITE SPECTRAL METHOD FOR GAUSSIAN-TYPE FUNCTIONS\*

TAO TANG†

**Abstract.** Although Hermite functions were widely used for many practical problems, numerical experiments with the standard (normalized) Hermite functions  $\psi_n(v)$  worked poorly in the sense that too many Hermite functions are required to solve differential equations. In order to obtain accurate numerical solutions, it is necessary to choose a scaling factor  $\alpha$  and use  $\psi_n(\alpha v)$  as the basis functions. In this paper the scaling factors are given for functions that are of Gaussian type, which have finite supports  $[-M, M]$ . The scaling factor used is  $\max_{0 \leq j \leq N} \{\gamma_j\}/M$ , where  $\{\gamma_j\}_{j=0}^N$  are the roots of  $\psi_{N+1}(v)$  and  $N + 1$  is the number of the truncated terms used. The numerical results show that after using this scaling factor, only reasonable numbers of the Hermite functions are required to solve differential equations.

**Key words.** spectral method, Hermite functions

**AMS subject classifications.** 65M70, 33C25, 35K05

**1. Introduction.** The normalized Hermite functions are

$$(1.1) \quad \psi_n(v) = \frac{1}{\sqrt{2^n n!}} H_n(v) \exp\left(-\frac{v^2}{2}\right),$$

where the  $H_n(v)$  are the usual (unnormalized) Hermite polynomials. For physical problems posed on  $v \in (-\infty, \infty)$  (i.e., infinite domain), a variety of spectral techniques have been developed in recent years. These include the use of Fourier series combined with domain truncation, sine function, Hermite functions, and algebraically mapped Chebyshev polynomials. Previous results for these techniques are summarized, for example in Boyd [5, Chap. 14]. Many researchers have noticed that the close connection of Hermite functions to the physics makes them a natural choice of basis functions for many fields of science and engineering. Numerical applications include many problems in continuum mechanics (see, e.g., [3]), particle physics (see, e.g., [9, 15] and [17]), tropical meteorology, and oceanography (see e.g., [2, 8], and [14]). Also one reason for using Hermite spectral methods is that Hermite system has some very attractive properties from the numerical point of view. For example, in a recent paper, Weideman [19] showed that the spectral radii for the first and second Hermite differentiation matrices are  $O(\sqrt{N})$  and  $O(N)$ , respectively, where  $N + 1$  is the number of truncated terms used. This places rather weak stability restrictions on the Hermite method. For example, if we consider the standard heat equation, then a maximum step size in the time direction of order  $O(N^{-1})$  is required, whereas for Fourier and Chebyshev methods it is of order  $O(N^{-2})$  and  $O(N^{-4})$ , respectively. In the actual calculations this means that we need not even consider implicit time integration methods with the Hermite method. A theoretical study of the Hermite method for the heat equation is given in recent paper, [11], which is concerned with the stability and convergence properties of the method.

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†Department of Mathematics and Statistics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6. This work was supported by Natural Sciences and Engineering Research Council of Canada grant OGP0105545

Although the Hermite spectral methods have some attractive properties, the direct spectral approach may not produce good approximations. In the practical calculations, it is necessary to choose a scaling factor  $\alpha$  since we can always use  $\psi_n(\alpha v)$  as the basis set for any finite  $\alpha$ . This freedom does not exist for a finite interval, but after a change of scale in  $v$ , an infinite domain is still an infinite domain. It was pointed out by Boyd [4]-[6] that  $\alpha$  should increase with the truncated terms used, but the theory of choosing an optimum scaling factor is still incomplete. In this paper, we study how to choose a proper scaling factor for a class of functions that decay at infinity at least like  $\exp(-pv^2)$  for some positive constants  $p$  (i.e., Gaussian type). Solutions of many practical problems behave like Gaussian-type functions at infinity, for example, the diffusion equations for heat flow and the Fokker-Planck equations for particle physics (see, e.g., [10] and [17]). The idea underlying our approach is the following: In using spectral collocation methods we choose a scaling factor  $\alpha$  which depends on the ratio of the maximum root of  $H_{N+1}(v)$  and the length of the finite support of the function. The usual method for dealing with the infinite interval is simply to truncate  $(-\infty, \infty)$  to a finite interval  $[-M, M]$ . The scaling factor  $\alpha$  is chosen so that all of the collocation points are within  $[-M, M]$ . The numerical results show that after using the scaling factor, reasonable numbers of Hermite functions are required to resolve a Gaussian-type function.

**2. Hermite collocation methods.** For a Gaussian-type function  $f$ , we have the expansion

$$(2.1) \quad f(v) = \sum_{n=0}^{\infty} a_n \psi_n(\alpha v), \quad |v| < \infty,$$

which is equivalent to

$$(2.2) \quad f(v/\alpha) = \sum_{n=0}^{\infty} a_n \psi_n(v), \quad |v| < \infty.$$

where  $\alpha$  is a positive constant. The spectral method of order  $N$  is to approximate the function  $f$  using the first  $N+1$  terms in the expansion series, i.e., the coefficients  $\{a_n\}_{n=N+1}^{\infty}$  are set equal to 0. Therefore, we have the spectral approximations

$$(2.3) \quad f_N(v/\alpha) = \sum_{n=0}^N a_n \psi_n(v).$$

When solving differential equations, we need to relate the coefficients of the derived function to those of the original function, as given by

$$(2.4) \quad f^{(k)}(v/\alpha) = \sum_{n=0}^N a_n \psi_n^{(k)}(v) = \sum_{n=0}^N a_n^{(k)} \psi_n(v).$$

Using the recurrence formulas of Hermite functions we can obtain that

$$(2.5) \quad a_n^{(1)} = \frac{\alpha}{\sqrt{2}} (-\sqrt{n} a_{n-1} + \sqrt{n+1} a_{n+1}),$$

$$(2.6) \quad a_n^{(2)} = \frac{\alpha^2}{2} \left( \sqrt{(n-1)n} a_{n-2} - (2n+1) a_n + \sqrt{(n+1)(n+2)} a_{n+2} \right),$$

with  $a_n = 0$  whenever  $n < 0$  or  $n > N$ .

In pseudospectral methods, the optimum pseudospectral points are the roots of  $H_{N+1}(v)$ , which are denoted by  $\{\gamma_j\}_{j=0}^N$  with the order  $\gamma_0 > \gamma_1 > \cdots > \gamma_N$ . Assuming that (2.3) is satisfied at the collocation points we have

$$(2.7) \quad f_N\left(\frac{\gamma_j}{\alpha}\right) = \sum_{n=0}^N a_n \psi_n(\gamma_j), \quad 0 \leq j \leq N.$$

Noting that

$$(2.8) \quad \sum_{n=0}^N \psi_n(\gamma_i) \psi_n(\gamma_j) = C_i \delta_{ij}, \quad 0 \leq i, j \leq N,$$

$$(2.9) \quad C_i = \sum_{n=0}^N [\psi_n(\gamma_i)]^2, \quad 0 \leq i \leq N,$$

we obtain from (2.7) that

$$(2.10) \quad a_n = \sum_{j=0}^N \frac{1}{C_j} f_N\left(\frac{\gamma_j}{\alpha}\right) \psi_n(\gamma_j), \quad 0 \leq n \leq N.$$

The above relations between  $\{a_n\}$  and  $\{f_N(\gamma_j/\alpha)\}$  give a simple evaluation of the derivatives of  $f_N(v)$  at the points  $\{\gamma_j/\alpha\}_{j=0}^N$ . Once  $\{f_N(\gamma_j/\alpha)\}_{j=0}^N$  are known, the coefficients  $\{a_n\}_{n=0}^N$  can be obtained by (2.10). Then, the first and second derivatives of  $f_N$  at points  $\{\gamma_j/\alpha\}_{j=0}^N$  can be computed by (2.4)–(2.6). A higher order of derivatives can be obtained in a similar way. If  $\{a_n\}_{n=0}^N$  are given, the function  $f_N(v)$  is computed by

$$(2.11) \quad f_N(v) = \sum_{n=0}^N a_n \psi_n(\alpha v).$$

**3. The scaling factor.** Suppose that the function  $f$  has a finite support  $[-M, M]$ , i.e.,  $f(v) \sim 0$  for  $|v| > M$ . In order to compute  $\{a_n\}_{n=0}^N$  by (2.10), we need to use information from the interval  $[-M, M]$  only, since outside of this region the function is almost zero and will not contribute much to  $a_n$ . This simple motivation suggests that

$$(3.1) \quad \left| \frac{\gamma_j}{\alpha} \right| \leq M, \quad \text{for all } 0 \leq j \leq N.$$

The above condition is satisfied by choosing

$$(3.2) \quad \alpha = \alpha_N = \max_{0 \leq j \leq N} \{\gamma_j\} = \gamma_0/M.$$

Since  $\gamma_0 \sim \sqrt{2N}$  (see, e.g., [1]), we obtain that

$$(3.3) \quad \alpha_N \sim \sqrt{2N}/M.$$

The Hermite spectral methods were rejected before because of their poor resolution properties. Gottlieb and Orszag [12] investigated the rate of convergence of Hermite

series by considering the expansion of the sine functions. They found that to resolve  $p$  wavelengths of the sine function requires  $O(p^2)$  polynomials. In the case when the function decays rapidly, we need to consider the sine functions which oscillate rapidly in a finite interval (i.e.,  $|v| \leq \text{Const.}$ ). Consider

$$(3.4) \quad \sin(pv) = \sum_{n=0}^{\infty} c_{2n+1} H_{2n+1}(v),$$

where

$$(3.5) \quad c_{2n+1} = (-1)^n \frac{p^{2n+1} \exp(-p^2/4)}{2^{2n+1} (2n+1)!},$$

for  $n = 0, 1, \dots$ . Using the asymptotic expansion of  $H_n(v)$  [1],

$$(3.6) \quad H_n(v) \sim \exp(v^2/2) \frac{n!}{(\frac{1}{2}n)!} \cos\left(\sqrt{2n+1}v - \frac{1}{2}n\pi\right),$$

and Sterling's formula

$$(3.7) \quad n! \sim \sqrt{2\pi} n^{n+1/2} \exp(-n),$$

we obtain the asymptotic behavior of the  $n$ th term of the right-hand side of (3.4) as

$$(3.8) \quad \text{term}_n \sim \frac{1}{\sqrt{2\pi}} \left(\frac{p^2}{4n}\right)^{n+1/2} \exp\left(n - p^2/4 + v^2/2\right).$$

It can be seen from the above equation that if  $n \approx p^2/4$  then the  $n$ th term behaves like  $\exp(v^2/2)/\sqrt{2\pi}$ , which is in general not small. That is, to resolve  $p$  wavelengths of the sine functions requires more than  $0.25p^2$  Hermite functions. This result is similar to that observed by Gottlieb and Orszag [12]. However, if we use the scaling factor  $\alpha_N$  of the form (3.2), i.e., if we expand

$$(3.9) \quad \sin(pv) = \sum_{n=0}^{\infty} d_{2n+1} H_{2n+1}(\alpha_N v),$$

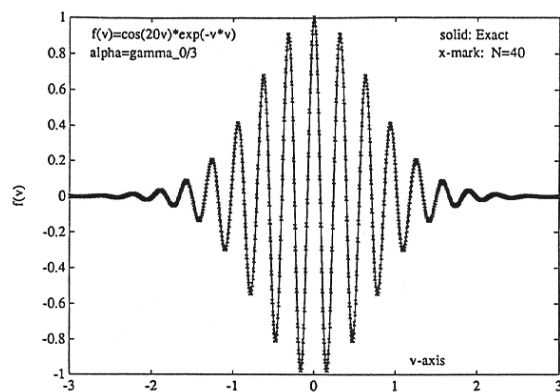
with  $\alpha_N = \gamma_0$ , then the  $n$ th expansion term is of the asymptotic form

$$(3.10) \quad \text{term}_n \sim \frac{1}{\sqrt{2\pi}} \left(\frac{p^2}{4n\alpha_N^2}\right)^{n+\frac{1}{2}} \exp\left(n - \frac{p^2}{4\alpha_N^2} + \frac{v^2}{2}\right).$$

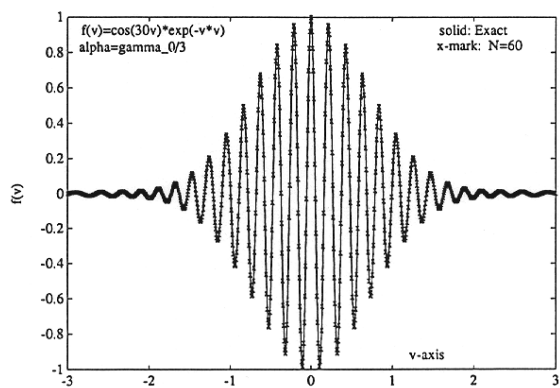
Noting that  $\alpha_N^2 \sim 2N$ , we obtain

$$(3.11) \quad \text{term}_n \sim \frac{p}{4\sqrt{\pi n N}} \left[\frac{p^2}{8nN} \exp\left(1 - \frac{p^2}{8nN}\right)\right]^n \exp\left(\frac{v^2}{2}\right).$$

The right-hand side of the above equation decays exponentially when  $n \geq N \approx p$ . This result shows that using the scaling factor can reduce the number of required polynomials to the best possible case. The above analysis is only given for the expansion in Hermite polynomials, but similar behavior can be seen for the expansion



(a)



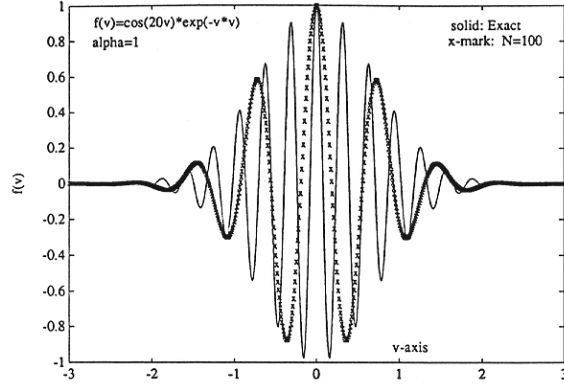
(b)

FIG. 1. (a) *Hermite spectral approximation for  $f(v) = \cos(20v) \exp(-v^2)$  with  $N = 40$  and  $\alpha = \gamma_0/3$* ; (b) *Hermite spectral approximation for  $f(v) = \cos(30v) \exp(-v^2)$  with  $N = 40$  and  $\alpha = \gamma_0/3$ .*

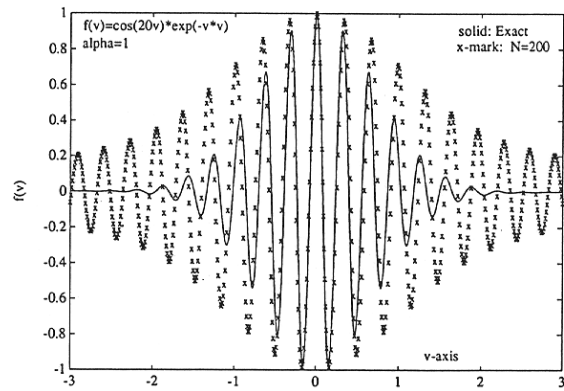
in the normalized Hermite functions (in this case, if the function has a finite support  $[-M, M]$ , then  $N \approx Mp$ ). To see this, we expand

$$(3.12) \quad \cos(pv) \exp(-v^2) = \sum_{n=0}^N a_n \psi_n(\alpha v).$$

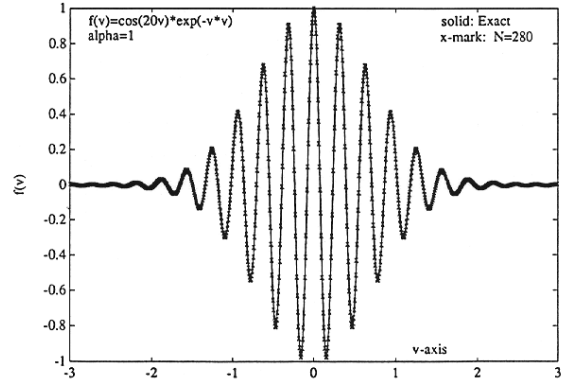
The coefficients  $\{a_n\}_{n=0}^N$  are obtained by using (2.10) and the numerical curve is given by (2.11). It can be seen from Fig. 1 that, after scaling (i.e.,  $\alpha = \alpha_N = \gamma_0/3$ ), 20 and 30 expansion terms give good approximations to the function  $\cos(pv) \exp(-v^2)$  is an even function and the number of the expansion term is  $N/2$  since the odd terms are zero). However, approximations without scaling (i.e.,  $\alpha = 1$ ) require more than 100 terms in case  $p = 20$ ; see Fig. 2. Furthermore, in Fig. 3 and 4, we have plotted the absolute values of the even coefficients in (3.12) (noting that the odd coefficients are zero) as a function of  $n$  in the case  $p = 20$ . In these two figures a log scale was used. Since  $\psi_n(\alpha v) = O(n^{-1/4})$ , the  $n$ th term of (3.12) is small only when its coefficient is small. Figure 3 suggests that in order to have the  $n$ th term less than  $10^{-3}$ , for all  $n \geq N$ , we need about 25 expansion terms (i.e.,  $N = 50$ ) when the scaling factor



(a)



(b)



(c)

FIG. 2. Hermite spectral approximation for  $f(v) = \cos(20v) \exp(-v^2)$  without using a scaling factor. (a)  $N = 100$ ; (b)  $N = 200$ ; and (c)  $N = 280$ .

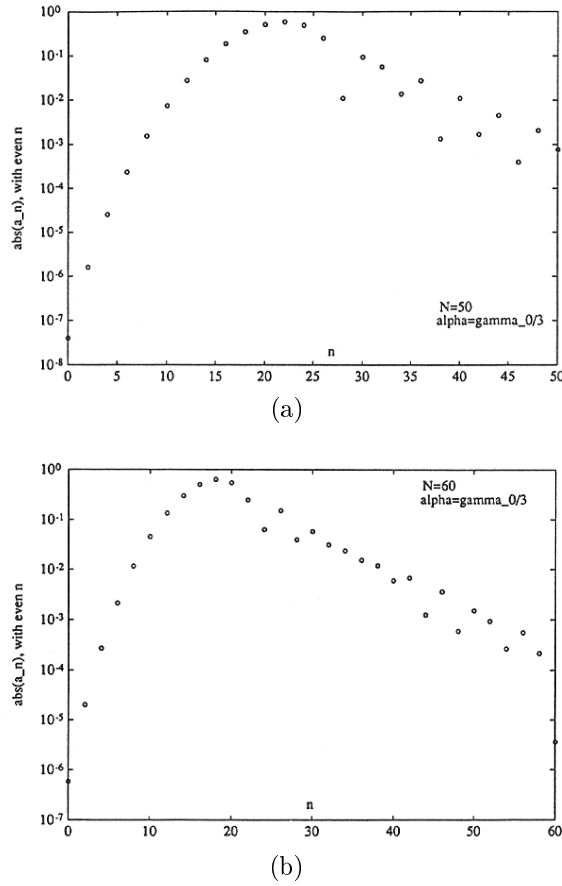


FIG. 3. The even coefficients of the Hermite expansions for  $f(v) = \cos(20v) \exp(-v^2)$ . (a)  $N = 50$  and  $\alpha = \gamma_0/3$ ; (b)  $N = 60$  and  $\alpha = \gamma_0/3$ .

is used. However, Fig. 4 shows that about 140 expansion terms are required for the conventional expansion (i.e.,  $\alpha = 1$ ).

Many practical problems require to approximate the distribution function of the form  $\exp(-pv^2)$  with moderate and large values of  $p$ , for example, the heat equations with Gaussian-type initial distribution with small viscosity coefficients, and the Fokker-Planck equations with small thermal velocity (cf. [17]) or with small particle response time (cf. [10]). Since

$$(3.13) \quad \exp(-pv^2) = \sum_{n=0}^{\infty} c_{2n} \psi_{2n}(v),$$

where

$$(3.14) \quad c_{2n} = \frac{(-1)^n}{\sqrt{2^{2n} (2n)! (p + \frac{1}{2})}} \left( \frac{p - \frac{1}{2}}{p + \frac{1}{2}} \right)^n \frac{(2n)!}{n!},$$

we obtain the asymptotic behavior of the  $n$ th term of the right hand side of (3.13) as

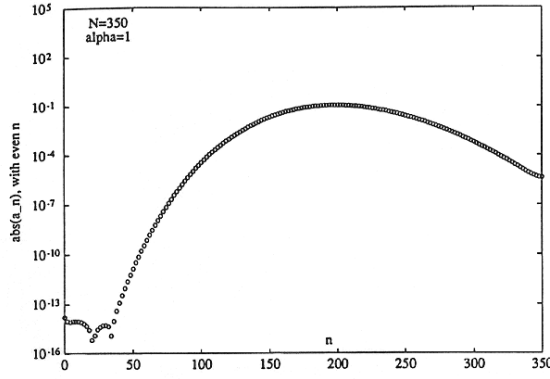


FIG. 4. The even coefficients of the standard Hermite expansions (i.e.,  $\alpha = 1$ ) for  $f(v) = \cos(20v) \exp(-v^2)$ ,  $N = 350$ .

$$(3.15) \quad \text{term}_n \sim \frac{1}{\sqrt{n\pi p}} \left( \frac{p - \frac{1}{2}}{p + \frac{1}{2}} \right)^n.$$

The above result is bad: for large  $p$  about  $O(p)$  terms are required. This can be seen from the following. Since

$$(3.16) \quad \left( 1 - \frac{1}{x} \right)^x \leq \lim_{a \rightarrow \infty} \left( 1 - \frac{1}{a} \right)^a = \frac{1}{e}, \quad \text{for all } x \geq 1,$$

then only when  $n \geq N \approx Cp$  with a positive constant  $C$  (which is quite large),

$$(3.17) \quad \text{term}_n \sim \frac{1}{\sqrt{n\pi p}} e^{-C}.$$

However, when applying the scaling technique to the same function, we obtain

$$(3.18) \quad \exp(-pv^2) = \sum_{n=0}^{\infty} d_{2n} \psi_{2n}(\alpha_N v)$$

with  $\alpha_N = \gamma_0/M$ , as given in (3.2). The asymptotic form of the  $n$ th term is

$$(3.19) \quad \text{term}_n \sim \frac{\alpha_N}{\sqrt{n\pi p}} \left( \frac{p/\alpha_N^2 - \frac{1}{2}}{p/\alpha_N^2 + \frac{1}{2}} \right)^n,$$

which yields that

$$(3.20) \quad \text{term}_n \sim \sqrt{\frac{2N}{n\pi p M^2}} \left( \frac{M^2 p/N - \frac{1}{2}}{M^2 p/N + \frac{1}{2}} \right)^n.$$

If  $p$  is large, then  $M$  can be chosen as one. If  $n \geq N$ , the right-hand side of (3.20) decays rapidly to zero when  $N \geq C(p/N + \frac{1}{2})$  with a positive constant  $C$ :

$$(3.21) \quad \begin{aligned} \text{term}_n &\sim \sqrt{\frac{2N}{n\pi p}} \left( 1 - \frac{1}{p/N + \frac{1}{2}} \right)^n \\ &\leq \sqrt{\frac{1}{p}} \left( 1 - \frac{1}{p/N + \frac{1}{2}} \right)^{C(p/N + 1/2)} \\ &\leq \sqrt{\frac{1}{p}} e^{-C}. \end{aligned}$$



The requirement  $N \geq C(p/N + \frac{1}{2})$  is satisfied when  $N = O(\sqrt{p})$ . In Figs. 5 and 6 we consider a test function  $f(v) = \exp(-2v^2) + \exp(-20v^2)$ . It can be seen from Fig. 5 that after scaling ten expansion terms (again, since the function  $f$  is an even function, the number of expansion terms is  $N/2$ ) give a good approximation. However, Fig. 6 shows that approximations without scaling need more than 50 expansion terms.

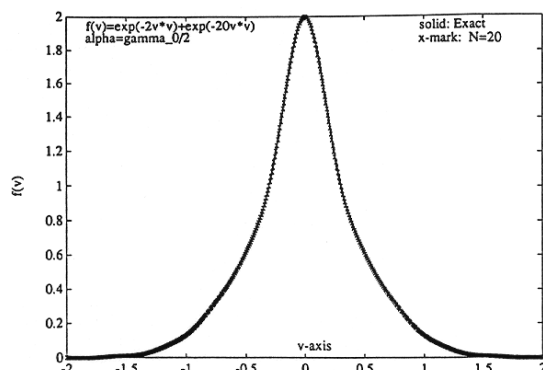


FIG. 5. Hermite spectral approximation for  $f(v) = \exp(-2v^2) + \exp(-20v^2)$ , with  $\alpha = \gamma_0/2$  and  $N = 20$ .

#### 4. Numerical Applications. Consider the eigenvalue problem [3, p. 126]

$$(4.1) \quad -u''(v) + v^4 u(v) = \lambda u(v).$$

By the WKB method, the solution of the above equation has the asymptotic behavior

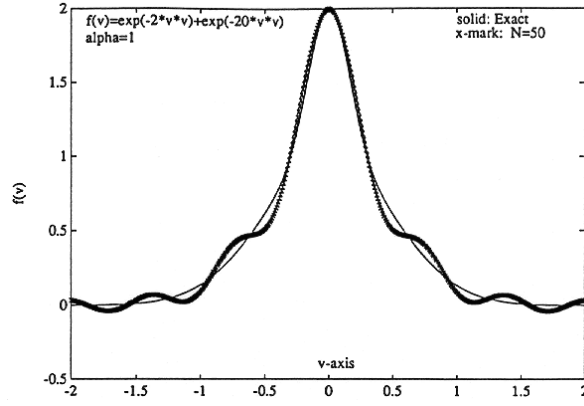
$$(4.2) \quad u(v) \sim \exp(-|v|^3/3).$$

It is obvious from (4.2) that  $u \sim 0$  if  $|v| \geq M \approx 5$ . In order to obtain accurate solutions of (4.1) efficiently, we need to choose the scaling factor  $\lambda = \gamma_0/M$ , where  $\gamma_0 = \max_{0 \leq j \leq N} \{\gamma_j\}$ , with  $\gamma_j$  the roots of  $H_{N+1}(\gamma)$ . Since the solutions of (4.1) are even functions, only  $N/2$  expansion terms are required in the actual calculations. For  $N = 60$ , we predict that the scaling factor  $\alpha \approx 10.16/5.0 \approx 2.0$ . Birkhoff and Fix[3] used Galerkin's method with 30 Hermite functions (i.e.,  $N = 60$ ) to solve (4.1). They found that the standard Hermite functions (i.e., without scaling) gave the first 18 eigenvalues to only three decimal places, whereas using a scaling factor  $\alpha = 2.154$  gave the same eigenvalues to 10 decimal places. That is, an increase of  $10^{-7}$  in accuracy is obtained. They obtained the optimum scaling factor through trial and error (the procedure requires a considerable amount of computer time), but the present work provides an accurate scaling factor in a very simple way.

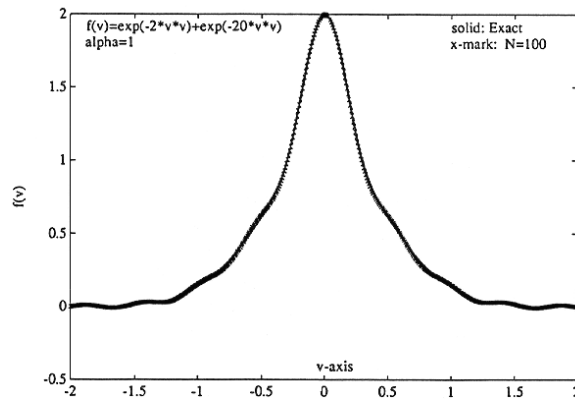
Finally, we apply the scaling technique to the one-dimensional heat equations. The numerical methods for heat equations have been studied extensively in the past (see, e.g., [16] and [18]). Consider the equation

$$(4.3) \quad \frac{\partial u}{\partial t} = \frac{\partial}{\partial v} \left( \nu \frac{\partial u}{\partial v} \right),$$

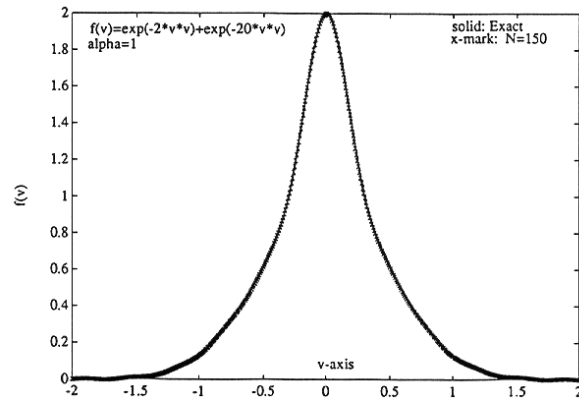
where  $\nu$  is the viscosity coefficient. If an initial temperature distribution is known, then the problem is to determine the temperature distribution at later times. If the



(a)



(b)



(c)

FIG. 6. Hermite spectral approximation for  $f(v) = \exp(-2v^2) + \exp(-20v^2)$  without using a scaling factor. (a)  $N = 50$ ; (b)  $N = 100$ ; and (c)  $N = 150$ .

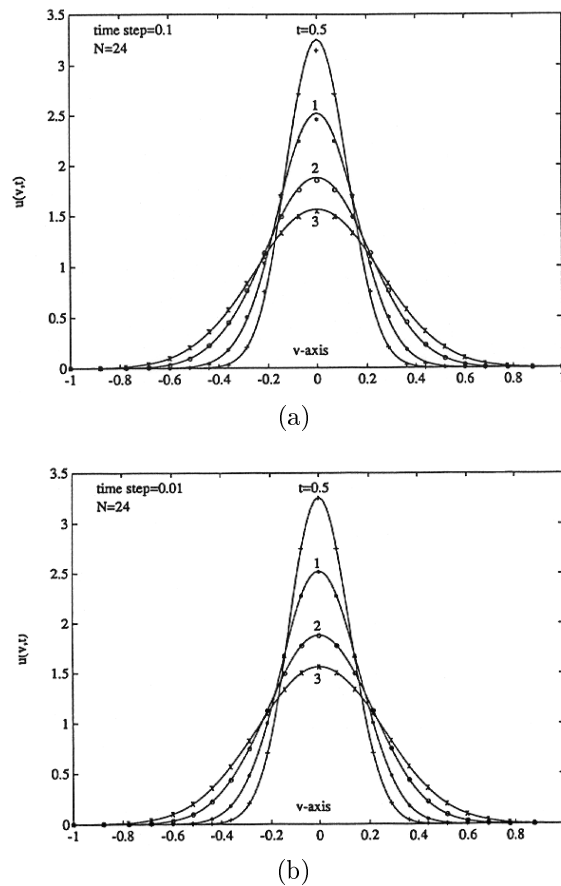


FIG. 7. Comparison between the exact (lines) and numerical (marks) solution for the diffusion equation at different times. (a)  $\Delta t = 0.1$  and  $N = 24$ ; (b)  $\Delta t = 0.01$  and  $N = 24$ .

viscosity coefficient is a constant and the initial distribution is given as

$$(4.4) \quad u(v, 0) = \frac{1}{\sqrt{\nu\pi}} \exp\left(-\frac{v^2}{\nu}\right),$$

then the exact solution of (4.3) and (4.4) is

$$(4.5) \quad u(v, t) = \frac{1}{\sqrt{\pi\nu(4t+1)}} \exp\left(-\frac{v^2}{\nu(4t+1)}\right).$$

Problem (4.3), (4.4) has been chosen since it has an analytic solution and this allows us to compare our numerical results with the exact solution (4.5). We use the pseudospectral method introduced in §2 to compute the numerical solutions. The numerical procedure can be applied to more complicated initial distributions and to variable viscosity coefficients. It can be seen from the previous section that the Hermite spectral methods work well for moderate values of  $\nu$ , but about  $O(1/\nu)$  expansion terms are needed when  $\nu$  is small. However, if we apply the scaling technique, then fewer terms are required. To illustrate this, we shall consider the case when  $\nu = 0.01$ .

Let  $U(t) = [u(\gamma_0/\alpha_N, t), \dots, u(\gamma_N/\alpha_N, t)]^T$ . Then (4.3) may be semidiscretized as

$$(4.6) \quad \frac{dU}{dt} = \nu D^{(2)} U,$$

where  $D^{(2)}$  is the second-order differentiation matrix, which can be computed by (2.4), (2.6), and (2.10). When an explicit method is used to integrate (4.6) in time, the maximum allowable time step needs to satisfy

$$(4.7) \quad \Delta t = O\left(\frac{1}{\nu sr(D^{(2)})}\right),$$

where  $sr(D^{(2)})$  denotes the spectral radius of the matrix  $D^{(2)}$ . Since  $sr(D^{(2)}) = O(\alpha_N^2 N)$  (see [19]) and  $N = O(\sqrt{1/\nu})$  (see §3),  $\alpha_N = O(\sqrt{N})$ , we obtain  $\Delta t = O(1)$ . This suggests that the time-step size can be independent of  $N$  when  $\nu$  is small, which is unlike the finite difference methods [16] and the particle methods [18]. Figure 7 gives a comparison between the exact solution and the numerical results. The solution domain is  $|v| \leq 1$  and  $N$  is 24 (which corresponds to 12 expansion terms, since the solution is an even function). Figure 7(a) shows that even for a quite large step size,  $\Delta t = 0.1$ , stable numerical results can be obtained. The results differ only slightly from those obtained by using a smaller time-step size (see Fig. 7(b)). The numerical results are obtained by using the forward Euler method with constant time-step size  $\Delta t$ .

**5. Discussions.** The method presented in this paper can be used in solving differential equations with solutions that decay exponentially as  $v \rightarrow \infty$ . The idea of using a scaling factor can also be extended to other spectral methods for unbounded intervals, for example, Laguerre spectral methods (see, e.g., [13]) and rational spectral methods (see, e.g., [7] and [19]). It is known that Hermite spectral methods cannot handle functions that decay algebraically with  $v$ , but Laguerre and rational spectral methods are appropriate in approximating slowly decay functions (see, e.g., [5]). It is expected that the use of Laguerre or rational spectral methods with a similar scaling technique can approximate solutions of some practical problems (e.g., problems in [7], [8], and [13]).

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