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Lagrange distributed approximating functional method for the solution of the Schrödinger equation

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Abstract

The utility and accuracy of a new distributed approximating functional (DAF), combining the Gaussian weighted DAF concept with Lagrange interpolation, is explored for the discrete spectrum solution of the Schrödinger equation. Two instructive examples, an I_2 Morse oscillator and the 2-dimensional Henon–Heiles potential, are considered in the present study. The present "Lagrange DAF" (LDAF) approach achieves extremely high accuracy for I_2 while using fewer grid points than previous approaches. The present results for the Henon–Heiles system are in excellent agreement with those of earlier established methods, such as that of Shizgal. © 1998 Elsevier Science B.V.

1. Introduction

Finding the discrete eigenvalues and eigenfunctions of the Schrödinger equation is of fundamental importance for both quantum dynamics calculations and spectroscopy. For quantum scattering calculations, solution of the time-dependent or time-independent Schrödinger equation generally requires knowledge of sets of eigenstates of subsystems for the construction of the initial state and the final state analysis. For spectroscopic applications, the differences of eigenvalues and various transition amplitudes are directly related to experimental measurements. There are many methods that have been developed for calculating eigenstates and eigenvalues [1–14]. Most computational methods involve two basic steps: the first step is to construct a matrix representation of the Hamiltonian, and the second step is to obtain the eigenvalues and eigenfunctions of the Hamiltonian matrix. Both steps can be accomplished in a variety of ways. For example, the second step can be realized either by direct matrix diagonalization or by time-dependent propagation [11,12]. The first step can be achieved either by local methods, such as finite difference and finite element methods, or by global methods, such as spectral and pseudospectral methods. Most global methods use classical basis functions which involve some well known polynomials, such as Jacobi, Laguerre, Legendre, Hermite and Chebyshev polynomials. Expan-

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sion coefficients are usually determined by the Galerkin method or by collocation. Shizgal's method [3,4] utilizes nonclassical weight functions which are adapted to the problem under study, and may further reduce the number of grid points. For classical weight functions, Shizgal's method reduces to the popular DVR method [5,6], which is widely used in chemical dynamics. Generally speaking, global methods are more accurate than local methods for solving linear equations *with relatively simple boundary conditions*. However, for systems with complex boundary conditions and geometries, the local methods, such as various finite element methods [15] and finite difference methods [16–18] are simpler and are the ones commonly used. It is desirable to have a class of methods that possess spectral or pseudospectral accuracy and local methods' flexibility for both simple and complicated systems. The distributed approximating functional (DAF) approach [19] is a method of this kind.

The DAFs can be considered as generalized sequences of the Dirac delta function for approximating functions of polynomial growth in the domain of definition, accurate to a given tolerance [19,20]. A useful approach, yielding a wide class of DAFs, is based on a pointwise least squares variational principle, the most general form of which uses a different basis set at every point in the domain of definition [19,20]. This typically leads to discrete DAFs that are not strictly interpolative but rather have similar accuracy both on and off the input grid (the "well-tempered DAF"). Viewed as a generalization of the familiar sequences of the Dirac delta function, DAFs tend to the Dirac delta measure δ in appropriate limits of the DAF parameters. In contrast to DAFs, however, the Dirac delta function (i.e. distribution), as well as the standard Gaussian test functions, do not have much numerical utility. The DAFs have been shown to provide the basis of very powerful methods for numerical applications. Various noninterpolating DAFs have been proposed, depending on the application of interest [21], and these have been successfully applied to a variety of computational problems, including scattering and eigenvalue problems in quantum mechanics [22,23], the linear and nonlinear Fokker–Planck equation [24,25] and nonlinear Burgers' equation with high Reynolds numbers [26,27]. We have recently proposed a new class of DAFs, "interpolating DAFs" or Lagrange DAFs, for treating dynamical problems [28,29]. For solving a particular time-dependent Fokker–Planck equation, the Lagrange DAF method has been found to be accurate to 13 significant figures with reasonable parameters for relatively long times. In this work we explore the usefulness and accuracy of these Lagrange DAFs for calculating the discrete eigenvalues and eigenfunctions of the Schrödinger equation. We find that the Lagrange DAF method easily provides 13 significant figure accuracy for the lower eigenvalues of the example systems we considered.

This paper is organized as follows: The Lagrange DAF hamiltonian is briefly summarized in Section 2. The numerical application of the Lagrange DAF method to calculate the eigenfunctions and eigenvalues of the Schrödinger equation is investigated in Section 3. We end with a brief conclusion.

2. The Lagrange DAF Hamiltonian

There are several classes of DAFs. One class of DAFs, typified by the Hermite DAF [19–21], is constructed in terms of certain polynomials (classical or nonclassical [3]) and their *associated* weight functions. The interpolating, or Lagrange DAFs combine the DAF concept with the general Lagrange interpolation expression of the Paley–Weiner theorem [25,29,30]. The LDAFs behave like a standard expansion basis set under summation over the grid [29]. Specifically, on the domain of R^1, the Lagrange DAF can be expressed as

$$\delta_{M,\sigma_k}(x\,|\,x_k) = C_k P_{M,k}(x) w_{\sigma_k}(x-x_k), \tag{1}$$

where k denotes the grid points and M is the number of the grid points used in constructing the function. The weight $w_{\sigma_k}(x-x_k)$ is to taken to be the Gaussian function,

$$w_{\sigma_k}(x-x_k) = \exp\left(-\frac{(x-x_k)^2}{2\sigma_k^2}\right), \tag{2}$$

the function $P_{M,k}(x)$ in Eq. (1) is the polynomial,

$$P_{M,k}(x) = \prod_{i\neq k}^{M}(x-x_i), \tag{3}$$

and the C_k is determined by

$$\int \mathrm{d}x\, \delta_{M,\sigma_k}(x \mid x_k) = 1. \tag{4}$$

It is noted that M is, in general, unrelated to the total number of grid points N used in the computational problem. Any function of polynomial growth can be approximated by the Lagrange DAFs through "discrete convolution"

$$f(x) \approx \sum_k \Delta_k \delta_{M,\sigma_k}(x \mid x_k) f(x_k), \tag{5}$$

where Δ_k is the grid spacing. We can approximate the lth derivative of a function by

$$f^{(l)}(x) \approx \sum_k \Delta_k \delta^{(l)}_{M,\sigma_k}(x \mid x_k) f(x_k), \tag{6}$$

where lth derivative of the Lagrange DAFs with an appropriate weight function is analytically expressed as

$$\delta^{(l)}_{M,\sigma_k}(x \mid x_k) = C_k \sum_{j=0}^{l} \frac{l!}{j!(l-j)!} P^{(j)}_{M,k}(x) \times w^{(l-j)}_{\sigma_k}(x - x_k). \tag{7}$$

The realization of the Lagrange DAFs used in this paper is the Gaussian Lagrange DAF,

$$\delta_{M,\sigma_k}(x \mid x_k) = C_k \prod_{i \neq k}^{M} (x - x_i) \exp\left(- \frac{(x - x_k)^2}{2\sigma_k^2} \right). \tag{8}$$

In the case of an even grid spacing Δ, Eq. (8) can be written as an explicit function of $x - x_k$ if we use

$$\prod_{i \neq k}^{M} (x - x_i) = \prod_{i=1}^{M/2} (x - x_k + i\Delta)(x - x_k - i\Delta). \tag{9}$$

This leads to a *uniform* Gaussian Lagrange DAF

$$\delta_{M,\sigma}(x - x_k) = C \prod_{i=1}^{M/2} (x - x_k + i\Delta)(x - x_k - i\Delta) \times \exp\left(- \frac{(x - x_k)^2}{2\sigma^2} \right). \tag{10}$$

This form is especially useful for solving partial differential equations on a grid. The derivatives of Eq. (8) can be carried out according to Eq. (7). The first two derivatives of the Gaussian Lagrange DAF (8) are found to be

$$\delta^{(1)}_{M,\sigma_k}(x \mid x_k) = \left(\sum_{j \neq k} \frac{1}{x - x_j} - \frac{x - x_k}{\sigma_k^2} \right) \delta_{M,\sigma_k}(x \mid x_k) \tag{11}$$

and

$$\delta^{(2)}_{M,\sigma_k}(x \mid x_k) = \left[\sum_{j_2 \neq j_1, k} \sum_{j_1 \neq k} \frac{1}{(x - x_{j_2})(x - x_{j_1})} - \frac{2(x - x_k)}{\sigma_k^2} \sum_{j \neq k} \frac{1}{x - x_j} - \frac{1}{\sigma_k^4} \left(\sigma_k^2 - (x - x_k)^2 \right) \right] \delta_{M,\sigma_k}(x \mid x_k), \tag{12}$$

and the Hamiltonian matrix on the grid is expressed in terms of the latter as

$$H_{jk} = - \frac{\hbar^2}{2m} \delta^{(2)}_{M,\sigma_k}(x_j \mid x_k) + V(x_k) \delta_{jk}. \tag{13}$$

These forms have been used for time-dependent quantum dynamics [28,29].

In the remainder of this Letter we explore the utility and test the accuracy of the Gaussian Lagrange DAF, Eq. (10), for calculating eigenfunctions and eigenvalues of the Schrödinger equation.

3. Numerical application

Two "standard" problems are considered to illustrate the use of the Gaussian Lagrange DAF method for calculating the eigenfunctions and eigenvalues of the s-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{s}\frac{\partial^2}{\partial x_i^2}+V(x_1,\cdots,x_s)\right]$$
$$\times\Phi_k(x_1,\cdots,x_s)=E_k\Phi_k(x_1,\cdots,x_s) \qquad (14)$$

where Φ_k and E_k are the kth eigenfunction and eigenvalue, respectively. The Lagrange DAF results for these problems are compared with those obtained by other authors using various methods. The results of these applications are reported in the following two subsections. In the present computations, the Gaussian Lagrange DAF parameters are taken as $M = 80$ and $\sigma/\Delta = 3.173$ for all examples, but the results are not highly sensitive to the specific values used. For a given M value, the σ/Δ can vary over a wide range and still deliver highly accurate results. The DAF-band width $2W+1$ used for all calculations is 71.

3.1. Morse potential for the I_2 molecule

Because it is analytically soluble and anharmonic, and permits dissociation, the Morse oscillator is one of the most popular potentials for modelling diatomic molecules for various applications. It is a standard testing problem for calibrating new numerical methods. If one considers heavy diatomics, one must carry out a longer time propagation to resolve its nearly degenerate eigenstates in the imaginary time relaxation method [11]. We shall use the Morse potential for the I_2 molecule to test the accuracy of

Table 1
Results for the 1D I_2 Morse oscillator

k	Analytical	Difference [a]	Difference [b]	Difference [c]
0	.8529966236266942E-03	$-.10E-10$	$-.14E-13$	$-.14E-13$
1	.1412462184629706E-02	$-.30E-10$	$-.43E-13$	$-.43E-13$
2	.1964568661834224E-02	$-.50E-10$	$-.70E-13$	$-.70E-13$
3	.2509316055240247E-02	$-.70E-10$	$-.98E-13$	$-.98E-13$
4	.3046704364847777E-02	$-.89E-10$	$-.13E-12$	$-.13E-12$
5	.3576733590656813E-02	$-.11E-09$	$-.15E-12$	$-.15E-12$
6	.4099403732667354E-02	$-.13E-09$	$-.18E-12$	$-.18E-12$
7	.4614714790879402E-02	$-.15E-09$	$-.20E-12$	$-.20E-12$
8	.5122666765292955E-02	$-.16E-09$	$-.23E-12$	$-.23E-12$
9	.5623259655908014E-02	$-.18E-09$	$-.26E-12$	$-.26E-12$
10	.6116493462724579E-02	$-.20E-09$	$-.28E-12$	$-.28E-12$
11	.6602368185742650E-02	$-.22E-09$	$-.30E-12$	$-.30E-12$
12	.7080883824962227E-02	$-.23E-09$	$-.32E-12$	$-.33E-12$
13	.7552040380383310E-02	$-.25E-09$	$-.33E-12$	$-.35E-12$
14	.8015837852005899E-02	$-.27E-09$	$-.32E-12$	$-.38E-12$
15	.8472276239829993E-02	$-.28E-09$	$-.25E-12$	$-.40E-12$
16	.8921355543855595E-02	$-.30E-09$	$-.43E-13$	$-.42E-12$
17	.9363075764082702E-02	$-.32E-09$	$.48E-12$	$-.43E-12$
18	.9797436900511314E-02	$-.33E-09$	$.17E-11$	$-.43E-12$
19	.1022443895314143E-01	$-.35E-09$	$.43E-11$	$-.40E-12$
20	.1064408192197306E-01	$-.36E-09$	$.96E-11$	$-.30E-12$
21	.1105636580700619E-01	$-.38E-09$	$.20E-10$	$-.37E-13$
22	.1146129060824082E-01	$-.39E-09$	$.40E-10$	$.55E-12$
23	.1185885632567697E-01	$-.41E-09$	$.78E-10$	$.18E-11$
24	.1224906295931461E-01	$-.42E-09$	$.14E-09$	$.43E-11$

[a] Braun et al. (Ref. [14], $N = 128$).
[b] Present ($N = 80$).
[c] Present ($N = 100$).

results obtained using the Lagrange DAF method. This potential for the I_2 molecule is given by

$$V(x) = D[e^{-2\alpha x} - 2e^{-\alpha x}] + D, \tag{15}$$

where $D = 0.0224$ au, $\alpha = 0.9374$ au. The reduced mass for this system is $\mu = 119406$ au. The analytical results for the eigenfunctions are the generalized Laguerre polynomials [31]

$$\Phi_k = N_k z^{p/2} e^{-z/2} L_k^p(z), \tag{16}$$

where $z = \beta e^{-\alpha x}, p = \beta - 2k - 1, \beta = 156.047612535$ and the normalization constant, obtained using the generating function of the generalized Laguerre polynomials, is [31]

$$N_k = \left[\frac{\Gamma(p)}{\alpha} \sum_{\gamma=0}^{k} (-1)^{\gamma} \binom{-p}{\gamma} \right]^{-1/2}. \tag{17}$$

The analytical expression for the eigenvalues is [31]

$$E_k = \kappa \left[k + \frac{1}{2} - \frac{1}{\beta} \left(k + \frac{1}{2} \right)^2 \right], \tag{18}$$

where $\kappa = 5.741837286 \times 10^{-4}$ au.

This system has been recently studied computationally by Braun et al. [14] using an efficient Chebyshev-Lanczos method to achieve an accuracy ranging from 7 to 9 digits using 128 grid points. Our calculation makes use of the direct diagonalization of our Lagrange DAF-Hamiltonian matrix. Totals of 80 ($N = 80, \Delta = 0.034568$) and 100 ($N = 100, \Delta = 0.027723$) grid points were used for the present computations. The results of our calculation and those of Braun et al. [14] are listed in Table 1. As seen from the table, our 100 grid point results are 100 to 1000 times more accurate than those of Braun et al., obtained with 128 grid points. Our 80 grid point results are still about 1000 times better than those of Braun et al. [14] for the low eigenvalues and are a few times better for the highest ones in the Table 1. Even higher accuracy can be achieved easily by increasing the number of grid points. In this regard, it should be noted that in the LDAF method, an increase in the total number of grid points does *not* require an increase in the degree of the DAF polynomial. Consequently, the computation time does not increase as rapidly as in the most commonly used spectral methods or pseudospectral methods.

3.2. *The Henon–Heiles potential system*

To demonstrate further the reliability and robustness of the Gaussian Lagrange DAF method for calculating the eigenfunctions and eigenvalues of the Schrödinger equation, we consider a widely-studied benchmark; the 2D anharmonic Henon–Heiles system [32]. This potential gives rise to chaotic classical motion, and when used to describe a resonating system, it provides a simple example for the study of Poincare surfaces and trajectories. The system is also important in numerical analysis. Various numerical methods, such as the symmetric split operator-FFT [10], Shizgal's [4], the Chebyshev-Lanczos [14], the potential optimized DVR [6], the semiclassical and a quantum mechanical Hermite basis set expansion [9,33] have been tested on the Henon–Heiles potential. A preliminary study, based on the Hermite DAF method, has been carried out using a Chebyshev expansion of the spectral density operator [34], and another recent study [24] using this method gave the same level of accuracy as Shizgal's method. The purpose of the present calculation is to demonstrate the accuracy and the speed of convergence of the Lagrange DAF approach for this 2D system.

The scaled "Schrödinger equation" for this system is given by

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \tfrac{1}{2}x^2 + \tfrac{1}{2}y^2 - \lambda x\left(\tfrac{1}{3}x^2 - y^2\right) \right]$$

$$\times \phi_{nm}(x,y) = \varepsilon_{nm} \phi_{nm}(x,y), \tag{19}$$

where the principal quantum number n and angular momentum quantum number m characterize the *quasi-bound states* of this system and have been discussed by Noid and Marcus [9]. Obviously the parameter λ is a measure of the anharmonicity of the two-dimensional system and is here taken to be $\sqrt{0.0125}$ to enable the comparison of our results with those of other authors. Earlier work by Marcus et al. [33] used basis sets with 990 and 1225 basis states. Feit et al. [10] have reported an accurate

Table 2
Eigenvalues of the 2D Henon–Heiles potential system

n	m	Feit et al. [a]	Shizgal et al. [b]	Present [c]
3	3	3.9825	3.982 417	3.982 417
3	−3	3.9859	3.985 761	3.985 761
5	3	5.8672	5.867 015	5.867 015
5	−3	5.8816	5.881 446	5.881 446
6	6	6.9991	6.998 932	6.998 932
6	−6	6.9996	6.999 387	6.999 387
7	3	7.6979	7.697 721	7.697 721
7	−3	7.7371	7.736 885	7.736 885
8	6	8.8116	8.811 327	8.811 327
8	−6	8.8154	8.815 188	8.815 188
9	3	9.4670	9.466 773	9.466 773
9	−3	9.5526	9.552 382	9.552 382
9	9	10.0356	10.035 413	10.035 413
9	−9	10.0359	10.035 592	10.035 592
10	6	10.5727	10.572 480	10.572 480
10	−6	10.5907	10.590 470	10.590 470
11	3	11.1603	11.160 258	11.160 259
11	−3	11.3253	11.325 231	11.325 231
11	9	11.7497	11.749 519	11.749 519
11	−9	11.7525	11.752 297	11.752 297
12	6	12.3335	12.333 785	12.333 785
12	−6	12.2771	12.277 192	12.277 192
12	12	12.7474	12.748 445	12.748 423
12	−12	13.0310	13.032 062	13.032 062
13	3	13.0868	13.086 873	13.086 873
13	−3	13.0800	13.081 196	13.081 196

[a] Ref. [10], 16384 time steps used in their split operator-FFT method.
[b] Ref. [4], $N_x = N_y = 50$.
[c] Present, $N_x = N_y = 50$.

calculation using their split operator-FFT method, that required 16384 time steps. A recent computation by Shizgal and Chen [4] achieved six significant figure accuracy for eigenvalues as high as $\epsilon_{13,3}$, using 50 or fewer grid points in each dimension. A potential optimized DVR calculation by Echave and Clary [6] using 55 primitive grid points in each dimension has shown a similar level of accuracy as Shizgal's method. (We note that by using a nonclassical weight function $[w(x) = \exp(-x^2 + 2\gamma x^3/9)]$ [4], designed specifically for the problem, Shizgal's method allows a further reduction in the number of grid points required, for the same accuracy.)

The present results are calculated using 50 grid points in x ($N_x = 50, \Delta_x = 0.357647$) and 50 grid points in y ($N_y = 50, \Delta_y = 0.357647$). As shown in Table 2, our Lagrange DAF approach achieves the same level of accuracy and rate of convergence as has been obtained by Shizgal's method. It is interesting to note that the present results are consistent with our Hermite DAF calculations [24]. The two results are identical to the first eight significant figures as shown in Table 2.

4. Conclusion

In this Letter, the utility of a new (interpolating) Lagrange DAF for calculating discrete eigenvalues and eigenfunctions of the Schrödinger equation is explored. Two different examples are chosen to demonstrate the usefulness and to test the accuracy of the present approach. In the first example, a Morse oscillator parameterized for the I_2 molecule is considered. Our method performs extremely well for this model. The first 23 eigenvalues are accurate to 12 significant figures when using 100 grid points, which is 1000 times better than those of Braun et al. [14] recently obtained by means of an efficient Chebyshev-Lanczos method, using 128 grid points. Additionally, our 80 grid point DAF results range from a few times to 1000 times more accurate than those of Braun et al. [14]. The other example studied in this paper is the two dimensional Henon–Heiles potential, which is also a standard benchmark problem for various numerical methods. The Lagrange DAF method converges very rapidly in this case. The first 97 eigenvalues converge to eight significant figures, when we use 50 grid points in each dimension. The present results are in excellent agreement with those of other methods. It appears that for this problem, Shizgal's method, with a specially tailored nonclassical weight function, provides the most rapidly convergent results. Our Lagrange DAF has been shown to yield the same level of accuracy and speed of convergence as Shizgal's method using a Gaussian weight. The present results are also consistent with our previous calculations using an entirely different, non-interpolating Hermite DAF method [24]. These two calculations show that the Lagrange DAF approach is an efficient, reliable and particularly simple method for the solving the Schrödinger equation.

There are two properties that ensure that the LDAF entails low CUP cost for large-scale computations. One is that the number of grid points is not restricted by the degree of the polynomial, so that an increase in the number of grid points does not lead to as large an increase in computation time as occurs for global methods. The other is that the DAF matrices are highly banded and Toeplitz. As a result, one needs to store only $(W+1)$-numbers in order to generate all the various DAF matrices.

References

[1] R. Friesner, Chem. Phys. Lett. 116 (1985) 39.
[2] D.O. Harris, G.G. Engerholm, W.D. Gwinn, J. Chem. Phys. 43 (1965) 1515.
[3] B. Shizgal, J. Comput. Phys. 41 (1981) 309.
[4] B. Shizgal, H. Chen, J. Chem. Phys. 104 (1996) 4137.
[5] J.V. Lill, G.A. Parker, J.C. Light, Chem. Phys. Lett. 89 (1982) 483.
[6] J. Echave, D.C. Clary, Chem. Phys. Lett. 190 (1992) 225.
[7] D.W. Schwenke, D.G. Truhlar, in: R. Glowinski, A. Lichnewsky (Eds.), Computing Methods in Applied Sciences and Engineering, SIAM, Philadelphia, 1990.
[8] W. Yang, A.C. Peet, Chem. Phys. Lett. 153 (1988) 98.
[9] D.W. Noid, R.A. Marcus, J. Chem. Phys. 62 (1975) 2119.
[10] M.D. Feit, J.A. Fleck Jr., A. Steiger, J. Comput. Phys. 47 (1982) 412.
[11] R. Kosloff, H. Tal-Ezer, Chem. Phys. Lett. 127 (1986) 223.
[12] D. Neuhauser, J. Chem. Phys. 93 (1990) 2611; 100 (1994) 5076.
[13] R.E. Wyatt, Phys. Rev. E 51 (1995) 3643.
[14] M. Braun, S.A. Sofianos, D.G. Papageorgiou, I.E. Lagaris, J. Comput. Phys. 126 (1996) 315.
[15] O.C. Ziekiewicz, The Finite Element Method in Engineering Science, McGraw-Hill, London, 1971.
[16] P.D. Lax, Commun. Pure Appl. Math. 6 (1953) 231.
[17] G.E. Forsythe, W.R. Wasow, Finite Difference Method for Partial Differential Equation, Wiley, New York, 1967.
[18] D.W. Schwenke, S.L. Mielke, D.G. Truhlar, Theor. Chem. Acta 79 (1991) 241.
[19] D.K. Hoffman, N. Nayar, O.A. Sharafeddin, D.J. Kouri, J. Phys. Chem. 95 (1991) 8299.
[20] D.J. Kouri, W. Zhu, X. Ma, B.M. Pettitt, D.K. Hoffman, J. Phys. Chem. 96 (1992) 9622.
[21] D.K. Hoffman, T.L. Marchioro II, M. Arnold, Y. Huang, W. Zhu, D.J. Kouri, J. Math. Chem. 20 (1996) 117.
[22] Y. Huang, D.J. Kouri, D.K. Hoffman, Chem. Phys. Lett. 238 (1995) 387.
[23] W. Zhu, Y. Huang, D.J. Kouri, M. Arnold, D.K. Hoffman, Phys. Rev. Lett. 72 (1994) 1310.
[24] D.S. Zhang, G.W. Wei, D.J. Kouri, D.K. Hoffman, J. Chem. Phys. 106 (1997) 5216.
[25] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, J. Chem. Phys., in press.
[26] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, Comput. Methods Appl. Mech. Engrg., submitted.
[27] D.S. Zhang, G.W. Wei, D.J. Kouri, D.K. Hoffman, Phys. Fluids 9 (1853) 1997.
[28] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, Phys. Rev. Lett. 79 (1997) 775.
[29] D.K. Hoffman, G.W. Wei, D.S. Zhang, D.J. Kouri, Phys. Rev. E., submitted; G.W. Wei, S.A. Althorpe, D.J. Kouri, D.K. Hoffman, Phys. Rev. A., submitted.
[30] R. Paley, N. Wiener, Fourier Transforms in the Complex Domain, Amer. Math. Soc. Colloq. Publs., Ser., vol. 19, Amer. Math. Soc., Providence, RI, 1934.
[31] S. Flügge, Practical Quantum Mechanics, Springer-Verlag, New York, Berlin, 1974.
[32] M. Henon, C. Heiles, Astron. J. 69 (1964) 73.
[33] D.W. Noid, M.L. Koszykowski, M. Tabor, R.A. Marcus, J. Chem. Phys. 72 (1980) 6169.
[34] W. Zhu, Y. Huang, D.J. Kouri, C. Chandler, D.K. Hoffman, Chem. Phys. Lett. 217 (1993) 73.