Journal of Approximation Theory **100**, 233–250 (1999)
Article ID jath.1999.3325, available online at http://www.idealibrary.com on IDEAL®

# Uniform Approximation of Functions with Discrete Approximation Functionals

Colston Chandler

*Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico 87131, U.S.A.*

and

Archie G. Gibson

*Department of Mathematics and Statistics, University of New Mexico, Albuquerque, New Mexico 87131, U.S.A.*

*Communicated by Alphonse P. Magnus*

Received May 28, 1996; accepted in revised form November 5, 1998

Hoffman, Kouri, and collaborators have calculated nonrelativistic quantum scattering amplitudes by numerically evaluating Feynman path integrals. They observed that the errors introduced by their numerical scheme were uniform in coordinate space, implying that their scheme accurately reproduces both the shape and the phase of functions. Furthermore, they observed that the size and the uniform nature of the errors were preserved when the functions were allowed to evolve in time under the action of the kinetic energy operator. In this paper it is established that these observed properties of the errors are not numerical artifacts but follow from analytical properties of a general class of approximations that include those of Hoffman, Kouri, and collaborators as a special case. 

## I. INTRODUCTION

In their very interesting program to calculate nonrelativistic quantum scattering amplitudes by numerically evaluating Feynman path integrals Hoffman, Kouri, and their collaborators [1–14] have introduced certain approximations to the identity operator. They observed numerically that the error introduced by their approximations was uniformly small in the position coordinate. Moreover, the size and the uniformity of the error was unchanged under propagation in time by the kinetic energy operator. That the errors are uniform is particularly intriguing because it implies that the approximations preserve both the shapes and the phases of functions relatively well. It is the purpose of this paper to prove that the observed



0021-9045/99 $30.00

uniformity is not a numerical artifact but is a consequence of the analytical properties of the approximations,

Nonrelativistic Feynman path integrals [15] can be considered a consequence of the Trotter product formula [16, Section X.11]. Solutions of the time-dependent Schrödinger equation have the form

$$\psi_t = e^{-iHt}\psi_0, \tag{1}$$

where $\psi_t \in L_2(\mathbb{R})$ for all real $t$, $i=\sqrt{-1}$, and $H$ is a self-adjoint operator of the form

$$H \equiv K + V. \tag{2}$$

The kinetic energy operator $K$ is defined by

$$(Kf)(x) \equiv -\frac{1}{2\mu}\frac{d^2 f}{dx^2}(x), \tag{3}$$

where the constant $\mu$ represents a mass. The potential energy operator $V$ is defined by

$$(Vf)(x) \equiv v(x)\, f(x), \tag{4}$$

where (for simplicity) $v\colon \mathbb{R} \to \mathbb{R}$, $v \in L_\infty(\mathbb{R}) \cap L_2(\mathbb{R})$. The Trotter product formula [17, Theorem VIII.31] implies that Eq. (5) can be rewritten,

$$\psi_t = \lim_{N\to\infty} \mathsf{U}_{t/N}^N \psi_0, \tag{5}$$

where $N$ assumes integer values. The unitary operator $\mathsf{U}_\tau$ is defined by

$$\mathsf{U}_\tau \equiv e^{-iV\tau} e^{-iK\tau} \tag{6}$$

and has the kernel [16, Section IX.7]

$$\mathsf{U}_\tau(x, y) = e^{-iv(x)\,\tau} \left\{ \left(\frac{\mu}{2\pi i\tau}\right)^{1/2} e^{i\mu\,|x-y|^2/(2\tau)} \right\}. \tag{7}$$

Writing out Eq. (5) in terms of the kernel functions given in Eq. (7) yields

$$\psi_r(x) = \lim_{N\to\infty} \int_{\mathbb{R}} dx_N \cdots \int_{\mathbb{R}} dx_1\, \mathsf{U}_{t/N}(x, x_N)\, \mathsf{U}_{t/N}(x_N, x_{N-1}) \cdots$$

$$\times\, \mathsf{U}_{t/N}(x_2, x_1)\, \psi_0(x_1), \tag{8}$$

the equation from which derivations of the Feynman path integral formalism commonly start.

Numerical calculations based on Eq. (8) involve choosing an initial function $\psi_0$, fixing $N$, restricting the integrations to some finite interval, and using some quadrature rule to evaluate the resulting $x$-integrations. For example, for the composite trapezoid rule, one would have the approximation

$$\psi_t(x) \approx \Delta^N \sum_{r_1, r_2, \ldots, r_N = -M}^{M} \mathsf{U}_{t/N}(x, r_N \Delta)\, \mathsf{U}_{t/N}(r_N \Delta, r_{N-1}\Delta) \cdots \\ \times \mathsf{U}_{t/N}(r_2 \Delta, r_1 \Delta)\, \psi_0(r_1 \Delta). \tag{9}$$

The values of $N$, $M$, and $\Delta$ would then be varied to obtain numerical convergence.

The numerical method just described is not practical, however, and a further approximation must be introduced. The problem is that the matrix $U_{r'r} \equiv \mathsf{U}_\tau(r'\Delta, r\Delta)$ is dense, as is apparent from the fact that all the matrix elements have the same norm ($|U_{r'r}| = (\mu/2\pi\tau)^{1/2}$). The key idea of Hoffman *et al.* [1–14] was to replace $\mathsf{U}_\tau$ by $\mathsf{U}_\tau \mathsf{D}_n$, where $n$ is a positive integer and the operators $\mathsf{D}_n$ are bounded and tend (in some sense) to the identity as $n \to \infty$. They constructed the operators $\mathsf{D}_n$ so that the kernel matrix $(\mathsf{U}_\tau \mathsf{D}_n)(r'\Delta, r\Delta)$ is strongly banded. Numerical calculations employing the operators $\mathsf{D}_n$ (which Hoffman *et al.* called *distributed approximation functionals*) proved to be efficient, accurate, and robust [5, 9, 12].

In their numerical studies Hoffman *et al.* noticed [18] that for every function $f$ used the function $(e^{-iK\tau}\mathsf{D}_n f)(x)$ approximated $(e^{-iK\tau}f)(x)$ to arbitrary accuracy uniformly in $x$ and $\tau$ for $n$ sufficiently large. It is the purpose of this paper to prove that this observed uniformity is a consequence of the analytical properties of the approximations, and to do this for a class of approximations to the identity operator that includes those of Hoffman *et al.* as a special case.

A general class of sequences of functions, called sequences of unity approximations, is defined and studied in Section II. In Section III both continuous and semi-discrete approximations to the identity operator are defined and proved to be bounded linear transformations on certain Banach spaces. The semi-discrete approximations are essentially discrete convolutions with more general kernels than those of previous theories that center on such convolutions (*e.g.*, moving least squares [19, 20] and shift-invariant spaces [21]). Theorems are then proved in Section IV that give the precise conditions under which the errors introduced by the approximations are uniform in coordinate space. The Schrödinger time evolution of the continuous and semi-discrete approximations is studied in Section V, and it is proved that the errors resulting from the approximations are not only uniform in coordinate space but remain so when propagated in time by the kinetic energy operator. While the results for the continuous approximations to the identity are not surprising and may well be known in other contexts, the results for the semi-discrete approximations, which are particularly relevant to numerical applications, are new.

## II. SEQUENCES OF UNITY APPROXIMATIONS

In this section notation is established and fundamental definitions are given. In particular, a definition is given of the general class of sequences of functions (called sequences of unity approximations) used to construct the approximations to the identity operator that are the main subject of this paper. The important properties of these sequences are also established in this section.

Throughout this paper certain standard notation will be used. $\mathbb{R}$ will denote the set of all real numbers, and $\mathbb{C}$ will denote the set of all complex numbers. $S(\mathbb{R})$ will denote the *functions of rapid decrease*, that is, the class of infinitely differentiable functions of a real variable satisfying $\lim_{|x|\to\infty} |x^\ell f^{(m)}(x)| = 0$, for all $\ell, m \geqslant 0$. $L_p(\mathbb{R})$, $1 \leqslant p < \infty$, will denote the space of measurable complex-valued functions of a real variable whose $p$th power is Lebesgue integrable, and $L_\infty(\mathbb{R})$ will denote the space of essentially bounded complex-valued functions of a real variable. Finally, $C_\infty(\mathbb{R}) \subset L_\infty(\mathbb{R})$ will denote the set of all continuous functions of a real variable that vanish at infinity.

The other needed spaces are specified in the following two definitions.

DEFINITION 1. For each integer $M \geqslant 0$, a measurable function $\hat{f}\colon \mathbb{R} \to \mathbb{C}$ will be said to belong to the space $S_M$ if

$$\|\hat{f}\|_{S_M} \equiv \int_{\mathbb{R}} dk\, w_M(k)\, |\hat{f}(k)| < \infty, \tag{10}$$

where

$$w_M(k) \equiv \sum_{m=0}^{M} |k|^m. \tag{11}$$

Note that the space $S_M$ is a complete normed linear vector space with norm $\|\cdot\|_{S_M}$ defined by Eqs. (10) and (11). Note also that $S_M \subseteq L_1(\mathbb{R})$.

DEFINITION 2. For each integer $M \geqslant 0$, a function $f\colon \mathbb{R} \to \mathbb{C}$ will be said to belong to the space $F_M$ if it is the Fourier transform $\mathscr{F}\{\hat{f}\}$ of $\hat{f} \in S_M$, where the Fourier transform $\mathscr{F}$ is defined by

$$f(x) = (\mathscr{F}\{\hat{f}\})(x) \equiv (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} \hat{f}(k). \tag{12}$$

The continuity properties of functions in $F_M$ are important for this paper and are established by the following well-known lemma (cf. [16, Theorem IX.7; 25, Theorem 3].

LEMMA 1. *Let $f \in F_M$ be the Fourier transform of $\hat{f} \in S_M$. Then, the Fourier transforms*

$$f^{(m)}(x) = \mathscr{F}\{(ik)^m \hat{f}\}$$
$$\equiv (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} (ik)^m \hat{f}(k), \qquad m = 0, 1, ..., M, \tag{13}$$

*exist, belong to $C_\infty(\mathbb{R}) \cap F_{M-m} \subset L_\infty(\mathbb{R}) \cap F_{M-m}$, and satisfy $\|f^{(m)}\|_\infty \leqslant (2\pi)^{-1/2} \|\hat{f}\|_{S_M}$. Moreover, $f = f^{(0)}$ and $f^{(m)} = d^m f/dx^m$.*

Note that $S(\mathbb{R}) \subset S_M$ and $S(\mathbb{R}) \subset F_M$. Note also that while $F_M \subset C_\infty(\mathbb{R}) \subset L_\infty(\mathbb{R})$, the set $F_M$ is not a subset of $L_p(\mathbb{R})$ nor is $L_p(\mathbb{R})$ a subset of $F_M$ for any $p$ satisfying $1 \leqslant p < \infty$. However, the following lemma holds.

LEMMA 2. *For each integer $M \geqslant 0$, $F_M \cap L_p(\mathbb{R})$ is dense in $L_p(\mathbb{R})$ for every $p$ satisfying $1 \leqslant p < \infty$.*

*Proof.* Let $C_0^\infty(\mathbb{R})$ denote the infinitely differentiable functions of compact support. Since for every $p$, $1 \leqslant p < \infty$, $C_0^\infty(\mathbb{R}) \subset S(\mathbb{R}) \subset F_M \cap L_p(\mathbb{R})$, and $C_0^\infty(\mathbb{R})$ is dense in $L_p(\mathbb{R})$ ([23], p. 3), it follows that $F_M \cap L_p(\mathbb{R})$ is dense in $L_p(\mathbb{R})$. ∎

This lemma is important for applications to nonrelativistic quantum mechanics for which the natural function space is $\mathscr{L}_2(\mathbb{R})$. It implies that all wave functions can be approximated by functions in $F_M$, $M \geqslant 0$, to arbitrary accuracy in $L_2$ norm.

The general class of sequences that specify the approximations that are the main subject of this paper are now defined.

DEFINITION 3. A sequence $\{\hat{\chi}_n\}_{n=1}^\infty$ of measurable functions $\hat{\chi}_n: \mathbb{R} \to \mathbb{C}$ will be called a *sequence of unity approximations* and $\hat{\chi}_n$ will be called a *unity approximation* if the following three properties are satisfied:

- ($\chi 1$) For each $n = 1, 2, ...,$ $\chi_n \equiv (2\pi)^{-1/2} \mathscr{F}\{\hat{\chi}_n\} \in L_1(\mathbb{R}) \cap F_1$;
- ($\chi 2$) $\|\hat{\chi}_n\|_\infty \leqslant C$ for some positive constant $C$ independent of $n$;
- ($\chi 3$) $\lim_{n \to \infty} \hat{\chi}_n(k) = 1$, for almost all $k \in \mathbb{R}$.

Note that if $\hat{\chi}_n \in S(\mathbb{R})$ for each $n$, ($\chi 1$) is automatically satisfied. Consequently, if ($\chi 2$) and ($\chi 3$) are also satisfied, then $\{\hat{\chi}_n\}_{n=1}^\infty$ is a sequence of unity approximations. This is the case, in particular, for the sequence of functions used in the work of Hoffman, Kouri, and their collaborators

[1–14] that stimulated this paper. Although they studied several sequences based on several different types of orthogonal polynomials, the functions they studied in greatest detail are based on Hermite polynomials

$$\chi_n(x) = (2\pi\sigma^2)^{-1/2}\, e^{-x^2/(2\sigma^2)} \sum_{\nu=0}^{n} \frac{(-1)^\nu}{2^{2\nu}\nu!} H_{2\nu}(x/(2^{1/2}\sigma)) \tag{14}$$

and

$$\hat{\chi}_n(k) = e^{(-\sigma k)^2/2} \sum_{\nu=0}^{n} \frac{[(\sigma k)^2/2]^\nu}{\nu!}. \tag{15}$$

Here $\sigma$ is a positive real constant and $H_{2\nu}$ is the Hermite polynomial of degree $2\nu$. It is evident that $\hat{\chi}_n \in S(\mathbb{R})$ for each fixed value of $n$. Moreover, the sum in Eq. (15) converges monotonically from below to $\exp[(\sigma k)^2/2]$ as $n \to \infty$, for every finite $k$. It immediately follows that ($\chi$2) and ($\chi$3) are satisfied with $C = 1$ and, consequently, that the functions in Eqs. (14) and (15) form a sequence of unity approximations.

The following lemma establishes several important properties of unity approximations.

LEMMA 3. *Let $\{\hat{\chi}_n\}$ be a sequence of unity approximations. Then the following hold*:

(a) *For each $n = 1, 2, \ldots$, both $\chi_n$ and its derivative $\chi_n'$ belong to $C_\infty(\mathbb{R}) \subset L_\infty(\mathbb{R})$ and are bounded in $L_\infty$ norm by $(2\pi)^{-1} \|\hat{\chi}_n\|_{S_1}$,*

(b) *For each $n = 1, 2, \ldots$, $\hat{\chi}_n(k)$ has the representation*

$$\hat{\chi}_n(k) = \int_{\mathbb{R}} dx\, e^{-ikx} \chi_n(x), \tag{16}$$

(c) *For each $n = 1, 2, \ldots$, both $\hat{\chi}_n$ and $\chi_n$ belong to $L_p(\mathbb{R})$ for all $1 \leqslant p \leqslant \infty$,*

(d) *The sequence $\{\chi_n\}$ is a delta sequence, i.e.,*

$$\lim_{n\to\infty} \int_{\mathbb{R}} dy\, \chi_n(x-y)\, \phi(y) = \phi(x), \tag{17}$$

*for any $\phi \in S(\mathbb{R})$.*

*Proof.* Let $\{\hat{\chi}_n\}$ be a sequence of unity approximations.

(a) By ($\chi$1), $\chi_n = (2\pi)^{-1/2}\, \mathcal{F}\{\hat{\chi}_n\} \in F_1$. Lemma 1 then implies that $\chi_n$ and its derivative $\chi_n' = (2\pi)^{-1/2}\, \mathcal{F}\{ik\hat{\chi}_n\}$ both belong to $C_\infty(\mathbb{R}) \subset L_\infty(\mathbb{R})$ and are bounded in $L_\infty$ norm by $(2\pi)^{-1} \|\hat{\chi}_n\|_{S_1}$.

(b) By assumption ($\chi 1$), part (a) of this proof, and the Fourier transform theorem [24, Theorem 7.1], $\hat{\chi}_n$ and $(2\pi)^{1/2}\chi_n$ are a Fourier transform pair, and $\hat{\chi}_n$, the inverse Fourier transform of $(2\pi)^{1/2}\chi_n$, is given by Eq. (16).

(c) Since $S_1 \subset L_1(\mathbb{R})$, ($\chi 1$) and ($\chi 2$) imply $\hat{\chi}_n \in L_1(\mathbb{R}) \cap L_\infty(\mathbb{R})$. This further implies that $\hat{\chi}_n \in L_p(\mathbb{R})$ for all $1 \leqslant p \leqslant \infty$ since

$$\|\hat{\chi}_n\|_p^p = \int_{\mathbb{R}} dk\, |\hat{\chi}_n(k)|^{p-1}\, |\hat{\chi}_n(k)| \leqslant \|\hat{\chi}_n\|_\infty^{p-1}\, \|\hat{\chi}_n\|_1 < \infty. \tag{18}$$

By ($\chi 1$) and part (a) of this proof, $\chi_n \in L_1(\mathbb{R}) \cap L_\infty(\mathbb{R})$. Therefore, Eq. (18) is valid without the hats, and $\chi_n \in L_p(\mathbb{R})$ for all $1 \leqslant p \leqslant \infty$.

(d) The sequence $\{\chi_n\}$ is a delta sequence if $\chi_n \in L_1^{\text{loc}}(\mathbb{R})$ and $\chi_n(x)$ converges in the sense of distributions to the delta function $\delta(x)$ [25, Chapter 2]. By assumption ($\chi 1$), $\chi_n$ is locally integrable on $\mathbb{R}$. Let $\phi \in S(\mathbb{R})$, and let $\langle f, \phi \rangle$ denote the action of the distribution $f$ on the test function $\phi$. Then

$$|\langle \chi_n - \delta, \phi \rangle| = |\langle \hat{\chi}_n - 1, \hat{\phi} \rangle| \leqslant \int_{\mathbb{R}} dk\, |\hat{\chi}_n(k) - 1|\, |\hat{\phi}(k)|, \tag{19}$$

where $\hat{\phi}$ is the Fourier transform of $\phi$. The right-hand side of Eq. (19) converges to zero as $n \to \infty$ by ($\chi 2$) and ($\chi 3$) and the Lebesgue dominated convergence theorem. ∎

## III. CONTINUOUS AND DISCRETE DAFS

In this section sequences of unity approximations are used to define two sequences of operators which approximate the identity. The nomenclature follows that of references [1–14].

The continuous approximations are defined by using the functions $\hat{\chi}_n$ of sequences of unity approximations as Fourier window functions.

DEFINITION 4. Let $\{\hat{\chi}_n\}$ be a sequence of unity approximations. The operators $\mathsf{C}_n$ defined by

$$(\mathsf{C}_n f)(x) \equiv (\mathscr{F}\{\hat{\chi}_n \hat{f}\})(x) = (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} \hat{\chi}_n(k)\, \hat{f}(k) \tag{20}$$

will be called *continuous distributed approximating functionals* (*continuous* DAFs).

The domain and corresponding range of the continuous DAFs is established by the following lemma which is doubtless well-known. Its proof will be omitted.

LEMMA 4. *Let* $\{\hat{\chi}_n\}$ *be a sequence of unity approximations, and let the operators of the sequence* $\{\mathsf{C}_n\}$ *be the corresponding continuous DAFs. Let* $M$, $M \geqslant 0$, *and* $n$, $1 \leqslant n < \infty$, *be arbitrary fixed integers. Then* $\mathsf{C}_n$ *maps* $F_M$ *into* $F_M \subset L_\infty(\mathbb{R})$, *and for each* $f \in F_M$

$$(\mathsf{C}_n f)(x) = \int_{\mathbb{R}} dy\, \chi_n(x-y)\, f(y), \tag{21}$$

*with* $\chi_n = (2\pi)^{-1/2} \mathscr{F}\{\hat{\chi}_n\}$.

Discrete versions of the continuous DAFs are now defined as follows.

DEFINITION 5. Let $\{\hat{\chi}_n\}$ be a sequence of unity approximations. Let $\{w_s, t_s\}_{s=1}^{S}$ be the positive weights and nodes for a quadrature rule for integrals on the interval $[-1, 1]$. Let $\Delta$ be a positive real number. The operators $\mathsf{D}_n$ defined by

$$(\mathsf{D}_n f)(x) \equiv (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} \hat{\chi}_n(k) \times \left\{ \frac{\Delta}{2\sqrt{2\pi}} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s e^{-ikx_{rs}} f(x_{rs}) \right\}, \tag{22}$$

where

$$x_{rs} = \left(r + \frac{1}{2}\right)\Delta + \frac{\Delta}{2} t_s, \tag{23}$$

will be called *discrete distributed approximating functionals* (*discrete* DAFs).

Equation (22) is recognized as a composite quadrature approximation of Eq. (20).

The following lemma provides a domain and range result for discrete DAFs that is analogous to that of Lemma 4 for the continuous DAFs.

LEMMA 5. *Let* $\{\hat{\chi}_n\}$ *be a sequence of unity approximations. Let* $\{w_s, t_s\}_{s=1}^{S}$ *be the positive weights and nodes for a quadrature rule for integrals on the interval* $[-1, 1]$. *Let* $\sum_{s=1}^{S} w_s = 2$, *and let* $\Delta$ *be a positive real number. Let the operators of the sequence* $\{\mathsf{D}_n\}_{n=1}^{\infty}$ *be the corresponding discrete DAFs. Let* $n$, $1 \leqslant n < \infty$, *be an arbitrary fixed integer. Let* $f$ *be a* *differentiable complex-valued function on* $\mathbb{R}$ *such that* $f,\ f' \equiv df/dx \in L_1(\mathbb{R})$. *Then,* $\mathsf{D}_n f \in F_0 \subset L_\infty(\mathbb{R})$ *and*

$$(\mathsf{D}_n f)(x) = \frac{\Delta}{2} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s \chi_n(x - x_{rs})\, f(x_{rs}), \tag{24}$$

*where* $\chi_n = (2\pi)^{-1/2}\, \mathscr{F}\{\hat{\chi}_n\}$.

*Proof.* A general consequence of standard numerical analysis [26, p. 70] is that for any function $\varphi$: $\mathbb{R} \to \mathbb{C}$ such that $\varphi,\ \varphi' \equiv d\varphi/dx \in L_1(\mathbb{R})$,

$$\int_{-1}^{1} dt\, \varphi(x_r(t)) - \sum_{s=1}^{S} w_s \varphi(x_{rs}) = \int_{-1}^{1} dt\, K_0(t) \frac{d}{dt}\, \varphi(x_r(t)), \tag{25}$$

where $x_r(t) = (r + 1/2)\, \Delta + (\Delta/2)\, t$ and $x_{rs} = x_r(t_s)$. The function $K_0(t)$ is the Peano kernel

$$K_0(t) \equiv \int_{-1}^{1} du\, H(u - t) - \sum_{s=1}^{S} w_s H(t_s - t), \tag{26}$$

where $H(\cdot)$ is the Heaviside function. Because $|H(u - t)| \leqslant 1$, $K_0 \in L_\infty([-1, 1])$ and

$$\left| \sum_{s=1}^{S} w_s \varphi(x_{rs}) \right| \leqslant \int_{-1}^{1} dt \{ |\varphi(x_r(t))| + (\|K_0\|_\infty\, \Delta/2)\, |\varphi'(x_r(t))| \}. \tag{27}$$

Transforming the integration variable from $t$ to $x = x_r(t)$ yields

$$\left| \sum_{s=1}^{S} w_s \varphi(x_{rs}) \right| \leqslant \frac{2}{\Delta} \int_{r\Delta}^{(r+1)\,\Delta} dx \{ |\varphi(x)| + (\|K_0\|_\infty\, \Delta/2)\, |\varphi'(x)| \}, \tag{28}$$

with the further consequence that

$$\frac{\Delta}{2} \sum_{r=-\infty}^{\infty} \left| \sum_{s=1}^{S} w_s \varphi(x_{rs}) \right| \leqslant \|\varphi\|_1 + (\|K_0\|_\infty\, \Delta/2)\, \|\varphi'\|_1. \tag{29}$$

Applying this analysis to $\varphi(x) = e^{-ikx} f(x)$ proves that the quantity in braces in Eq. (22) is a continuous function of $k$ that satisfies

$$\left| \frac{\Delta}{2\sqrt{2\pi}} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s e^{-ikx_{rs}} f(x_{rs}) \right| \leqslant (2\pi)^{-1/2} \{ \|f\|_1 + (\|K_0\|_\infty\, \Delta/2)(|k|\ \|f\|_1 + \|f'\|_1) \}. \tag{30}$$

The quantity in braces in Eq. (22) times $\hat{\chi}_n$ consequently belongs to $S_0$ and $\mathsf{D}_n f \in F_0 \subset L_\infty(\mathbb{R})$. Equation (28) implies that the order of integration and infinite summation can be reversed in Eq. (22), yielding Eq. (24). ∎

*Remark.* The discrete DAF reminds one of other well developed approximations, but the similarity is only superficial. It is true, for example, that the continuous DAF specified by Eqs. (14) and (15) is a special case of the moving least squares method [19, 20]. The discrete DAF is different, on the other hand, from the discrete moving least squares method, which does not, in general, have the form of a discrete convolution. The form of the discrete DAF is also suggestive of approximations involving shift-invariant space theory [21]. In shift-invariant space theory, however, there is a scale parameter and a mesh size that are set equal. In discrete DAF theory, on the other hand, the mesh size $\Delta$ is prominent but there is no scaling parameter. In addition the Strang-Fix conditions, which are prominent in both the moving least squares and the sift-invariant space theories, are absent in discrete DAF theory. The discrete DAFs seem to be new, with more general kernels than those allowed by these other theories.

It is important for applications that the approximations in Eq. (24) be uniform in $x$, and we address this question in the next section.

## IV. UNIFORM APPROXIMATION THEOREMS

The convergence in Eq. (17) of Lemma 3 is in the sense of distributions and is not strong enough for applications. The following theorem establishes that any function in $F_M$ may be approximated *uniformly in x* by a continuous DAF. The results contained in the theorem are surely well-known, and we omit the proof.

THEOREM 1. *Let $\{\hat{\chi}_n\}$ be a sequence of unity approximations, and let the operators of the sequence $\{\mathsf{C}_n\}$ be the corresponding continuous DAFs. Let $M$, $M \geqslant 0$, be an arbitrary fixed integer, and let $f \in F_M$. Let $f^{(0)}$ denote $f$, $f^{(m)}$ denote $d^m f/dx^m$ for $1 \leqslant m \leqslant M$, and let $(\mathsf{C}_n f)^{(m)}$ denote the corresponding derivatives of $\mathsf{C}_n f$. Then, $f^{(m)} - (\mathsf{C}_n f)^{(m)} \in F_M \subset L_\infty(\mathbb{R})$, with*

$$\|f^{(m)} - (\mathsf{C}_n f)^{(m)}\|_\infty \leqslant (2\pi)^{-1/2} \|(ik)^m (1-\hat{\chi}_n) \hat{f}\|_1 \leqslant (2\pi)^{-1/2}(1+C) \|\hat{f}\|_{S_M}. \tag{31}$$

*Moreover,*

$$\lim_{n \to \infty} \|(ik)^m (1-\hat{\chi}_n) \hat{f}\|_1 = 0. \tag{32}$$

The next theorem establishes that any function in a certain subset of $F_{M+1}$ may be approximated *uniformly in* $x$ by a discrete DAF.

THEOREM 2. *Let* $\{\hat{\chi}_n\}$ *be a sequence of unity approximations. Let* $\{w_s, t_s\}_{s=1}^{S}$ *be the positive weights and nodes for a quadrature rule for integrals on the interval* $[-1, 1]$ *that is exact for polynomials of degree through* $P$, $P \geqslant 0$. *Let* $\Delta$ *be a positive real number. Let the operators of the sequence* $\{\mathsf{D}_n\}_{n=1}^{\infty}$ *be the corresponding discrete DAFs. Let* $M$, $M \geqslant 0$, *be an arbitrary fixed integer, and let* $\hat{\chi}_n \in S_{M+P+1}$. *Let* $f^{(p)} \in L_1(\mathbb{R})$, $0 \leqslant p \leqslant P+1$. *Then,* $\mathsf{C}_n f - \mathsf{D}_n f \in F_M$ *and*

$$\|(\mathsf{C}_n f)^{(m)} - (\mathsf{D}_n f)^{(m)}\|_\infty \leqslant (2\pi)^{-1} \Delta^{P+1} \|K_P\|_\infty \|\hat{\chi}_n\|_{S_{M+P+1}} \max_{p=0, ..., P+1} \|f^{(p)}\|_1, \tag{33}$$

$0 \leqslant m \leqslant M$, *where*

$$K_P(t) \equiv \frac{1}{P!} \left\{ \int_{-1}^{1} du\, H(u-t)(u-t)^P - \sum_{s=1}^{S} w_s H(t_s - t)(t_s - t)^P \right\}, \tag{34}$$

*with* $H$ *the Heaviside function.*

*Proof.* By Eqs. (20) and (22), $(\mathsf{C}_n f)^{(m)} - (\mathsf{D}_n f)^{(m)}$ can be written in the form

$$([\mathsf{C}_n - \mathsf{D}_n] f)^{(m)}(x) = \int_{\mathbb{R}} dk\, e^{ikx} (ik)^m \hat{\chi}_n(k) \hat{J}(k), \tag{35}$$

where

$$\hat{J}(k) \equiv \frac{1}{\sqrt{2\pi}} \hat{f}(k) - \frac{\Delta}{4\pi} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s e^{-ikx_{rs}} f(x_{rs}) \tag{36}$$

$$= \frac{\Delta}{4\pi} \sum_{r=-\infty}^{\infty} \left\{ \int_{-1}^{1} dt\, e^{-ikx_r(t)} f(x_r(t)) - \sum_{s=1}^{S} w_s e^{-ikx_{rs}} f(x_{rs}) \right\}, \tag{37}$$

with $x_r(t) = (r + 1/2)\,\Delta + (\Delta/2)\, t$.

For a general function $\varphi: \mathbb{R} \to \mathbb{C}$, with $\varphi^{(m)} \in L_1(\mathbb{R})$ for $1 \leqslant m \leqslant P+1$, Eq. (25) can be rewritten [26, p. 70]

$$\int_{-1}^{1} dt\, \varphi(x_r(t)) - \sum_{s=1}^{S} w_s \varphi(x_{rs}) = \int_{-1}^{1} dt\, K_P(t) \frac{d^{(P+1)}}{dt^{(P+1)}} \varphi(x_r(t)), \tag{38}$$

where $K_P$ is the Peano kernel defined in Eq. (34). Because the quadrature rule is exact for polynomials of degree through $P$, $P \geqslant 0$, it is exact for constants, with the consequence that $\sum_{s=1}^{S} w_s = 2$. Because $|H(u-t)(u-t)^P| < 2^P$, $K_P \in L_\infty([-1, 1])$. The same sort of analysis that led from Eq. (25) to Eq. (28) now yields

$$\left| \int_{-1}^{1} dt\, \varphi(x_r(t)) - \sum_{s=1}^{S} w_s \varphi(x_{rs}) \right| \leqslant \frac{2\, \|K_P\|_\infty}{\Delta} \left(\frac{\Delta}{2}\right)^{P+1} \int_{r\Delta}^{(r+1)\Delta} dx\, |\varphi^{(P+1)}(x)| \tag{39}$$

and

$$\frac{\Delta}{2} \sum_{r=-\infty}^{\infty} \left| \int_{-1}^{1} dt\, \varphi(x_r(t)) - \sum_{s=1}^{S} w_s \varphi(x_{rs}) \right| \leqslant \|K_P\|_\infty \left(\frac{\Delta}{2}\right)^{P+1} \|\varphi^{(P+1)}\|_1. \tag{40}$$

Combining Eqs. (37) and (40) for $\varphi(x) = e^{-ikx} f(x)$ yields

$$|\hat{J}(k)| \leqslant \frac{\|K_P\|_\infty}{2\pi} \left(\frac{\Delta}{2}\right)^{P+1} \sum_{p=0}^{P+1} \binom{P+1}{p} |k|^{P+1-p}\, \|f^{(p)}\|_1, \tag{41}$$

where $\binom{P+1}{p}$ denotes the binomial coefficient. From Eq. (41) it follows that $\hat{\chi}_n \hat{J} \in S_M$ and, consequently, that $\mathsf{C}_n f - \mathsf{D}_n f \in F_M$. Moreover, combining Eqs. (35) and (41) yields

$$\|([\mathsf{C}_n - \mathsf{D}_n]\, f)^{(m)}\|_\infty \leqslant \frac{\|K_P\|_\infty}{2\pi} \left(\frac{\Delta}{2}\right)^{P+1} \|\hat{\chi}_n\|_{S_{M+P+1}} \sum_{p=0}^{P+1} \binom{P+1}{p} \|f^{(p)}\|_1, \tag{42}$$

from which Eq. (33) immediately follows. ∎

We present in the following table values of $\|K_0\|_\infty$, $P$ and $\|K_P\|_\infty$ for some simple quadrature rules.

| Quadrature rule | $\|K_0\|_\infty$ | $P$ | $\|K_P\|_\infty$ |
|---|---|---|---|
| Trapezoid | 1 | 1 | 0.500000 |
| Simpson's | 2/3 | 3 | 0.013889 |
| Gauss–Legendre (2 point) | $1/\sqrt{3}$ | 3 | 0.009592 |
| Gauss–Legendre (3 point) | 4/9 | 5 | 0.000098 |

## V. SCHRÖDINGER DYNAMICS

Let $K$ denote the kinetic energy operator defined for $f \in F_2$ by Eq. (3). Then, $e^{-iK\tau}f$ is defined by [27, Section 3-3]

$$(e^{-iK\tau}f)(x) \equiv (\mathscr{F}\{e^{-i(k^2/2\mu)\tau}\hat{f}\})(x)$$
$$= (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} e^{-i(k^2/2\mu)\tau} \hat{f}(k). \tag{43}$$

Some properties of the operator $e^{-iK\tau}$ are collected in Lemma 6.

LEMMA 6. *Let $e^{-iK\tau}$ be defined by Eq.* (43). *Then the following hold:*

(a) $e^{-iK\tau}$: $L_p(\mathbb{R}) \to L_q(\mathbb{R})$, *for all* $\tau \in \mathbb{R}$ *and all* $p$, $2 \leqslant p \leqslant \infty$, *with* $q \equiv (1 - p^{-1})^{-1}$.

(b) $e^{-iK\tau}$: $F_M \to F_M$, *for all* $\tau \in \mathbb{R}$.

*Furthermore, if* $\{\hat{\chi}_n\}$ *is a sequence of unity approximations, then the following hold for each* $n = 1, 2, ....$

(c) $|(e^{-iKt}\chi_n)(x)|$ *and* $|\partial(e^{-iK\tau}\chi_n)(x)/\partial x|$ *are both continuous and bounded above uniformly in* $x$ *and* $t$ *by* $(2\pi)^{-1} \|\hat{\chi}_n\|_{S_1}$.

(d) $e^{-iK\tau}\chi_n \in L_q(\mathbb{R})$, *for all* $q$, $2 \leqslant q \leqslant \infty$.

*Proof.* (a) See ([16], Theorem IX.30).

(b) This follows immediately from Eq. (43) because $e^{-i(k^2/2\mu)\tau}\hat{f}(k) \in S_M$ for all $\hat{f} \in S_M$.

(c) This is proved by replacing $\hat{\chi}_n(k)$ by $e^{-i(k^2/2\mu)\tau}\hat{\chi}_n(k)$ in the proof of Lemma 3(a).

(d) This follows immediately from Lemma 3(c) and part (a) of this lemma. ∎

It follows from Eqs. (20) and (43) that the operators $e^{-iK\tau}\mathsf{C}_n$ are given by

$$(e^{-iK\tau}\mathsf{C}_n f)(x) = (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} e^{-i(k^2/2\mu)\tau} \hat{\chi}_n(k)\, \hat{f}(k), \tag{44}$$

for all $f \in F_M$ and $n = 1, 2, ....$ The following lemma establishes some properties of these operators.

LEMMA 7. *Let the hypotheses of Lemma* 4 *hold. Then,* $e^{-iK\tau}\mathsf{C}_n$ *maps* $F_M$ *into* $F_M$*, and for each* $f \in F_M$

$$(e^{-iK\tau}\mathsf{C}_n f)(x) = \int_{\mathbb{R}} dy\, (e^{-iK\tau}\chi_n)(x-y)\, f(y), \tag{45}$$

*with* $\chi_n = (2\pi)^{-1/2}\, \mathscr{F}\{\hat{\chi}_n\}$.

*Proof.* The proof is obtained by replacing $\hat{\chi}_n(k)$ by $e^{-i(k^2/2\mu)\tau}\hat{\chi}_n(k)$ in the proof of Lemma 4. ▮

Equation (44) gives the Schrödinger time evolution of continuous DAFs. The corresponding equation for the discrete DAFs is

$$(e^{-iK\tau}\mathsf{D}_n f)(x) = (2\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{ikx} e^{-i(k^2/2\mu)\tau} \hat{\chi}_n(k) \times \left\{ \frac{\Delta}{2\sqrt{2\pi}} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s e^{-ikx_{rs}} f(x_{rs}) \right\}, \tag{46}$$

where $\Delta$ is some positive real number. The following lemma establishes some useful properties.

LEMMA 8. *Let the hypotheses of Lemma* 5 *hold. Then* $e^{-iK\tau}\mathsf{D}_n f \in F_0 \subset L_\infty(\mathbb{R})$ *and*

$$(e^{-iK\tau}\mathsf{D}_n f)(x) = \frac{\Delta}{2} \sum_{r=-\infty}^{\infty} \sum_{s=1}^{S} w_s (e^{-iK\tau}\chi_n)(x - x_{rs})\, f(x_{rs}), \tag{47}$$

*where* $\chi_n = (2\pi)^{-1/2}\, \mathscr{F}\{\hat{\chi}_n\}$.

*Proof.* By inserting the Fourier representation of $(e^{-iK\tau}\chi_n)(x - x_{rs})$ into Eq. (47), one obtains Eq. (46), thus establishing their equivalence. The interchange of the summation and the integration is justified by the uniform absolute convergence of the sum in the braces. As noted in the proof of Lemma 5, the sum in the braces in Eq. (22) is continuous and is bounded by a first order polynomial in $|k|$. Therefore, $e^{-i(k^2/2\mu)t}\hat{\chi}_n(k)$ times the sum in the braces belongs to $S_0$ by ($\chi_1$). Since $(e^{-iKt}\mathsf{D}_n f)$ is the Fourier transformation of this function, it belongs by definition to $F_0$. ▮

Our final theorem establishes that the Schrödinger time evolution of certain functions may be approximated *uniformly in x and t* by both continuous and discrete DAFs.

THEOREM 3. (a) *Let the assumptions of Theorem 1 hold. Then,*

$$\lim_{n\to\infty} \sup_{\tau\in\mathbb{R}} \|(e^{-iK\tau}f)^{(m)} - (e^{-iK\tau}\mathsf{C}_n f)^{(m)}\|_\infty = 0, \tag{48}$$

*uniformly in m,* $0 \leqslant m \leqslant M$.

(b) *Let the assumptions of Theorem 2 hold. Then, for each finite n,*

$$\lim_{\Delta\to 0} \sup_{\tau\in\mathbb{R}} \|(e^{-iK\tau}\mathsf{C}_n f)^{(m)} - (e^{-iK\tau}\mathsf{D}_n f)^{(m)}\|_\infty = 0, \tag{49}$$

*uniformly in m,* $0 \leqslant m \leqslant M$.

(c) *Let the assumptions of Theorems 1 and 2 hold. Then,*

$$\lim_{n\to\infty} \lim_{\Delta\to 0} \sup_{\tau\in\mathbb{R}} \|(e^{-iK\tau}f)^{(m)} - (e^{-iK\tau}\mathsf{D}_n f)^{(m)}\|_\infty = 0, \tag{50}$$

*uniformly in m,* $0 \leqslant m \leqslant M$.

(d) *Let the assumptions of Theorems 1 and 2 hold, and let* $\mathsf{U}_\tau$ *be defined by Eq. (6) with* $v^{(m)}(x) \in \mathscr{L}_\infty(\mathbb{R})$, $0 \leqslant m \leqslant M$. *Then*

$$\lim_{n\to\infty} \lim_{\Delta\to 0} \sup_{\tau\in\mathbb{R}} \|(\mathsf{U}_\tau f)^{(m)} - (\mathsf{U}_\tau \mathsf{D}_n f)^{(m)}\|_\infty = 0. \tag{51}$$

*Proof.* (a) Replacing $\hat{f}(k)$ by $e^{-ik^2\tau/2\mu}\hat{f}(k)$ in the proof of Theorem 1 proves that $\|(e^{-iK\tau}f)^{(m)} - (e^{-iK\tau}\mathsf{C}_n f)^{(m)}\|_\infty$ is bounded by the expressions given in Eq. (31). Application of Eq. (32) then completes the proof of Theorem 3(a).

(b) Replacing $\hat{\chi}_n(k)$ by $e^{-i(k^2/2\mu)t}\hat{\chi}_n(k)$ in the proof of Theorem 2 proves that $\|(e^{-iK\tau}\mathsf{C}_n f)^{(m)} - (e^{-iK\tau}\mathsf{D}_n f)^{(m)}\|_\infty$ is bounded by the expression on the right-hand side of Eq. (33), immediately yielding Theorem 3(b).

(c) Theorem 3(c) is an immediate consequence of Theorem 3(a), Theorem 3(b), and the triangle inequality

$$\begin{aligned} &\|(e^{-iK\tau}f)^{(m)} - (e^{-iK\tau}\mathsf{D}_n f)^{(m)}\|_\infty \\ &\quad \leqslant \|(e^{-iK\tau}f)^{(m)} - (e^{-iK\tau}\mathsf{C}_n f)^{(m)}\|_\infty \\ &\qquad + \|(e^{-iK\tau}\mathsf{C}_n f)^{(m)} - (e^{-iK\tau}\mathsf{D}_n f)^{(m)}\|_\infty. \end{aligned} \tag{52}$$

(d) Because $(\mathsf{U}_\tau\varphi)(x) = e^{-iv(x)\tau}(e^{-iK\tau}\varphi)(x)$ for all functions $\varphi$, Eq. (51) is a trivial consequence of Theorem 3(c). ∎

Theorem 3(a) states, in other words, that the sequence $\{e^{-iK\tau}\chi_n\}_{n=1}^{\infty}$ is a delta sequence for which the expected pointwise limit Eq. (17) is achieved uniformly in $x$, $\tau \in \mathbb{R}$. That this delta sequence property persists in a discrete context is the surprising content of Theorem 3(c), which at the same time establishes that the uniformity noticed numerically by Hoffman *et al.* is not a numerical artifact but has its roots in the analytical properties of DAFs.

The distributed approximating functionals are tailored to make them useful for practical calculations.

- The class of functions $f$ for which Theorems 1-3 hold includes the class $S(\mathbb{R})$ of functions of rapid decrease. In particular it holds for the Gaussian wave functions often used in quantum mechanical calculations.
- For the $\chi_n$ defined in Eq. (14), the functions $e^{-iK\tau}\chi_n$ are known analytically,

$$(e^{-iK\tau}\chi_n)(x) = (2\pi\eta^2(\tau))^{-1/2}\, e^{-x^2/(2\eta^2(\tau))} \times \sum_{\nu=0}^{n} \frac{(-1)^\nu}{2^{2\nu}\nu!}\left(\frac{\sigma}{\eta(\tau)}\right)^{2\nu} H_{2\nu}(x/(2^{1/2}\eta(\tau))), \tag{53}$$

with $\eta(\tau) \equiv (\sigma^2 + i\tau/\mu)^{1/2}$. This greatly facilities the calculation of the kernel functions $(\mathsf{U}_\tau \mathsf{D}_n)(x, y)$ for the operators $\mathsf{U}_\tau \mathsf{D}_n$.

- The matrix with elements $(\mathsf{U}_\tau \mathsf{D}_n)(x_{rs}, x_{r's'})$ is strongly banded and block Toeplitz, greatly reducing demands on computer memory and allowing the use of very efficient specialized codes for matrix manipulation.

Theorem 3(d), which establishes a delta sequence property for the discrete operators $\mathsf{U}_\tau \mathsf{D}_n$, is only a beginning if those operators are to be used as a basis for practical solutions of the Schrödinger equation. Powers of $\mathsf{U}_\tau \mathsf{D}_n$ must be analyzed, especially as there is numerical evidence of a strong relation between the index $n$ and the maximum power that may be used before accuracy degrades. The effect of truncating the infinite sum in the definition of $\mathsf{D}_n$ needs study. Clearly there is much yet to be done to provide a solid mathematical foundation for this interesting numerical method.

## ACKNOWLEDGMENTS

The problem treated in this paper was brought to our attention by D. K. Hoffman and D. J. Kouri. We thank them for several stimulating conversations. We are grateful for the support of the U.S. National Science Foundation (Grants PHY-9505615 and INT-9222354). Finally, C. Chandler thanks the Flinders University of South Australia for its hospitality and the Australian–American Educational Foundation for its support (through its Fulbright Senior Scholar Program) during a portion of this work.

## REFERENCES


1. D. K. Hoffman, N. Nayar, O. A. Sharafeddin, and D. J. Kouri, Analytic banded approximation for the discretized free propagator, *J. Phys. Chem.* **95** (1991), 8299–8305.
2. D. K. Hoffman and D. J. Kouri, Distributed approximating function theory: A general, fully quantal approach to wave propagation, *J. Phys. Chem.* **96** (1992), 1179–1184.
3. D. K. Hoffman, M. Arnold, and D. J. Kouri, Properties of the optimum distributed approximating function class propagator for discretized and continuous wave packet propagations, *J. Phys. Chem.* **96** (1992), 6539–6545.
4. D. J. Kouri, W. Zhu, X. Ma, B. M. Pettitt, and D. K. Hoffman, Monte Carlo evaluation of real-time Feynman path integrals for quantal many-body dynamics: Distributed approximating functions and Gaussian sampling, *J. Phys. Chem.* **96** (1992), 9622–9630.
5. D. J. Kouri and D. K. Hoffman, Toward a new time-dependent path integral formalism based on restricted quantum propagators for physically realizable systems, *J. Phys. Chem.* **96** (1992), 9631–9636.
6. N. Nayar, D. K. Hoffman, X. Ma, and D. J. Kouri, A computational demonstration of the distributed approximating function approach to real time quantum dynamics, *J. Phys. Chem.* **96** (1992), 9637–9643.
7. D. J. Kouri, M. Arnold, and D. K. Hoffman, Time-to-energy transform of wavepackets using absorbing potentials. Time-independent wavepacket–Schrödinger and wavepacket–Lippmann–Schwinger equations, *Chem. Phys. Lett.* **203** (1993), 166–174.
8. D. K. Hoffman, M. Arnold, and D. J. Kouri, Traveling distributed approximating function approach to wave packet propagation: Explicit inclusion of a local wave velocity, *J. Phys. Chem.* **97** (1993), 1110–1118.
9. Y. Huang, D. J. Kouri, M. Arnold, T. L. Marchioro II, and D. K. Hoffman, Distributed approximating function approach to time-dependent wave-packet propagation in more than one dimension: Inelastic collinear atom–diatom collisions, *J. Chem. Phys.* **99** (1993), 1028–1034.
10. D. K. Hoffman, M. Arnold, W. Zhu, and D. J. Kouri, Interacting distributed approximating functions for real-time quantum dynamics, *J. Chem. Phys.* **99** (1993), 1124–1134.
11. T. L. Marchioro II, D. K. Hoffman, W. Zhu, Y. Huang, and D. J. Kouri, Extensions to the distributed approximating functional: The harmonic propagator, *Phys. Rev. E* **50** (1994), 2320–2330.
12. Y. Huang, D. J. Kouri, M. Arnold, T. L. Marchioro II, and D. K. Hoffman, Distributed approximating function approach to time-dependent wavepacket propagation in 3-dimensions: Atom-surface scattering, *Comput. Phys. Commun.* **80** (1994), 1–16.
13. A. M. Frishman, D. K. Hoffman, R. J. Rakauskas, and D. J. Kouri, Distributed approximating functional approach to fitting and predicting potential surfaces. 1. Atom–atom potentials, *Chem. Phys. Lett.* **252** (1996), 62–70.
14. D. K. Hoffman, T. L. Marchioro II, M. Arnold, Y. Huang, W. Zhu, and D. J. Kouri, Variational derivation and extensions of distributed approximating functionals, *J. Math. Chem.* **20** (1996), 117–140.
15. R. P. Feynman and A. R. Hibbs, "Quantum Mechanics and Path Integrals," McGraw–Hill, New York, 1965.
16. M. Reed and B. Simon, "Methods of Modern Mathematical Physics, Vol. II," Academic Press, New York, 1975.
17. M. Reed and B. Simon, "Methods of Modern Mathematical Physics, Vol. I," Academic Press, New York, 1972.
18. D. K. Hoffman and D. J. Kouri, personal communication.

19. W.-K. Liu, S. Li, and T. Belytscho, Moving least-square reproducing kernel methods. I. Methodology and convergence, *Comput. Methods Appl. Mech. Engrg.* **143** (1997), 113–154.
20. S. Li and W. K. Liu, Moving least-square reproducing kernel methods. II. Fourier analysis, *Comput. Methods Appl. Mech. Engrg.* **139** (1996), 159–193.
21. M. J. Johnson, On the approximation order of principal shift-invariant subspaces of $L_p(\mathbb{R}^d)$, *J. Approx. Theory* **91** (1997), 279–319.
22. S. Bochner and S. Chandrasekharan, "Fourier Transforms," Princeton Univ. Press, Princeton, 1949.
23. L. Hörmander, "Linear Partial Differential Operators,"Academic Press, New York, 1963.
24. J. P. Keener, "Principles of Applied Mathematics, Transformation and Approximation," Addison–Wesley, Redwood City, CA, 1988.
25. I. Stakgold, "Green's Functions and Boundary Value Problems," Wiley, New York, 1979.
26. P. J. Davis, "Interpolation and Approximation," Blaisdell, Waltham, MA, 1963.
27. W. O. Amrein, J. M. Jauch, and K. B. Sinha, "Scattering Theory in Quantum Mechanics," Benjamin, Reading, MA, 1977.