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# Discrete approximation of the radial contribution to the Schrödinger time evolution operator in three-dimensional Euclidean space

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**Abstract**
The Laplace operator $\nabla^2$ on $N$-dimensional Euclidean space $\mathbb{E}_N$ in spherical coordinates $(r, \theta_1, \ldots, \theta_{N-1}) \equiv (r, \overrightarrow{\theta})$ is $\nabla^2 = \triangle_r + \frac{1}{r^2}\triangle_0(\overrightarrow{\theta})$. The free-particle Schrödinger time evolution operator may be constructed by exponentiation, $\mathrm{e}^{\frac{\mathrm{i}}{2}\xi\nabla^2} = \cdots \mathrm{e}^{-\frac{1}{2}\xi^2[\triangle_r, \frac{1}{r^2}\triangle_0]}\,\mathrm{e}^{\frac{\mathrm{i}}{2r^2}\xi\triangle_0}\,\mathrm{e}^{\frac{\mathrm{i}}{2}\xi\triangle_r}$. Denoting a central finite difference approximation of $\triangle_r$ by $\frac{1}{\Delta r^2}\mathbb{T}^{\langle N\rangle}$, the matrix $\mathbb{S}^{\langle N\rangle} \equiv \mathrm{e}^{\frac{\mathrm{i}}{2}\lambda\mathbb{T}^{\langle N\rangle}}$, with $\lambda = \frac{1}{\Delta r^2}\xi$, is investigated and explicitly evaluated for $N = 3$. $\mathbb{S}^{\langle N\rangle}$ provides an approximation of the leading term of the radial component of the kinetic energy contribution to the evolution operator. An unconditionally stable numerical algorithm for quantum mechanical scattering is proposed based on this approximation when $N = 3$.

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## 1. Introduction

Let $\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2$ denote the Hamiltonian of a free spinless particle of mass $m$ moving in $\mathbb{E}_N$, and let $\Psi(r, \overrightarrow{\theta}, t)$ denote the Schrödinger wavefunction of this particle. Integration of the Schrödinger equation gives

$$\Psi(r, \overrightarrow{\theta}, t+\delta t) = \mathrm{e}^{\delta t\,\partial_t}\Psi(r, \overrightarrow{\theta}, t) = \mathrm{e}^{\frac{\mathrm{i}\hbar\delta t}{2m}\nabla^2}\Psi(r, \overrightarrow{\theta}, t). \tag{1}$$

The evolution operator may be expanded using the Zassenhaus formula as

$$\mathrm{e}^{\frac{\mathrm{i}\hbar\delta t}{2m}\nabla^2} = \cdots \mathrm{e}^{A_3\delta t^3}\,\mathrm{e}^{A_2\delta t^2}\,\mathrm{e}^{\frac{\mathrm{i}\hbar\delta t}{2m}\frac{1}{r^2}\triangle_0(\overrightarrow{\theta})}\,\mathrm{e}^{\frac{\mathrm{i}\hbar\delta t}{2m}\triangle_r}, \tag{2}$$

where the $A_2, A_3, \ldots$ are anti-Hermitian operators. This decomposition of the evolution operator is in terms of unitary operators, so that the norm of $\Psi$ is preserved as the 'dynamics' unfolds. We seek a discrete (and unitary, up to a similarity transformation) approximation to $e^{\frac{i\hbar\delta t}{2m}\triangle_r}$ for $N = 3, \ldots$ (the results for $N = 1$ and $N = 2$ are known [1, 2]).

Following Vilenkin [3] we introduce spherical coordinates $(r, \theta_1, \ldots, \theta_{N-1}) \equiv (r, \overrightarrow{\theta})$ in $N$-dimensional Euclidean space $\mathbb{E}_N$, which are related to Cartesian coordinates $x_n, n = 1, \ldots, N$ by

$$
\begin{aligned}
x_1 &= r\sin(\theta_{N-1})\cdots\sin(\theta_2)\sin(\theta_1)\\
x_2 &= r\sin(\theta_{N-1})\cdots\sin(\theta_2)\cos(\theta_1)\\
&\cdots\cdots\cdots\\
x_N &= r\cos(\theta_{N-1}).
\end{aligned}
$$

The Laplacian may be realized as $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\triangle_0(\overrightarrow{\theta})$, where $\triangle_0(\overrightarrow{\theta})$ has eigenvalues $-\ell(\ell + N - 2), \ell = 0, 1, 2, \ldots$ [3]. Let $\triangle_r = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r}\frac{\partial}{\partial r}$. Employing a uniform discrete lattice approximation with lattice spacing $\Delta r$ for the radial coordinate $r \to r_n = \left(n + \frac{1}{2}\right)\Delta r, n \in \mathbb{N}\,(n = 0, 1, 2, \ldots)$, the action of $\triangle_r$ on $\Psi$ may be approximated as $\{\triangle_r\Psi\}_n \approx \frac{1}{\Delta r^2}(\mathbb{T}^{\langle N\rangle}\Psi)_n$ where $(\mathbb{T}^{\langle N\rangle}\Psi)_n = \Psi_{n+1} - 2\Psi_n + \Psi_{n-1} + \frac{N-1}{2\left(n+\frac{1}{2}\right)}(\Psi_{n+1} - \Psi_{n-1})$. The matrix elements of $\mathbb{T}^{\langle N\rangle}$ are

$$
\mathbb{T}^{\langle N\rangle}_{nn'} = -2\delta_{nn'} + \delta_{nn'-1}\left(1 + \frac{N-1}{2n+1}\right) + \delta_{nn'+1}\left(1 - \frac{N-1}{2n+1}\right), \tag{3}
$$

where $n, n' \in \mathbb{N}$. Let $\lambda = \frac{\hbar\delta t}{m\Delta r^2}$. We compute a (unitary, up to a similarity transformation) approximation to $e^{\frac{i\hbar\delta t}{2m}\triangle_r}$ as

$$
\mathbb{S}^{\langle N\rangle} = e^{\frac{i}{2}\lambda\mathbb{T}^{\langle N\rangle}} = e^{-i\lambda}\, e^{\frac{i}{2}\lambda\widehat{\mathbb{T}}^{\langle N\rangle}}, \tag{4}
$$

where

$$
\widehat{\mathbb{T}}^{\langle N\rangle}_{nn'} = \delta_{nn'-1}\left(1 + \frac{N-1}{2n+1}\right) + \delta_{nn'+1}\left(1 - \frac{N-1}{2n+1}\right). \tag{5}
$$

At this point, it is convenient to define $\widehat{\mathbb{S}}^{\langle N\rangle}$ as

$$
\widehat{\mathbb{S}}^{\langle N\rangle} = e^{\frac{i}{2}\lambda\widehat{\mathbb{T}}^{\langle N\rangle}} \tag{6}
$$

and to compute $\widehat{\mathbb{S}}^{\langle N\rangle}$.

## 2. Evaluation of the $\widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda)$

Let $\mu = 1 - \frac{N}{2} = \frac{1}{2}, 0, -\frac{1}{2}, -1, \ldots$. Note that $\mu \leqslant -\frac{1}{2}$ for $N \geqslant 3$. The matrix elements $\widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda)$ may be investigated by considering

$$
h^{\langle N\rangle}_n(\lambda, \xi) \equiv \sum_{n'=0}^{\infty} \widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda) P^{\mu}_{n'}(\xi). \tag{7}
$$

Here, $P^{\mu}_{\nu}(\xi)$ denotes an associated Legendre function of the first kind of degree $\nu$ and order $\mu$. This series for $h^{\langle N\rangle}_n(\lambda, \xi)$ is convergent for $-1 \leqslant \xi \leqslant 1$ and $\lambda \in \mathbb{R}$ because $\left|P^{\pm\mu}_{\nu}(\xi)\right| \leqslant \sqrt{\left(\frac{8}{\nu\pi}\right)\frac{\Gamma(\nu\pm\mu+1)}{\Gamma(\nu+1)}}\sin(\cos^{-1}(\xi))^{-\mu-\frac{1}{2}}$ [4] and, for each $n$, $\left\{\widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda)\right\}_{n'\in\mathbb{N}} \in \ell^2(\mathbb{E}_N)$.

$P^{\mu}_{\nu}(\xi)$ satisfies the well-known recurrence relations

$$
(\nu - \mu + 1)P^{\mu}_{\nu+1}(\xi) + (\nu + \mu)P^{\mu}_{\nu-1}(\xi) = \xi(2\nu + 1)P^{\mu}_{\nu}(\xi) \tag{8}
$$

for $\nu, \mu, \xi \in \mathbb{C}$. We note that when $\mu = 1 - \frac{N}{2}$ these recurrence relations imply that

$$
\sum_{n'=0}^{\infty} \widehat{\mathbb{T}}^{\langle N\rangle}_{kn'} P^{\mu}_{n'}(\xi) = \begin{cases} 2\xi P^{\mu}_{k}(\xi) & \text{if} \quad k > 0 \\ (2\xi + N - 2)P^{\mu}_{k}(\xi) & \text{if} \quad k = 0. \end{cases} \tag{9}
$$

For future reference we record several other facts.

*2.1. Other facts/preliminary results*

When $n, k \in \mathbb{N}$, $\mu \in \mathbb{Z}$ and $|\mu| \leqslant n, k$ the orthogonality relations

$$\int_{-1}^{+1} P_n^{\mu}(\xi) P_k^{\mu}(\xi)\, \mathrm{d}\xi = \frac{2}{(2n+1)} \frac{(n+\mu)!}{(n-\mu)!} \delta_{nk} \tag{10}$$

hold. The orthogonality relations for odd $N$ require some discussion. For $N$ odd, $\mu = 1 - \frac{N}{2}$ is negative and half-odd-integral. For the case $N = 3$, $\mu = 1 - \frac{3}{2} = -\frac{1}{2}$. Let us put $\beta_\nu = [\xi + \sqrt{\xi^2 - 1}]^{\nu + \frac{1}{2}} = \mathrm{e}^{\mathrm{i}(\nu + \frac{1}{2})\theta}$, where $\xi = \cos(\theta)$. For the case $N = 3$, $\mu = -\frac{1}{2}$ we define the associated Legendre function $P_\nu^{-\frac{1}{2}}(\xi)$ as $\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} \times$ {the definition of Erdélyi *et al* [4] for $P_\nu^{-\frac{1}{2}}(\xi)$},

$$\begin{aligned} P_\nu^{-\frac{1}{2}}(\xi) &= \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} \frac{1}{2\nu+1} \sqrt{\frac{2}{\pi}} (\xi^2 - 1)^{-\frac{1}{4}} \left(\beta_\nu - \frac{1}{\beta_\nu}\right) \\ &= \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} \frac{2\mathrm{i}}{2\nu+1} \sqrt{\frac{2}{\pi}} (\xi^2 - 1)^{-\frac{1}{4}} \sin\left[\left(\nu + \frac{1}{2}\right)\theta\right]. \end{aligned} \tag{11}$$

Then for $\nu = n$, $\nu' = n' \in \mathbb{N}$ the following orthogonality relations apply:

$$\begin{aligned} &\int_{-1}^{+1} P_n^{-\frac{1}{2}}(\xi) P_{n'}^{-\frac{1}{2}}(\xi)\, \mathrm{d}\xi \\ &\qquad = \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}} \frac{2\,(2\mathrm{i})^2}{\mathrm{i}\pi(2n+1)(2n'+1)} \int_0^\pi \sin\left[\left(n + \frac{1}{2}\right)\theta\right] \sin\left[\left(n' + \frac{1}{2}\right)\theta\right] \mathrm{d}\theta \\ &\qquad = \left(\frac{2}{2n+1}\right)^2 \delta_{nn'}. \end{aligned} \tag{12}$$

This integral is the value obtained by formal analytic continuation of equation (10).

We shall also need the following integral (with $\xi = \cos(\theta)$):

$$\begin{aligned} &\int_{-1}^{+1} \mathrm{e}^{\mathrm{i}\lambda\xi} P_n^{-\frac{1}{2}}(\xi) P_k^{-\frac{1}{2}}(\xi)\, \mathrm{d}\xi \\ &\qquad = -\mathrm{i}(-4) \frac{2}{\pi} \frac{1}{(2n+1)(2k+1)} \\ &\qquad\quad \times \int_{-1}^{+1} \mathrm{e}^{\mathrm{i}\lambda\xi} \frac{1}{\mathrm{i}\sqrt{1-\xi^2}} \sin\left[\left(n + \frac{1}{2}\right)\theta\right] \sin\left[\left(k + \frac{1}{2}\right)\theta\right] \mathrm{d}\xi \\ &\qquad = \frac{8}{\pi(2n+1)(2k+1)} \int_0^\pi \mathrm{e}^{\mathrm{i}\lambda\cos(\theta)} \sin\left[\left(n + \frac{1}{2}\right)\theta\right] \sin\left[\left(k + \frac{1}{2}\right)\theta\right] \mathrm{d}\theta \\ &\qquad = \frac{4}{\pi(2n+1)(2k+1)} \int_0^\pi \mathrm{e}^{\mathrm{i}\lambda\cos(\theta)} \{\cos[(n-k)\theta] - \cos[(n+k+1)\theta]\}\, \mathrm{d}\theta \\ &\qquad = \frac{4}{(2n+1)(2k+1)} \{\mathrm{i}^{|n-k|} J_{|n-k|}(\lambda) - \mathrm{i}^{n+k+1} J_{n+k+1}(\lambda)\}. \end{aligned} \tag{13}$$

Here, we have used the well-known integral representation

$$\frac{1}{\pi} \int_0^\pi \mathrm{e}^{\mathrm{i}\lambda\cos(\theta)} \cos(n\theta)\, \mathrm{d}\theta = \mathrm{i}^{|n|} J_{|n|}(\lambda). \tag{14}$$

*2.2.* $\widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda)$

To evaluate $h_n^{\langle N\rangle}(\lambda,\xi)$ of equation (7), we begin by differentiating $h_n^{\langle N\rangle}(\lambda,\xi)$ with respect to $\lambda$. This yields

$$\begin{aligned}\frac{\partial}{\partial\lambda}h_n^{\langle N\rangle}(\lambda,\xi) &= \frac{\mathrm{i}}{2}\sum_{k=0}^{\infty}\widehat{\mathbb{S}}^{\langle N\rangle}_{nk}(\lambda)\sum_{n'=0}^{\infty}\widehat{\mathbb{T}}^{\langle N\rangle}_{kn'}P^{\mu}_{n'}(\xi)\\ &= \mathrm{i}\sum_{k=0}^{\infty}\widehat{\mathbb{S}}^{\langle N\rangle}_{nk}(\lambda)\left[\xi P^{\mu}_{k}(\xi)+\left(\frac{N}{2}-1\right)P^{\mu}_{0}(\xi)\delta_{k0}\right]\\ &= \mathrm{i}\xi h_n^{\langle N\rangle}(\lambda,\xi)+\mathrm{i}\left(\frac{N}{2}-1\right)\widehat{\mathbb{S}}^{\langle N\rangle}_{n0}(\lambda)P^{\mu}_{0}(\xi).\end{aligned}$$

Integration and application of the initial condition $h_n^{\langle N\rangle}(0,\xi) = P_n^{\mu}(\xi)$ for $h_n^{\langle N\rangle}(\lambda,\xi)$ gives

$$\begin{aligned}h_n^{\langle N\rangle}(\lambda,\xi) &= \sum_{n'=0}^{\infty}\widehat{\mathbb{S}}^{\langle N\rangle}_{nn'}(\lambda)P_{n'}^{1-\frac{1}{2}N}(\xi)\\ &= P_n^{1-\frac{1}{2}N}(\xi)\,\mathrm{e}^{\mathrm{i}\lambda\xi}+\mathrm{i}\left(\frac{N}{2}-1\right)\mathrm{e}^{\mathrm{i}\lambda\xi}\int_0^{\lambda}\widehat{\mathbb{S}}^{\langle N\rangle}_{n0}(\lambda')\,\mathrm{e}^{-\mathrm{i}\lambda'\xi}\,\mathrm{d}\lambda'\,P_0^{1-\frac{1}{2}N}(\xi).\end{aligned}\tag{15}$$

Here,

$$\begin{aligned}P_0^{1-\frac{1}{2}N}(\xi) &= \frac{1}{\Gamma\left(\frac{N}{2}\right)}\left(\frac{1-\xi}{1+\xi}\right)^{\frac{N-2}{4}}\\ &= \begin{cases}\dfrac{1}{\left(\frac{N}{2}-1\right)!}\left(\dfrac{1-\xi}{1+\xi}\right)^{\frac{N-2}{4}} & \text{if}\quad N=2,4,\ldots\\[2ex] \dfrac{2^{\frac{N-1}{2}}}{(N-2)!!\sqrt{\pi}}\left(\dfrac{1-\xi}{1+\xi}\right)^{\frac{(N-2)}{4}} & \text{if}\quad N=3,5,\ldots.\end{cases}\end{aligned}\tag{16}$$

For the case $N=3$, $\mu$ is negative and half-odd-integral: $\mu = 1-\frac{N}{2} = -\frac{1}{2}$. To simplify $\widehat{\mathbb{S}}^{\langle N\rangle}_{nk}(\lambda)$ in this case, we multiply equation (15) by $P_k^{\mu}(\xi)\,\mathrm{d}\xi$, integrate over $-1\leqslant\xi\leqslant+1$, use the orthogonality relations, equation (12), the Bessel function representation, equation (13), and $\frac{(k-\mu)!}{(k+\mu)!} = k+\frac{1}{2}$. This yields

$$\begin{aligned}\widehat{\mathbb{S}}^{\langle 3\rangle}_{nk}(\lambda) &= \frac{2k+1}{2}\frac{(k-\mu)!}{(k+\mu)!}\int_{-1}^{+1}\mathrm{e}^{\mathrm{i}\lambda\xi}P_n^{\mu}(\xi)P_k^{\mu}(\xi)\,\mathrm{d}\xi-\mathrm{i}\mu\frac{2k+1}{2}\frac{(k-\mu)!}{(k+\mu)!}\int_0^{\lambda}\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda')\\ &\quad\times\left[\int_{-1}^{+1}\exp(\mathrm{i}(\lambda-\lambda')\xi)P_0^{\mu}(\xi)P_k^{\mu}(\xi)\,\mathrm{d}\xi\right]\mathrm{d}\lambda'\\ &= \frac{2k+1}{2}\frac{(k-\mu)!}{(k+\mu)!}\frac{4}{(2n+1)(2k+1)}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda)-\mathrm{i}^{n+k+1}J_{n+k+1}(\lambda)\}\\ &\quad-\mathrm{i}\mu\frac{2k+1}{2}\frac{(k-\mu)!}{(k+\mu)!}\int_0^{\lambda}\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda')\\ &\quad\times\left[\frac{4}{(2k+1)}\{\mathrm{i}^{k}J_k(\lambda-\lambda')-\mathrm{i}^{k+1}J_{k+1}(\lambda-\lambda')\}\right]\mathrm{d}\lambda'\\ &= \frac{2k+1}{2n+1}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda)-\mathrm{i}^{n+k+1}J_{n+k+1}(\lambda)\}\\ &\quad+\frac{1}{2}\mathrm{i}^{k+1}(2k+1)\int_0^{\lambda}\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda')[J_k(\lambda-\lambda')-\mathrm{i}J_{k+1}(\lambda-\lambda')]\,\mathrm{d}\lambda'.\end{aligned}\tag{17}$$

Putting $k = 0$ into this result gives

$$\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda) = \frac{\mathrm{i}^n}{2n+1}\{J_n(\lambda) - \mathrm{i}J_{n+1}(\lambda)\} + \frac{\mathrm{i}}{2}\int_0^\lambda \widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda')[J_0(\lambda-\lambda') - \mathrm{i}J_1(\lambda-\lambda')]\,\mathrm{d}\lambda'. \tag{18}$$

We solve for $\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda) \equiv f(\lambda)$ using the Laplace transform $\mathcal{L}[f](s)$ and its inverse. The Laplace transform of equation (18) gives

$$\begin{aligned}\mathcal{L}[f](s) &= \frac{\mathrm{i}^n}{2n+1}\mathcal{L}[J_n - \mathrm{i}J_{n+1}](s) + \frac{\mathrm{i}}{2}\mathcal{L}[f](s)\mathcal{L}[J_0 - \mathrm{i}J_1](s)\\ &= \frac{\mathrm{i}^n}{2n+1}\frac{\mathcal{L}[J_n - \mathrm{i}J_{n+1}](s)}{\left\{1 - \frac{\mathrm{i}}{2}\mathcal{L}[J_0 - \mathrm{i}J_1](s)\right\}}\\ &= \mathrm{i}^n\frac{2}{2n+1}\left(s+\sqrt{1+s^2}\right)^{-(n+1)},\end{aligned} \tag{19}$$

and the inverse Laplace transform of this expression is

$$\widehat{\mathbb{S}}^{\langle 3\rangle}_{n0}(\lambda) = \mathrm{i}^n\frac{2(n+1)}{2n+1}\frac{J_{n+1}(\lambda)}{\lambda}. \tag{20}$$

Substituting this result back into equation (17), and using

$$\int_0^\lambda J_\mu(\lambda')J_\nu(\lambda-\lambda')\frac{\mathrm{d}\lambda'}{\lambda'} = \frac{1}{\mu}J_{\mu+\nu}(\lambda) \tag{21}$$

(cf [5], equation (11.3.40)) yields

$$\begin{aligned}\widehat{\mathbb{S}}^{\langle 3\rangle}_{nk}(\lambda) &= \frac{2k+1}{2n+1}\Bigg\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda) - \mathrm{i}^{n+k+1}J_{n+k+1}(\lambda)\\ &\quad + \mathrm{i}^{n+k+1}(n+1)\int_0^\lambda J_{n+1}(\lambda')[J_k(\lambda-\lambda') - \mathrm{i}J_{k+1}(\lambda-\lambda')]\frac{\mathrm{d}\lambda'}{\lambda'}\Bigg\}\\ &= \frac{2k+1}{2n+1}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda) - \mathrm{i}^{n+k+1}J_{n+k+1}(\lambda) + \mathrm{i}^{n+k+1}[J_{n+k+1}(\lambda) - \mathrm{i}J_{n+k+2}(\lambda)]\}\\ &= \frac{2k+1}{2n+1}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda) + \mathrm{i}^{n+k}J_{n+k+2}(\lambda)\}.\end{aligned} \tag{22}$$

Or

**Theorem 1** $\left(\widehat{\mathbb{S}}^{\langle 3\rangle}_{nk}\right)$**.**

$$\widehat{\mathbb{S}}^{\langle 3\rangle}_{nk}(\lambda) = \frac{2k+1}{2n+1}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda) + \mathrm{i}^{n+k}J_{n+k+2}(\lambda)\}. \tag{23}$$

## 3. Free Feynman propagator

As is well known, there is a closed expression for the free-particle propagator in any dimension $D$: $K(\vec{r}, t; \vec{r}', t' = \left(\frac{m}{2\pi\mathrm{i}\hbar(t-t')}\right)^{D/2}\exp\left(\frac{\mathrm{i}m}{2\hbar(t-t')}|\vec{r}-\vec{r}'|^2\right)$. How does this result relate to the discretized formula (23)?

To answer this question we first examine the case $D = 1$. According to a previous result [1], in 1-dimension and using Cartesian coordinates

$$\mathbb{S}(\lambda)_{nn'} = \left[\mathrm{e}^{\frac{\mathrm{i}\lambda}{2}\mathbb{T}}\right]_{nn'} = \mathrm{i}^{n-n'}\mathrm{e}^{-\mathrm{i}\lambda}J_{n-n'}(\lambda). \tag{24}$$

Here, $\lambda = \frac{\hbar\delta t}{m\Delta x^2}$.

We may employ the asymptotic expansion

$$J_\nu\left(\frac{\nu}{\cosh(\alpha)}\right) \sim \frac{1}{\sqrt{2\pi\nu\tanh\alpha}}\,\mathrm{e}^{\nu(\tanh\alpha-\alpha)}\left\{1+O\left(\frac{1}{\nu}\right)\right\}, \tag{25}$$

which is valid for large order $\nu$ [5] to compute the free Feynman propagator from equation (24). Let $x - x' = (n-n')\Delta x = \nu\Delta x$ where $\nu = n - n'$ and define $t - t' = N\delta t$. We consider the limits $\Delta x \to 0$, $\nu \to \infty$ with

$$x - x' = \lim_{\substack{\Delta x\to 0\\ \nu\to\infty}} \nu\Delta x$$

fixed, and the limits $\delta t \to 0$, $N \to \infty$ with

$$t - t' = \lim_{\substack{\delta t\to 0\\ N\to\infty}} N\delta t$$

fixed. If we define $\alpha$ by $\cosh(\alpha) = \frac{\nu}{N\lambda}$ then $\tanh(\alpha) = \frac{1}{\nu}\sqrt{\nu^2 - N^2\lambda^2}$ and we find that

$$\begin{aligned}
\mathbb{S}(N\lambda)_{nn'} &= \Bigg[\overbrace{\mathbb{S}(\lambda)\cdot\mathbb{S}(\lambda)\cdot\cdots\cdot\mathbb{S}(\lambda)}^{\text{N times}}\Bigg]_{nn'}\\
&= \mathrm{i}^{n-n'}\,\mathrm{e}^{-\mathrm{i}N\lambda}J_{n-n'}(N\lambda).\\
&= \frac{\mathrm{e}\left(-\mathrm{i}\lambda N + \sqrt{-(\lambda^2N^2)+\nu^2} + \frac{\mathrm{i}}{2}\nu\pi - \nu\,\mathrm{arcsech}\left(\frac{\lambda N}{\nu}\right)\right)}{(-(\lambda^2N^2)+\nu^2)^{\frac{1}{4}}\sqrt{2\pi}}\left\{1+O\left(\frac{1}{\nu}\right)\right\}\\
&= \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t-t')}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{m(x-x')^2}{2(t-t')}}\,\Delta x\{1+O(\Delta x)\},
\end{aligned} \tag{26}$$

which yields the very well-known free Feynman propagator $U(x-x';t-t')$ in the limit $\psi_n(t) = \sum_{n'=-\infty}^{\infty}\mathbb{S}(N\lambda)_{nn'}\psi_{n'}(t') \to \Psi(x,t) = \int_{-\infty}^{\infty}U(x-x';t-t')\Psi(x',t')\,\mathrm{d}x'$.

Unfortunately this type of limit does not exist when using spherical coordinates, even in a one-dimensional space. In a spherical coordinate system, even for problems with manifest spherical symmetry, the free Feynman propagator must contain an angular dependence to allow the particle to sample all paths. Even if a classical path is purely radial, quantum excursions from this path ensure that a non-trivial angular dependence exists in the propagator. We conclude that the full free propagator in spherical coordinates cannot be factored into radial and angular contributions, and hence its radial contribution cannot be calculated as any limit of equation (23). We should emphasize that in this paper we have not assumed spherical symmetry, and have only computed the leading radial contribution to the full free propagator. Angular (and smaller order radial) contributions are manifest in equation (2) and may be included as required.

## 4. Unconditional stability

The matrix with elements $\mathrm{e}^{-\mathrm{i}\lambda\widehat{\mathbb{S}}^{\langle 3\rangle}_{nk}}(\lambda)$ provides a concrete unitary approximation to $\mathrm{e}^{\frac{\mathrm{i}\hbar\delta t}{2m}\Delta_r}$, up to a similarity transformation. Here, $\lambda = \frac{\hbar\delta t}{m\Delta r^2}$. This similarity transformation is defined by a diagonal 'weight' matrix $\mathbb{W}$ with matrix elements

$$\mathbb{W}_{nn'} = \delta_{nn'}\left(n+\tfrac{1}{2}\right), \tag{27}$$

$n, n' \in \mathbb{N}$. $\mathbb{W}$ corresponds to the square root of the radial weight function $r^2$ in a standard spherical coordinate system in 3-space (recall that $r \to r_n = (n+\frac{1}{2})\Delta r$). The similarity transform of $\widehat{\mathbb{S}}^{\langle 3\rangle}$ by $\mathbb{W}$, $\widehat{\mathbb{U}} = \mathbb{W}\widehat{\mathbb{S}}^{\langle 3\rangle}\mathbb{W}^{-1} = \mathbb{W}\,\mathrm{e}^{\frac{\mathrm{i}}{2}\lambda\widehat{\mathbb{T}}^{\langle 3\rangle}}\mathbb{W}^{-1} = \mathrm{e}^{\frac{\mathrm{i}}{2}\lambda\mathbb{W}\widehat{\mathbb{T}}^{\langle 3\rangle}\mathbb{W}^{-1}}$, is a unitary matrix that naturally appears in the formalism. ($\widehat{\mathbb{U}}$ is a unitary matrix because $\mathbb{W}\widehat{\mathbb{T}}^{\langle 3\rangle}\mathbb{W}^{-1}$ is a real symmetric matrix (with non-zero matrix elements equal to +1 above and below the main diagonal).) A numerical algorithm for solving a quantum mechanical scattering problem in $N = 3$ dimensions based on this approximation for $\mathrm{e}^{\frac{i\hbar\delta t}{2m}\triangle_r}$ is unconditionally stable because $\widehat{\mathbb{U}}$ is a unitary matrix. It is expected, based on $N = 1$ known results and simulations [1], that scattering data obtained using such an algorithm may be as accurate as approximations computed using a Crank–Nicolson implicit second-order method [9].

To exhibit the unconditional stability of this approach it is sufficient to consider the following: let $\Phi$, $\Psi$ denote two column vectors representing, say, two discretized solutions to the Schrödinger equation at time $t$, with components $\Phi_n(\theta, \phi; t)$, $\Psi_n(\theta, \phi; t)$, $n = 0, 1, 2, \ldots$. $\mathbb{W}\Phi$ and $\mathbb{W}\Psi$ are employed in the construction of the scalar product $[\mathbb{W}\Psi]^\dagger\mathbb{W}\Phi = \Psi^\dagger\mathbb{W}^2\Phi$, and correspond to $\int_0^\infty \Psi^\dagger(r, \theta, \phi)\Phi(r, \theta, \phi)r^2\,\mathrm{d}r$ in the standard formalism. Moreover, according to equation (2), suppressing angular degrees of freedom, the leading order radial contribution to the propagator due to the kinetic energy is represented by $\mathrm{e}^{-\mathrm{i}\lambda}\widehat{\mathbb{U}}(\lambda)$: $\mathbb{W}\Psi(t + \delta t) = \cdots \mathbb{W}\,\mathrm{e}^{-\mathrm{i}\lambda}\widehat{\mathbb{S}}^{\langle 3\rangle}(\lambda)\mathbb{W}^{-1}\,[\mathbb{W}\Psi(t)] = \cdots \mathrm{e}^{-\mathrm{i}\lambda}\widehat{\mathbb{U}}(\lambda)[\mathbb{W}\Psi(t)]$. We see that the norm of $\mathbb{W}\Psi$ is preserved as the dynamics unfolds.

## 5. Conclusion

For $N = 3$, $\mathbb{S}^{\langle 3\rangle}$ of equation (23) provides a unitary (up to a similarity transformation by the weight matrix $\mathbb{W}$) approximation of the leading term of the radial component of the kinetic energy contribution to the evolution operator. An unconditionally stable numerical algorithm for quantum mechanical scattering may be based on this approximation. Let $V$ denote the effective potential energy of the spinless system, $\widehat{\mathbb{V}}$ denote the matrix representing $V$ and $b = \frac{m}{\hbar^2}\Delta r^2$. Since $\widehat{\mathbb{V}}$ is diagonal, equations (2) and (23) yield, to $O\big(\big[\frac{\hbar\delta t}{m\Delta r^2}\big]^2\big)$,

$$\Psi_n(t + \delta t) = \sum_{k=0}^{\infty}\left[\exp\left(\frac{\mathrm{i}\lambda}{2}T - \mathrm{i}\lambda b\widehat{\mathbb{V}}\right)\right]_{nk}\Psi_k(t), \tag{28}$$

where

$$\begin{aligned}\left[\exp\left(\frac{\mathrm{i}\lambda}{2}T - \mathrm{i}\lambda b\widehat{\mathbb{V}}\right)\right]_{nk} &= \left[\cdots \mathrm{e}^{-\mathrm{i}\lambda b\widehat{\mathbb{V}}}\,\mathrm{e}^{\frac{\mathrm{i}\lambda}{2}T}\right]_{nk} \\ &\approx \mathrm{e}^{-\mathrm{i}\lambda(1+b\widehat{\mathbb{V}}_{nn})}\frac{2k+1}{2n+1}\{\mathrm{i}^{|n-k|}J_{|n-k|}(\lambda) + \mathrm{i}^{n+k}J_{n+k+2}(\lambda)\}.\end{aligned} \tag{29}$$

The $J_n(\lambda)$ are calculated only once at the beginning of the procedure. If one examines the asymptotic expansion of $J_n$ then one sees that it decreases exponentially [8, 6] for large $\left|\frac{n}{\lambda}\right|$. It is expected, based on $N = 1$ known results and simulations [1], that scattering data obtained using such an algorithm will be as accurate as approximations computed using a Crank–Nicolson implicit second-order method [9].

This calculation recalls the associated Legendre function of the first kind, $P_\nu^\mu(\xi)$, which we employ to outline a general approach for attacking this problem; then particular results for $N = 3$ are illustrated. One of the referees has kindly pointed out that in $N = 3$ a simpler derivation of the $N = 3$ result may be obtained by defining polynomials $u_n(\xi) = \frac{1}{n+\frac{1}{2}}\frac{\sin((n+1)\arccos(\xi))}{\sin(\arccos(\xi))}$ (related to ordinary Chebyshev polynomials of the second kind). One finds that $\sum_{n'=0}^{\infty}\widehat{\mathbb{T}}_{kn'}^{\langle N\rangle}u_{n'}(\xi) = 2\xi u_k(\xi)$ for $k = 0, 1, 2, \ldots$. A simple homogeneous differential equation follows from this, and integration reproduces the result (23).

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