A variational approach to the Dirichlet–Gabor wavelet-distributed approximating functional

D.K. Hoffman^a, G.W. Wei^b and D.J. Kouri^{c,*}

^a Department of Chemistry and Ames Laboratory**, Iowa State University, Ames, IA 50011, USA

^b Department of Computational Sciences, National University of Singapore, 10 Kent Ridge Cresent, Singapore 119260

^c Department of Chemistry and Department of Physics, University of Houston, Houston, TX 77204-5641, USA

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We show that the Dirichlet–Gabor wavelet-distributed approximating functional (DAF) can be derived from the same variational principle used to obtain non-interpolating wavelet-DAFs (such as the Hermite DAF). This variational approach for such interpolating DAFs complements the original viewpoint that they are generated by regularizing interpolating shells or through two-parameter Dirac delta sequences.

1. Introduction

Recently, we have introduced several new types of distributed approximating functionals (DAFs) [2,5–8,13] and related wavelet bases associated with them [1,8–10,14,16]. In the course of that work, it was observed that DAFs could be generated in several ways. The first approach [5–7] leads to a systematic way of approximating a given discrete set of input data with an infinitely smooth function. The most intensively studied DAF of this type is called the Hermite DAF, or HDAF. The fundamental unit of its construction is a product of a Hermite polynomial and its generating function, referenced to an origin that is located at each point, x. A variational method was introduced for deriving such DAFs [5], and they have been applied to a large number of problems, ranging from solving various linear and nonlinear partial differential equations (PDEs) to the entire gamut of signal processing [1,11,12,14,15,17]. A distinctive property of the first DAFs is that they are not interpolative on the input grid points [5–7]. That is, the first type of DAF approximation to the function at any grid point, x_j , is not exactly equal to the input data value. In place of the interpolative property, this DAF approach to functional approximation has the property that there

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are no "special points". Said another way, such DAFs deliver similar accuracy for approximating the function either on or off the grid; similarly, the DAF approximation to a function, sampled discretely, yields an approximation to the derivatives of the function comparable in accuracy to the function itself. This is strictly true only for functions belonging to the "DAF class", which is that set of functions whose Fourier transform is sufficiently contained under the DAF window in Fourier space [5].

More recently, we have developed another general type of DAF which does interpolate on the grid, but which still can be "tuned" to yield highly accurate derivatives for DAF-class functions [1,2,8,11,12,14,15,17]. The essence of this approach is to modify an "interpolating shell" (such as that for Lagrange interpolation [5], etc.) by an appropriate weighting function. By far the most attractive choice has been a Gaussian weight function, which has the property of "regularizing" the interpolation so that it delivers an infinitely smooth approximation to discretely sampled functions [1,2,8,14], and the accuracy is ensured so long as the function being considered is in the DAF class. Again, these have been shown to be enormously robust for the class of PDEs and signal processing problems considered earlier [1,2,11,12,14,15,17].

An alternative way of viewing these DAFs results from observing that continuous DAFs constitute two-parameter Dirac delta sequences [8]. That is, they are approximate identity transforms that depend on two adjustable parameters. In the case, e.g., of the HDAFs, the two parameters are the Gaussian width, σ , and the highest degree polynomial, M (where M is even):

$$\delta_{\text{DAF}}^{(M)}(x-x'|\sigma) = \frac{1}{\sigma} \exp\left[\frac{-(x-x')^2}{2\sigma^2}\right] \sum_{n=0}^{M/2} \left(\frac{-1}{4}\right)^n \frac{1}{\sqrt{2\pi}n!} H_{2n}\left(\frac{x-x'}{\sqrt{2}\sigma}\right).$$
(1)

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Here it is easily shown that

$$\lim_{M \to \infty} \delta_{\text{DAF}}^{(M)} \left(x - x' | \sigma \right) = \delta \left(x - x' \right)$$
(2)

for any $\sigma > 0$, and also that

$$\lim_{\sigma \to 0} \delta_{\text{DAF}}^{(M)} \left(x - x' | \sigma \right) = \delta \left(x - x' \right) \tag{3}$$

for any fixed M. The availability of two independent parameters, either of which can be used to generate the identity kernel or Dirac delta function, can be viewed as the source of robustness of the DAFs as computational tools [8].

Of the recently introduced regularized interpolation DAFs, a potentially very useful one is the Dirichlet–Gabor wavelet-DAF (DGWD) [8]. It was constructed by combining a Gaussian with the Dirichlet kernel for generating the Fourier series of a function, to give

$$\delta_{\text{DAF}}^{(M)}(x-x'|\sigma) = C_{M,\sigma} \,\mathrm{e}^{-(x-x')^2/2\sigma^2} \frac{\sin[(M+1/2)2\pi x/L]}{2\sin(\pi x/L)}.$$
(4)

As with all of the regularized interpolating DAFs, this product generates a scaling wavelet that at once is infinitely smooth and rapidly decaying in both physical and Fourier space [8]. The constant, $C_{M,\sigma}$, was determined by requiring that the zero-frequency Fourier transform, $\hat{\delta}_{DGWD}^{(M)}(0|\sigma)$, be normalized to unity, that is,

$$\widehat{\phi}(0) = \widehat{\delta}_{\text{DGWD}}^{(M)}(0|\sigma) = \int_{-\infty}^{\infty} \mathrm{d}x \, \delta_{\text{DGWD}}^{(M)}(x|\sigma) = 1.$$
(5)

Then the "father wavelet" basis is generated by translating and scaling, so that [8]

$$\phi_{mn}(x) = a^{-m/2} \phi\left(\frac{x-nb}{a^m}\right). \tag{6}$$

A corresponding "mother wavelet" can be defined as

$$\psi(x) = C_{M,\sigma} \left[e^{-x^2/2\sigma^2} \frac{\sin[(M+1/2)2\pi x/L]}{2\sin(\pi x/L)} - \frac{e^{-x^2/2\sigma^2 a^2}}{a} \frac{\sin[(M+1/2)2\pi x/(aL)]}{2\sin(\pi x/(aL))} \right].$$
(7)

Because of the constraint on $\hat{\phi}(0)$, equation (6), it is verified that $\psi(x)$ is a "small wave", so its zero-frequency transform satisfies

$$\widehat{\psi}(0) = \int_{-\infty}^{\infty} \mathrm{d}x \,\psi(x) = 0. \tag{8}$$

The computational usefulness of the DGWD was shown by several example applications to the solution of differential equations [2,11,12,15,17]. A multiresolution analysis has been developed based on these wavelets [1,2,14].

In this paper we enquire as to whether these regularized interpolation DAFs can also be obtained in a systematic manner from the same variational principle [5] used for the non-interpolating DAFs, especially the HDAF [5–7]. We shall see that the DGWD can indeed be obtained directly from our variational principle, and the derivation bears a similarity to that used for the Hermite DAFs. In the next section, we give the detailed derivation of the DGWD from the variational principle. The last section contains our conclusions.

2. Variational principle applied to the Dirichlet DAF

A general construction of the DAF approximation to a function proceeds by first developing a suitable approximation to the function at every point x in its domain. This is typically accomplished by making a basis set expansion of the form

$$f(x'|x) = \sum_{j} B_j(x'|x) b_j(x).$$
(9)

Here f(x'|x) is an approximation to the function f(x') about the point x, i.e., parameterized by x. The quantity $B_j(x'|x)$ is the *j*th basis function for the point x and $b_j(x)$ is the corresponding coefficient of this basis function for the expansion centered on the point x. The coefficients $b_j(x)$ remain to be determined as functionals of the known values of f(x). A succinct expression for the DAF approximation can then be given by

$$f_{\text{DAF}}(x) = f(x|x) \tag{10}$$

(although, as previously mentioned, other, more general, definitions, e.g., as parameterized delta sequences, are also possible [8]). To complete the definition, one must specify how the x-dependent coefficients are to be obtained.

There are various ways that the set of coefficients $\{b_j(x)\}$ can be determined. Perhaps the most straightforward is by the technique of "moving least squares". In this approach one defines a variational function $\lambda(x)$ for the point x of the form

$$\lambda(x) = \sum_{l} \omega(x_l - x) \left| f(x_l | x) - f(x_l) \right|^2,\tag{11}$$

where the summation over l is over all points in the domain of x where the value of the function is known. (We replace the sum by an integral over all continuous regions of the domain where the function is known.) The quantity $\omega(x_l - x)$ is a weight function of arbitrary form, restricted only in that it is non-negative. For concreteness we will take ω to be of the Gaussian form

$$\omega(x) = \mathrm{e}^{-x^2/2\sigma^2},\tag{12}$$

where σ is a parameter with units of length. It should be pointed out that, in general, the form of the weight can also vary as a function of x as can the basis functions themselves in both type and number. (For example, we could make σ vary with x, and/or choose $B_j(x'|x)$ from different complete sets for each distinct value of x.) We then write

$$f(x_k|x) = \sum_j B_j(x_k|x)b_j(x)$$
(13)

and determine the optimal values of these coefficients at a particular value of x by minimizing the "cost" function $\lambda(x)$. In general, the expansion coefficients can be complex. In anticipation of this eventuality, we minimize the cost function with respect to both the coefficients and their complex conjugates to obtain 2N equations to solve for the real and imaginary parts of the N coefficients. This leads to the set of linear equations

$$\sum_{l=-\infty}^{\infty} \omega(x_l - x) B_j^*(x_l | x) f(x_l) = \sum_{j'} \left\{ \sum_{l=-\infty}^{\infty} \omega(x_l - x) B_j^*(x_l | x) B_{j'}(x_l | x) \right\} b_{j'}, \quad (14)$$

which can be written compactly as

$$A_j = \sum_j C_{jj'} b_{j'} \tag{15}$$

by defining

$$A_j = \sum_{l=-\infty}^{\infty} \omega(x_l - x) B_j^*(x_l | x) f(x_l)$$
(16)

and

$$C_{jj'} = \sum_{l=-\infty}^{\infty} \omega(x_l - x) B_j^*(x_l | x) B_{j'}(x_l | x).$$
(17)

We immediately have that

$$b_j = \sum_{j'} \left(\underline{\underline{C}}^{-1}\right)_{jj'} A_{j'}.$$
(18)

It is important to recall that all of the quantities in this equation are implicit functions of x.

To proceed, we confine our discussion to functions on the real line and represent f(x'|x), our local approximation to the function centered on the point x, as a Fourier series. The basis functions then are

$$B_j(x'|x) = \frac{1}{\sqrt{N}} e^{-2\pi i (x'-x)j/(N\Delta)},$$
(19)

where j assumes the N values $-(N-1)/2 \leq j \leq (N-1)/2$. (Note that j takes on integer values for odd N and half-integer values for even N.) Here Δ is the grid spacing, which is assumed to be uniform. As a function of x', f(x'|x) is obviously periodic with a period domain of N Δ . From equation (17) it is seen that \underline{C} is a kind of overlap matrix for the basis functions centered at x under the weight function $\omega(x'-x)$ of the basis functions; we can express it solely as a function of $\eta = \text{mod}_{\Delta}(x'-x)$. As we now show, it is possible to invert the matrix $\underline{C}(\eta)$ in closed form. However, it is an *approximation* to the inverse that, when valid, gives rise to the DAF representation of the function which is of interest to us here.

It is useful to write the sum in equation (16) in the form

$$\sum_{l=-\infty}^{\infty} (\cdot)_l = \sum_{p=-\infty}^{\infty} \sum_q (\cdot)_{p,q},$$
(20)

where l = Np + q. Here we have divided the grid into domains, each with N points. The *p*-sum is over all domains and the *q*-sum is over all points within a given domain. We take the point of origin (i.e., p = 0, q = 0) to be the grid point closest to x. Then

$$x_l - x = (Np + q)\Delta + \eta, \tag{21}$$

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where $-\Delta/2 \leq \eta \leq \Delta/2$. That is, $x + \eta$ is the grid point closest to x. This leads to

$$C_{jj'} = \frac{1}{N} \sum_{p=-\infty}^{\infty} \sum_{q=0}^{N-1} \omega(x_l - x) e^{2\pi i (q+\eta/\Delta)(j-j')/N}$$
$$= \sum_{q=0}^{N-1} \lambda_{q+\eta/\Delta} \psi_j^{(q+\eta/\Delta)} \psi_{j'}^{(q+\eta/\Delta)*},$$
(22)

where

$$\lambda_{q+\eta/\Delta} = \sum_{p=-\infty}^{\infty} \omega \left([Np + q + \eta/\Delta] \Delta \right)$$
(23)

and

$$\psi_j^{(q+\eta/\Delta)} = \sqrt{\frac{1}{N}} e^{2\pi i (q+\eta/\Delta)j/N}.$$
(24)

The quantity $\psi_j^{(q+\eta/\Delta)}$ can be taken as the *j*th component of an orthonormal basis set of N vectors indexed on q. That is,

$$\sum_{j=-(N-1)/2}^{(N-1)/2} \psi_j^{(q+\eta/\Delta)*} \psi_j^{(\bar{q}+\eta/\Delta)} = \delta_{q,\bar{q}},$$
(25)

which is a standard result from Fourier theory. From this point of view, equation (22) simply gives an expression for the $C_{jj'}$ matrix element of $\underline{C}(\eta)$ in its spectral representation. (Here we have indicated explicitly that the matrix is a function of η .) From this it follows immediately that

$$\left(\underline{C}(\eta)^{-1}\right)_{jj'} = \sum_{q} \frac{1}{\lambda_{q+\eta/\Delta}} \psi_j^{(q+\eta/\Delta)} \psi_{j'}^{(q+\eta/\Delta)*}$$
(26)

and, further, from equation (18) that

$$b_{j}(\eta) = \sum_{j'} \left(\underline{C}(\eta)^{-1}\right)_{jj'} A_{j'}$$
$$= \sum_{j'} \sum_{q} \frac{1}{\lambda_{q+\eta/\Delta}} \psi_{j}^{(q+\eta/\Delta)} \psi_{j'}^{(q+\eta/\Delta)*} \sum_{l'=-\infty}^{\infty} w(x_{l'} - x) \psi_{j'}^{(q'+\eta/\Delta)} f(x_{l'}).$$
(27)

The sum over j^\prime here produces the Kronecker delta $\delta_{qq^\prime},$ where

$$q' + \eta/\Delta = \max_{N} \left(\frac{x_{l'} - x}{\Delta}\right).$$
(28)

Summing over q then leads to

$$b_j(\eta) = \sum_{l'=-\infty}^{\infty} \frac{1}{\lambda_{q'+\eta/\Delta}} \omega(x_{l'} - x) \psi_j^{(q'+\eta/\Delta)} f(x_{l'}), \tag{29}$$

which is the desired variational expression for the expansion coefficients. Finally, from equations (10), (13) and (19) we have that

$$f_{\text{DAF}}(x) = \frac{1}{\sqrt{N}} \sum_{j=-(N-1)/2}^{(N-1)/2} b_j(\eta)$$

= $\sum_{l'=-\infty}^{\infty} \frac{1}{\lambda_{q'+\eta/\Delta}} \omega(x_{l'} - x) \left[\frac{1}{\sqrt{N}} \sum_{j=-(N-1)/2}^{(N-1)/2} \psi_j^{(q'+\eta/\Delta)} \right] f(x_{l'})$
= $\sum_{l'=-\infty}^{\infty} \frac{(-1)^{q'}}{\lambda_{q'+\eta/\Delta}} \left[\frac{\sin(\pi\eta/\Delta)}{N\sin(\pi(q'+\eta/\Delta)/N)} \right] \omega(x_{l'} - x) f(x_{l'}),$ (30)

which is the formal-DAF expression without approximation.

If f(x) is periodic with period $N\Delta$, then $f(x_{l'})$ depends only on q' (i.e., not on p'), and the final result of equation (30) reduces to

$$\sum_{q'=0}^{N-1} (-1)^{q'} \left[\frac{\sin(\pi\eta/\Delta)}{N\sin(\pi(q'+\eta/\Delta)/N)} \right] f\left(q'\Delta+\eta+x\right),\tag{31}$$

where we have made use of equations (21) and (23). (Recall that $x + \eta$ is the grid point closest to x.) This is just the standard Fourier approximation to a periodic function known on N equally spaced grid points. It is interpolative (i.e., $f_{\text{DAF}}(x_l) = f(x_l)$, where x_l is any grid point and, hence, for which $\eta = 0$). This is, of course, the anticipated result for a least-squares fit of a periodic function using a Fourier basis.

If f(x) is not periodic, then $f_{DAF}(x)$ is nowhere exact (unless accidentally so), and, in particular, the DAF approximation is *not* interpolative. The quantity $f(q'\Delta + \eta + x)$ in equation (31) is replaced by

$$\bar{f}_{q'} = \sum_{p'=-\infty}^{\infty} \frac{\omega(x_{l'} - x)}{\lambda_{q'+\eta/\Delta}} f(x_{l'}), \tag{32}$$

which is a weight average across the infinite grid of functional values on grid points separated by multiples of $N\Delta$.

It is clear that the DAF approximation of equation (30) (being basically a Fourier sum) suffers from the principal drawback of the Fourier representation, namely that the approximation is not tightly banded. That is (off the grid), all of the N values of \bar{f}_q contribute more or less equivalently to the approximation. Said another way, each grid point contributes through the *normalized* probability $\omega(x_l - x)/\lambda_{q+\eta/\Delta}$, which falls off much more slowly than $\omega(x_l - x)$ itself as q is varied. To introduce a more

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tightly banded DAF representation of the function, we now assume that $\underline{C}(\eta)$ can be effectively replaced by a matrix that is independent of η . In so doing we, of course, ignore variations in $\underline{C}(\eta)$ over the distance of the grid spacing. There are various ways that this can be done. In previous studies, where we employed a polynomial basis set rather than the circular functions of equation (19), it proved convenient to replace $\underline{C}(\eta)$ by its average. This allowed us to use the properties of orthogonal polynomials to construct the corresponding approximation to \underline{C}^{-1} . We referred to the resulting representation of the function as *well-tempered*, because it has the property that for functions where the approximation is applicable (so-called DAF-class functions) the fit is of comparable accuracy both on and off the grid. In contrast, in the present case it is convenient to make an η -independent approximation to $\underline{C}(\eta)$ for which the grid points are special.

The idea is that, as N becomes large and the grid spacing becomes small in such a way that $N\Delta$ is held constant, every point becomes effectively a grid point (assuming continuity of the function to be fit). Then, to controllable accuracy we can replace $\underline{C}(\eta)$ by $\underline{C}(\eta = 0)$ to obtain

$$\left(\underline{C}^{-1}\right)_{jj'} \approx \sum_{q} \frac{1}{\lambda_q} \psi_j^{(q)} \psi_{j'}^{(q)*},\tag{33}$$

$$b_j \approx \sum_{j'} \sum_q \frac{1}{\lambda_q} \psi_j^{(q)} \psi_{j'}^{(q)*} \sum_{l'=-\infty}^{\infty} \omega(x_{l'} - x) \psi_j^{(q'+\eta/\Delta)} f(x_{l'})$$
(34)

and

$$f_{\text{DAF}}(x) \approx \frac{1}{\lambda_0} \sum_{l'=-\infty}^{\infty} \omega(x_{l'} - x) \frac{1}{\sqrt{N}} \sum_{j'=-(N-1)/2}^{(N-1)/2} \psi_{j'}^{(q'+\eta/\Delta)} f(x_{l'})$$
$$= \frac{\Delta}{\lambda_0 L} \sum_{l'=-\infty}^{\infty} \omega(x_{l'} - x) \sum_{j'=-(N-1)/2}^{(N-1)/2} e^{-2\pi i (x_{l'} - x)j'/L} f(x_{l'}), \quad (35)$$

where $L = N\Delta$. The applicability of this approximation depends of course on the appropriate choice of the DAF parameters, which has been discussed elsewhere. The sum can be written in terms of the *M*th order Dirichlet kernel, $D_M(y)$, defined by

$$D_M(y) = \frac{1}{\pi} \left[\frac{1}{2} + \sum_{k=1}^M \cos(ky) \right] = \frac{\sin[(M+1/2)y]}{2\pi \sin(y/2)},$$
(36)

which leads to the expression

$$f_{\text{DAF}}(x) = \frac{2\pi\Delta}{\lambda_0 L} \sum_{l'=-\infty}^{\infty} \omega(x_{l'} - x) D_{(N-1)/2} \left(\frac{2\pi(x_{l'} - x)}{L}\right) f(x_{l'}).$$
(37)

This result is parameterized by the three quantities L, N (which are related by the grid spacing Δ) and σ (see the form of ω of equation (12)).

Since our approximation $\underline{C}(\eta) \approx \underline{C}(\eta = 0)$ is exact on the grid, this approximation is interpolative for functions that are periodic on a domain of length L. If we take limit $N \to \infty$ and $L \to \infty$ in such a way that $\Delta = L/N$ is fixed, then the approximation assumes the sine-DAF form

$$f_{\text{DAF}}(x) = \frac{\Delta}{2\pi} \sum_{l'=-\infty}^{\infty} \omega(x_{l'} - x) \frac{\sin(2\pi(x_{l'} - x)/\Delta)}{(x_{l'} - x)} f(x_{l'}),$$
(38)

where we have used the fact that $\lambda_0 = 1$ in this limit. This result is interpolative on all grid points.

3. Conclusions

We have shown that the variational principle used earlier for generating noninterpolating DAFs (which could be used to generate associated wavelets) can also be used to derive interpolating DAFs, with a Gaussian weight, that were first obtained by multiplying various interpolation shells with a Gaussian, which regularized the function (making it infinitely differentiable) and ensured that it decays rapidly both in physical and Fourier space. We therefore conclude that the interpolating and noninterpolating DAFs are very closely related, corresponding to different ways of solving the moving least-squares variational algebraic equations. This result complements the earlier procedure used to construct the interpolating DAFs and provides another framework in which to develop robust approximation and estimation algorithms. Both the interpolating and non-interpolating DAFs, of course, have been shown previously to be computationally robust [1,3,4,6,7,11-15,17].

References

- [1] C.K. Chui, An Introduction to Wavelets (Academic Press, San Diego, CA, 1992).
- [2] I. Daubechies, *Ten Lectures on Wavelets*, CBMS-NSF Ser. in Appl. Math. (SIAM, Philadelphia, PA, 1992).
- [3] A. Frishman, D.K. Hoffman and D.J. Kouri, J. Chem. Phys. 107 (1997) 804.
- [4] D.K. Hoffman and D.J. Kouri, in: Proc. 3rd Internat. Conf. on Math. Numer. Aspects Wave Prop., ed. G. Cohen (SIAM, Philadelphia, PA, 1995) pp. 56–63.
- [5] D.K. Hoffman, T.L. Marchioro, M. Arnold, Y. Huang, W. Zhu and D.J. Kouri, J. Math. Chem. 20 (1996) 117.
- [6] D.K. Hoffman, N. Nayar, O.A. Sharafeddin and D.J. Kouri, J. Phys. Chem. 95 (1991) 8299.
- [7] D.J. Kouri, W. Zhu, X. Ma, B.M. Pettitt and D.K. Hoffman, J. Phys. Chem. 96 (1992) 1179.
- [8] Y. Meyer, Wavelets and Operators, Cambridge Stud. Adv. Math., Vol. 37 (Cambridge University Press, Cambridge, 1992).
- [9] Z. Shi, D.J. Kouri, G.W. Wei and D.K. Hoffman, Comput. Phys. Comm., in press.
- [10] Z. Shi, G.W. Wei, D.J. Kouri and D.K. Hoffman, in: *IEEE Sympos. on Time-Frequency and Time-Scale Analysis*, Vol. 144 (Pittsburgh, PA, 6–9 October 1998) pp. 469–472.

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- [11] G.W. Wei, S.C. Althorpe, D.J. Kouri and D.K. Hoffman, J. Chem. Phys. 108 (1998) 7065.
- [12] G.W. Wei, S.C. Althorpe, D.S. Zhang, D.J. Kouri and D.K. Hoffman, Phys. Rev. A 57 (1998) 3309.
- [13] G.W. Wei, D.J. Kouri and D.K. Hoffman, Comput. Phys. Comm. 112 (1998) 1.
- [14] G.W. Wei, D.J. Kouri and D.K. Hoffman, to be published.
- [15] G.W. Wei, D.S. Zhang, D.J. Kouri and D.K. Hoffman, J. Chem. Phys. 107 (1997) 3239.
- [16] G.W. Wei, D.S. Zhang, D.J. Kouri and D.K. Hoffman, Phys. Rev. Lett. 79 (1997) 775.
- [17] D.S. Zhang, G.W. Wei, D.J. Kouri and D.K. Hoffman, Phys Rev. E 56 (1997) 1197.