The commutators of the Poincaré group generators will be unchanged in form if a unitary transformation relates the free generators to the generators of an interacting relativistic theory. We test the concept of unitary transformations of generators in the nonrelativistic case, requiring that the free and interacting Hamiltonians be related by a unitary transformation. Other authors have applied this concept to time-dependent perturbation theory to give unitarity of the time evolution operator to each order in perturbation theory, with results that show improvement over the standard perturbation theory. In our case, a stationary perturbation theory can be constructed to find approximate solutions of the radial Schrödinger equation for scattering from a spherically symmetric potential. General formulae are obtained for the phase shifts at first and second order in the coupling constant. We test the method on a simple system with a known exact solution and find complete agreement between our first- and second-order contributions to the s-wave phase shifts and the corresponding expansion to second order of the exact solution.

I. INTRODUCTION

The motivation for this paper came from general considerations of interacting relativistic, quantum-mechanical theories. The proposal arising from those considerations was that the Poincaré generators of the interacting theory be related to those of the free theory by a unitary transformation. In this paper, we test that proposal on a nonrelativistic system, that of scattering of one spinless particle from a spherically symmetric potential. There, the interacting Hamiltonian is to be the unitary transformation of the free Hamiltonian. We find that a perturbation theory can be constructed by expanding the generator of the unitary transformation in powers of the coupling constant. This perturbation theory, because of the unitarity of the transformation acting on the state vectors, has the property that normalization is unchanged at each order in the coupling constant. Such is not the case for the conventional Green function method, with which we compare in section V.

Casas et al. [1] considered time-dependent perturbation theory, but their unitary transformation result carries over to the stationary perturbation theory considered here. They proposed that a unitary transformation of the original Hamiltonian be constructed to make an alternative Hamiltonian that is easier to solve

\[ H'_i = T^\dagger H_i T, \]

with \( T \), unitary, to be determined. The simplest choice is making \( H' \) equal to \( H_f \), which we assume can be solved exactly. This case is then the one considered here, with

\[ T = U_{if} \]

in our notation, a unitary transformation that depends on the coupling constant. In their examples it can also depend explicitly on time. Then the unitarity of their time evolution operator,

\[ U(t) = T e^{-iH_f t}, \]

is guaranteed at every order in their perturbation expansion. Their tests of the method on two-level systems show improvements over the standard time-dependent perturbation theory.

Ali [2] also considered time-dependent perturbation theory and the importance of unitarity. He noted that the Born series [3] for the time evolution operator is not unitary to any finite order. He proposed an exponentiation of

*Electronic address: scott.hoffmann@uqconnect.edu.au
the terms to a finite order, with modifications necessary to guarantee unitarity. For example, at first order he takes

\[ U^{(1)}(t) \rightarrow \exp(-i \int_0^t dt' H_I(t')) \]

instead of

\[ U^{(1)}_{\text{Born}}(t) = 1 - i \int_0^t dt' H_I(t'), \]

which is only unitary to first order. His tests of the method on two-level systems show improvements over the standard time-dependent perturbation theory.

For a free, special-relativistic, quantum-mechanical theory, we must have representations of the Poincare generators \( P^\mu \) (the four components of total energy-momentum which are the generators of spacetime translations) and \( M^{\mu \nu} \) (with \( K^i = M^{0i} \), the boost generators and \( J^k = \frac{1}{2} \epsilon_{kij} M^{ij} \), the angular momenta, generators of rotations) satisfying the commutation relations

\[
\begin{align*}
[P^\mu, P^\nu] &= 0, \\
[M^{\mu \nu}, P^\lambda] &= ig^{\nu \lambda} P^\mu - g^{\mu \lambda} P^\nu, \\
[M^{\mu \nu}, M^{\rho \sigma}] &= i(g^{\rho \sigma} M^{\mu \nu} - g^{\mu \nu} M^{\rho \sigma} - g^{\mu \rho} M^{\nu \sigma} - g^{\nu \sigma} M^{\mu \rho}).
\end{align*}
\]

(1)

For an interacting theory we must have different generators, \( P^\mu_i \) and \( M^{\mu \nu}_i \), satisfying commutators of the same form

\[
\begin{align*}
[P^\mu_i, P^\nu_i] &= 0, \\
[M^{\mu \nu}_i, P^\lambda_i] &= ig^{\nu \lambda} P^\mu_i - g^{\mu \lambda} P^\nu_i, \\
[M^{\mu \nu}_i, M^{\rho \sigma}_i] &= i(g^{\rho \sigma} M^{\mu \nu}_i - g^{\mu \nu} M^{\rho \sigma}_i - g^{\mu \rho} M^{\nu \sigma}_i - g^{\nu \sigma} M^{\mu \rho}_i).
\end{align*}
\]

(2)

We note that the form of a commutator is invariant under a unitary transformation. If

\[
[A, B] = iC
\]

(3)

and

\[
A' = UAU^\dagger, \quad B' = UBU^\dagger, \quad C' = UCU^\dagger,
\]

(4)

then

\[
[A', B'] = [UAU^\dagger, UBU^\dagger] = U[A, B]U^\dagger = iUCU^\dagger = iC'.
\]

(5)

So we propose that the free generators and interacting generators be related by a unitary transformation

\[
P^\mu_i = U_{if} P^\mu_f U_{if}^\dagger \quad \text{and} \quad M^{\mu \nu}_i = U_{if} M^{\mu \nu}_f U_{if}^\dagger.
\]

(6)

This unitary transformation will contain all the information on the interaction, so must depend on the charge. Also state vectors will be related by

\[
|\psi_i\rangle = U_{if} |\psi_f\rangle,
\]

(7)

where \(|\psi_f\rangle\) is a free state vector and \(|\psi_i\rangle\) is the corresponding interacting state vector. The consequences of this proposal will be considered in a future work.

We test the proposal on a nonrelativistic problem, the scattering of a spinless particle from a spherically symmetric potential. There, in the free theory, the first of the commutators

\[
[J_f, H_f] = 0 \quad \text{and} \quad \{J^j_f, J^j_f\} = i\epsilon_{ijk} J^k_f
\]

(8)

expresses the rotational invariance of the Hamiltonian. In the interacting theory, we require commutators of the same form,

\[
[J_i, H_i] = 0 \quad \text{and} \quad \{J^j_i, J^j_i\} = i\epsilon_{ijk} J^k_i.
\]

(9)
So we propose a unitary connection between the free operators and the interacting operators,

\[ H_i = U_{if} H_f U_{if}^\dagger \quad \text{and} \quad J_f = U_{if} J_f U_{if}^\dagger. \]  

We must also be able to write the interacting Hamiltonian in terms of a potential,

\[ H_i = H_f + V = H_f + \lambda U, \]

where \( \lambda \) is a dimensionless coupling constant. Note \( U \) is Hermitian but not unitary.

As we will see below, these equations can be solved for the generator of \( U_{if} \) as a series in powers of \( \lambda \), giving a perturbation theory that differs from those previously considered. In particular, once \( U_{if} \) is obtained to the desired order, the unitary transformation of the state vectors, for example the energy eigenvectors, is

\[ |E; i\rangle = U_{if} |E; f\rangle. \]  

Normalization will be preserved to each order, with no need for renormalization.

The organization of this paper is as follows. In section II we develop the unitary transformation theory for a spherically symmetric potential in nonrelativistic quantum mechanics. The result will be expressions for the unitary transformation generator at first and second order in \( \lambda \). In section III we consider a particular model, the spherical well or barrier, for which an exact solution is known. We will find agreement with the exact solution for the phase shifts to order \( \lambda^2 \). In section IV, we find general forms for the first and second order phase shifts using the phase shift formula derived using the Wronskian theorem. We then compare our results with the conventional Green function method, which is not designed to preserve normalization, in section V. Conclusions follow in section VI.

II. UNITARY TRANSFORMATION FOR SPHERICALLY SYMMETRIC POTENTIALS

Our aim is to solve the radial Schrödinger equation

\[ \{- \frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l + 1)}{2mr^2} + V(r)\} y^{(i)}_l(r, p) = \frac{p^2}{2m} y^{(i)}_l(r, p) \]  

on \( r \geq 0 \), with boundary condition \( y^{(i)}_l(0, k) = 0 \). We write

\[ V(r) = \lambda U(r). \]  

We take as the free Hamiltonian

\[ H_f = - \frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l + 1)}{2mr^2}. \]  

The free solutions that vanish at the origin are

\[ y^{(f)}_l(r, p) = \sqrt{\frac{2}{\pi}} kr j_{l}(pr), \]  

normalized to

\[ \int_0^\infty dr y^{(f)}_l(r, k_1) y^{(f)}_l(r, k_2) = \delta(k_1 - k_2). \]  

There are also solutions singular at the origin (for \( l \geq 1 \))

\[ \tilde{y}^{(f)}_l(r, p) = \sqrt{\frac{2}{\pi}} pr n_{l}(pr), \]  

which we will require in section V.

We write the unitary transformation in terms of an Hermitian generator, \( \Theta \), as

\[ U_{if} = e^{-i\Theta}. \]
We write $\Theta$ as a series in powers of $\lambda$, noting that it must vanish for $\lambda = 0$ to return the free theory:

$$\Theta = \lambda \Theta^{(1)} + \frac{1}{2} \lambda^2 \Theta^{(2)} + \ldots$$

Then

$$U_{if} = 1 - i\lambda \Theta^{(1)} - \frac{i}{2} \lambda^2 \Theta^{(2)} - \frac{1}{2} \lambda^2 \Theta^{(1)2} + \ldots$$

(21)

to this order.

Then from the two representations of $H_1$ in Eqs. (10) and (11), we require

$$U_{if} H_f U_{if}^\dagger = H_f + \lambda U.$$ 

(22)

To $O(\lambda^2)$, this is

$$H_f + i\lambda[H_f, \Theta^{(1)}] + \frac{i\lambda^2}{2} [H_f, \Theta^{(2)}] - \frac{1}{2} \lambda^2 [\Theta^{(1)}, [\Theta^{(1)}, H_f]] = H_f + \lambda U.$$ 

(23)

Equating like powers of $\lambda$, this gives

$$i[H_f, \Theta^{(1)}] = U \quad \text{and} \quad [H_f, \Theta^{(2)}] = [\Theta^{(1)}, U].$$ 

(24)

Taking matrix elements in the free basis, with

$$\Theta_i^{(n)}(k_1, k_2) \equiv \langle k_1, l | \Theta^{(n)} | k_2, l \rangle \quad \text{for} \quad n = 1, 2, 3, \ldots \quad \text{and} \quad U_i(k_1, k_2) \equiv \langle k_1, l | U | k_2, l \rangle,$$

(25)

gives the solutions

$$\Theta_i^{(1)}(k_1, k_2) = -i \frac{2m U_i(k_1, k_2)}{k_1^2 - k_2^2}$$

(26)

and

$$\Theta_i^{(2)}(k_1, k_2) = \frac{2m}{k_1^2 - k_2^2} \int_0^\infty dk \{ \Theta_i^{(1)}(k_1, k)U_i(k, k_2) - U_i(k_1, k)\Theta_i^{(1)}(k, k_2) \}
= -i \frac{2m}{k_1^2 - k_2^2} \int_0^\infty dk \{ \frac{2m U_i(k_1, k)U_i(k, k_2)}{k_1^2 - k^2} - \frac{2m U_i(k_1, k)U_i(k, k_2)}{k_2^2 - k^2} \}.$$ 

(27)

Note that from the Hermiticity of $U$, $U_i(k_1, k_2)$ is always symmetric in $k_1$ and $k_2$. In general (and in the example we consider in section [V]) it will not vanish at $k_1 = k_2$. So the expression in Eq. (26) is singular at $k_1 = k_2$. We deal with this singularity by imposing a rule of principal part integration. The justification for this is that, at first order, it ensures that the correction state vector is orthogonal to the unperturbed state vector, as required for unit normalization to first order. This leads to finite results in agreement with previous calculations.

We note the similarity of our result to the expression from first order perturbation theory of a discrete spectrum:

$$| n (1) \rangle = | n (0) \rangle - \lambda \sum_{n' \neq n} | n' (0) \rangle \frac{\langle n' (0) | V | n (0) \rangle}{E_{n'}^{(0)} - E_n^{(0)}},$$

where the absence of the contribution with $n' = n$ gives a finite result and unitarity of the transformation to first order. We can consider our method to be the continuum limit of the discrete method.

Then the unitarily transformed solution, to $O(\lambda)$, for momentum eigenvalue $p$, is

$$\langle r | p, l; i (1) \rangle = \int_0^\infty dk \langle r | k, l; f \rangle \langle k, l; f | U_{if} | p, l; f \rangle,$$

$$y_{i}^{(1)}(r, p) = y_{i}^{(f)}(r, p) - \lambda P \int_0^\infty dk y_{i}^{(f)}(r, k) \frac{2m U_i(k, p)}{(k^2 - p^2)}.$$ 

(28)

There are two ways to extract the phase shifts from this expression. The first is to evaluate the integral, then find the asymptotic behaviour of $y_{i}^{(1)}(r, p)$ as $r \to \infty$. We will do this to $O(\lambda^2)$ for a simple example potential in section [III] as a test of our method. The other method is to use the result derived using the Wronskian theorem [4]

$$\sin \delta_i(p) = \frac{-\pi m}{p} \int_0^\infty dr y_{i}^{(1)}(r, p)V(r)y_{i}^{(f)}(r, p).$$ 

(29)

To use this formula to find the phase shifts correct to $O(\lambda^2)$ only requires the interacting wavefunction to $O(\lambda)$. We will consider this method in section [IV].
III. THE SPHERICAL WELL OR BARRIER

In this section we test the unitary continuum perturbation method on a simple example, the spherical well or barrier. The potential is defined as

\[ V(r) = \begin{cases} \frac{\lambda}{R} & 0 \leq r \leq R, \\ 0 & r > R. \end{cases} \]  

(30)

For simplicity, we only consider the case \( l = 0 \), where the pair of free fundamental solutions is

\[ y_0^{(f)}(r, p) = \sqrt{\frac{2}{\pi}} \sin(pr), \quad \hat{y}_0^{(f)}(r, p) = -\sqrt{\frac{2}{\pi}} \cos(pr). \]  

(31)

We find that the matrix elements of the potential are

\[ \langle k_1, 0; f | V | k_2, 0; f \rangle = \lambda U_0(k_1, k_2) = \frac{\lambda}{\pi} \{\text{sinc}((k_1 - k_2)R) - \text{sinc}((k_1 + k_2)R)\}. \]  

(32)

Our method gives the normalized solution to \( O(\lambda) \)

\[ y_0^{(i,1)}(r, p) = \sqrt{\frac{2}{\pi}} \sin(pr) - \lambda \int_0^\infty dk \sqrt{\frac{2}{\pi}} \sin(kr) \frac{2mU_0(k, p)}{(k^2 - p^2)}. \]  

(33)

With \( q = k - p \), the principal part integral becomes

\[ P \int_0^\infty dk \sqrt{\frac{2}{\pi}} \sin(kr) \frac{2mU_1(k, p)}{(k^2 - p^2)} = P \int_{-p}^0 dq \sqrt{\frac{2}{\pi}} \sin((p+q)r) \frac{2mU_1(p + q, p)}{(2p + q)q} + \int_0^\infty dk \sqrt{\frac{2}{\pi}} \sin(kr) \frac{2mU_1(k, p)}{(k^2 - p^2)}. \]  

(34)

We are only interested in the asymptotic behaviour of these integrals as \( r \to \infty \), to obtain the phase shifts. The second integral will vanish like \( 1/r \) since the integrand is analytic in this region and the factor \( \sin(kr) \) oscillates rapidly with \( k \). In the principal part integration, the integrand is separated into parts odd in \( q \) and even in \( q \). The integral of the odd part on the symmetric interval \( q \in [-p, p] \), even if it is singular at \( q = 0 \), will vanish. The principal part integral is defined as the integral from \(-p\) to \(-\epsilon\) plus the integral from \(+\epsilon\) to \(+p\) for \( \epsilon \ll p \), with the limit as \( \epsilon \to 0^+ \) taken of the result.

This gives

\[ P \int_{-p}^0 dq \sqrt{\frac{2}{\pi}} \sin((p+q)r) \frac{2mU_1(p + q, p)}{(2p + q)q} = \sqrt{\frac{2}{\pi}} \sin(pr) \int_{-p}^0 dq \cos(qr) \left\{ \frac{4mp[U_1(p + q, p)]_+ - 2m [U_1(p + q, p)]_+}{(4p^2 - q^2)q} \right\} \]

\[ + \sqrt{\frac{2}{\pi}} \cos(pr) \int_{-p}^0 dq \sin(qr) \left\{ \frac{4mp[U_1(p + q, p)]_+ - 2m [U_1(p + q, p)]_+}{(4p^2 - q^2)} - \frac{2mU_1(p + q, p)}{(4p^2 - q^2)} \right\}, \]  

(35)

where

\[ [U_1(p + q, p)]_{\pm} = \frac{1}{2} \{U_1(p + q, p) \pm U_1(p - q, p)\} \]  

(36)

are the parts even (\( + \)) and odd (\( - \)) in \( q \). The first term will vanish like \( 1/r \) as \( r \to \infty \) since the integrand is without singularities and \( \cos(qr) \) oscillates rapidly as a function of \( q \). Then we note

\[ \frac{\sin(qr)}{q} = r \text{sinc}(qr) \sim \pi \delta(q). \]  

(37)

This factor approaches a delta function in \( q \) as \( r \to \infty \). This will give the only nonvanishing contribution as \( r \to \infty \)

\[ y_0^{(i,1)}(r, p) \to \sqrt{\frac{2}{\pi}} \sin(pr) - \lambda \sqrt{\frac{2}{\pi}} \cos(pr) \int_{-p}^0 dq \sin(qr) \frac{2mU_0(p + q, p)}{2p + q} \]

\[ = \sqrt{\frac{2}{\pi}} \sin(pr) + \left\{ -\frac{\pi \lambda}{p/m} U_0(p, p) \right\} \sqrt{\frac{2}{\pi}} \cos(pr). \]  

(38)
This is of the form, to $\mathcal{O}(\lambda)$,

$$y_0^{(1,1)}(r, p) \to \sqrt{\frac{2}{\pi}} \sin(pr + \delta_0^{(1)}(p)), \quad (39)$$

with phase shift

$$\delta_0^{(1)}(p) = -\frac{\pi \lambda}{p/m} U_0(p, p) = -\frac{\lambda}{p/m}(1 - \text{sinc}(2pR)). \quad (40)$$

We note that the size of the phase shift at high energies ($pR \gg 1$) is controlled by the factor

$$\eta \equiv \frac{\lambda}{p/m}. \quad (41)$$

This is very similar to the case of the Coulomb potential, where

$$\eta_C = \frac{Z_1 Z_2 \alpha}{p/m} \quad (42)$$

controls the size of the phase shifts. Here $Z_1$ and $Z_2$ are the atomic numbers of the target and projectile, respectively and $\alpha \approx 1/137$ is the fine structure constant.

At second order, using Eqs. (26,27), we find the contribution

$$\langle r \mid -\frac{1}{2} \lambda^2 (\Theta^{(1,2)} + i\Theta^{(2)}) \mid p, 0; f \rangle \to \sqrt{\frac{2}{\pi}} \sin(pr) \{ -\frac{1}{\eta^2 (1 - 2 \text{sinc}(2pR))} \} + \sqrt{\frac{2}{\pi}} \cos(pr) \{ -\frac{1}{\eta^2 (1 + 2 \cos(2pR))} \} + \mathcal{O}(\frac{1}{pR^2}). \quad (43)$$

We perform the $k$ integral first. In the first term, there is only a pole at $k = k'$, which we treat similarly to the first order calculation just given. In the second term, there are poles at $k = k'$ and $k = p$. We use expansions of $\sin(kr)$ around each of these points separately. To proceed with the remaining $k'$ integral, we choose to consider only the regime $pR \gg 1$ and obtain results to order $1/pR$. We encounter factors

$$\frac{\sin(qR)}{q} \sim \pi \delta(q) \quad \text{and} \quad \text{sinc}^2(qR) \sim \frac{\pi}{R} \delta(q), \quad (44)$$

approximations to delta functions in this regime. The net result is

$$\langle r \mid -\frac{1}{2} \lambda^2 (\Theta^{(1,2)} + i\Theta^{(2)}) \mid p, 0; f \rangle \to \sqrt{\frac{2}{\pi}} \sin(pr) \{ -\frac{1}{\eta^2 (1 - 2 \text{sinc}(2pR))} \} + \sqrt{\frac{2}{\pi}} \cos(pr) \{ -\frac{1}{\eta^2 (1 + 2 \cos(2pR))} \} + \mathcal{O}(\frac{1}{pR^2}). \quad (45)$$

The factor in the first term is

$$-\frac{1}{2} \eta^2 (1 - 2 \text{sinc}(2pR)) = -\frac{1}{2} \delta_0^{(1)}(p)^2 + \mathcal{O}(\frac{1}{pR^2}), \quad (46)$$

as required for unitarity. The second term gives the prediction

$$\delta_0^{(2)}(p) = -\eta^2 \frac{(1 + 2 \cos(2pR))}{2pR} + \mathcal{O}(\frac{1}{pR^2}). \quad (47)$$

The spherical well and barrier problems can be solved exactly with elementary methods. The energy shift on $0 \leq r \leq R$ gives free solutions with momenta

$$p' = \sqrt{p^2 + \frac{2m\lambda}{R}} = p\sqrt{1 + \frac{2\eta}{pR}}. \quad (48)$$
To satisfy the boundary condition, the solution must be proportional to \( y_0^{(f)}(r, p') \) in that region. For \( r > R \), the solution is a linear combination of the fundamental solutions \( y_0^{(f)}(r, p) \) and \( \tilde{y}_0^{(f)}(r, p) \). Requiring the wavefunction and its first derivative to be continuous across the boundary gives the solution, which then only needs normalization.

We find that the \( l = 0 \) phase shifts, \( \delta_0(p) \), are given by

\[
e^{i2\delta_0(p)} = \frac{(A_0 - iB_0)^2}{A_0^2 + B_0^2},
\]

with

\[
A_0 = \kappa' j_0(\kappa')n'_0(\kappa) - \kappa' \kappa n_0(\kappa)j'_0(\kappa'), \\
B_0 = \kappa' j_0(\kappa')j'_0(\kappa') - \kappa^2 j_0(\kappa')j'_0(\kappa),
\]

and \( \kappa = pR, \kappa' = p'R \).

We expand

\[
\kappa' = \kappa + \eta - \frac{1}{2} \eta^2 \frac{1}{\kappa}
\]

to \( \mathcal{O}(\eta^2) \), noting that this series only converges on \( \eta < \frac{1}{2}pR \), which is \( |V_0| < E \), where \( |V_0| = |\lambda|/R \) is the height or depth of the potential and \( E = p^2/2m \) is the energy of the projectile. For \( |\eta| > \frac{1}{2}pR \), the solutions are real exponentials on \( 0 \leq r \leq R \). For a small number of terms of a perturbative expansion to give a good approximation requires the further constraint \( |\eta| < 1 \). Expanding the expression for \( \exp(i2\delta_0(p)) \) in Eq. (49) to \( \mathcal{O}(\eta^2) \) with Mathematica gives phase shifts in agreement with Eqs. (40) and (47).

**IV. THE WRONSKIANS FORMULA**

A useful formula regarding phase shifts was obtained using the Wronskian theorem. We consider the two second order differential equations

\[
\{- \frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + V(r)\}y_1^{(i)}(r, p) = \frac{p^2}{2m}y_1^{(i)}(r, p)
\]

and

\[
\{- \frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2}\}y_1^{(f)}(r, p) = \frac{p^2}{2m}y_1^{(f)}(r, p).
\]

The Wronskian theorem gives

\[
W(y_1^{(i)}(r, p), y_1^{(f)}(r, p))|_0^M = \int_0^M dr \{y_1^{(i)}(r, p)y_1^{(f)f}(r, p) - y_1^{(f)i}(r, p)y_1^{(f)}(r, p)\}
\]

\[
= -2m \int_0^M dr y_1^{(i)}(r, p)V(r)y_1^{(f)}(r, p).
\]

For potentials, \( V(r) \), that fall off faster than \( 1/r \) as \( r \to \infty \) and may diverge at the origin no faster than \( 1/r^2 \), we know the asymptotic behaviour

\[
y_1^{(f)}(r, p) \to \sqrt{\frac{2}{\pi}} \sin(pr - l\frac{\pi}{2}) \quad \text{and} \quad y_1^{(i)}(r, p) \to \sqrt{\frac{2}{\pi}} \sin(pr - l\frac{\pi}{2} + \delta_1(p)).
\]

The Wronskian vanishes at the origin and, for \( pM \gg 1 \) approaches

\[
W(y_1^{(i)}(M, p), y_1^{(f)}(M, p)) \to \frac{2p}{\pi} \sin(\delta_1(p)),
\]

so

\[
\sin(\delta_1(p)) = -\frac{\pi m}{p} \int_0^\infty dr y_1^{(i)}(r, p)V(r)y_1^{(f)}(r, p).
\]
Hamiltonian equation that is the radial Schrödinger equation. This is an iterative perturbation method. We take as the “free”

\[
\langle \sin(\delta_1^{(1)}(p) + \delta_1^{(2)}(p)) = \delta_1^{(1)}(p) + \delta_1^{(2)}(p)
\]

\[
= -\frac{\pi m}{p} \int_0^\infty dr y_l^{(f)}(r,p)V(r)y_l^{(f)}(r,p) + \frac{\pi m}{p} \int_0^\infty dk y_l^{(f)}(r,k) \frac{2m\langle k,l;f|V|p,l;f \rangle}{k^2 - p^2} V(r)y_l^{(f)}(r,p)
\]

\[
= -\frac{\pi m}{p} \langle p,l;f|V|p,l;f \rangle + \frac{2\pi m^2}{p} \int_0^\infty dk \langle k,l;f|V|p,l;f \rangle^2.
\]

(58)

So the contributions to the phase shifts are

\[
\delta_1^{(1)}(p) = -\frac{\pi m}{p} \langle p,l;f|V|p,l;f \rangle, \quad \delta_1^{(2)}(p) = \frac{2\pi m^2}{p} \int_0^\infty dk \langle k,l;f|V|p,l;f \rangle^2.
\]

(59)

We verified that these two expressions give results in agreement with Eqs. (40) and (71) for the spherical well or barrier in the regime \( pR \gg 1 \).

V. COMPARISON WITH THE GREEN FUNCTION METHOD

We compare our method with the commonly used Green function method [3] for solving the second order differential equation that is the radial Schrödinger equation. This is an iterative perturbation method. We take as the “free” Hamiltonian

\[
H_0 = -\frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2},
\]

(60)

with known fundamental solutions

\[
\tilde{j}_l(kr) = \sqrt{\frac{2}{\pi}} kr \tilde{j}_l(kr) \quad \text{and} \quad \tilde{n}_l(kr) = \sqrt{\frac{2}{\pi}} kr \tilde{n}_l(kr),
\]

(61)

the latter being singular at the origin for \( l \geq 1 \). So we want to solve

\[
\langle r | H_0 - \frac{k^2}{2m} | k;i \rangle = -V(r)\langle r | k;i \rangle.
\]

(62)

We define the Green function, \( G(r,r') \), as a solution of

\[
\left\{-\frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} - \frac{k^2}{2m}\right\} G(r,r') = \delta(r-r').
\]

(63)

Then we note that the solutions, \( \langle r | k;i \rangle \), of the integral equation

\[
\langle r | k;i \rangle = \langle r | k;f \rangle - \int_0^\infty dr' G(r,r') V(r') \langle r' | k;i \rangle
\]

(64)

satisfy Eq. (62), the radial Schrödinger equation.

The integral equation is solved by iteration, first inserting the free solution that vanishes at the origin, \( \tilde{j}_l(kr) \), in place of \( \langle r' | k;i \rangle \) on the right hand side to generate \( \langle r | k;i(1) \rangle \) to first order in \( \lambda \). Next \( \langle r | k;i(1) \rangle \) is inserted on the right hand side to generate \( \langle r | k;i(2) \rangle \) and so on.

For the Green function, there is freedom in the definition, and we take the symmetric form

\[
G(r,r') = -\frac{\pi m}{k} \begin{cases} 
\tilde{j}_l(kr)\tilde{n}_l(kr') & \text{for } r < r', \\
\tilde{n}_l(kr')\tilde{j}_l(kr) & \text{for } r > r'.
\end{cases}
\]

(65)

Unlike the method presented in this paper, the Green function method is not designed to preserve the normalization of the solution. Using the symmetric Green function guarantees that the solution has the correct normalization to
\( \mathcal{O}(\lambda) \), but not at second and higher order, as we have found. A process of renormalization is necessary. If we find that the asymptotic form of the \( n \)-th order solution as \( r \to \infty \) is

\[
\langle r \mid k; i \rangle (n) = \sqrt{\frac{2}{\pi}} \sin(kr - \frac{l}{2}) A_l^{(n)}(r) + \sqrt{\frac{2}{\pi}} \cos(kr - \frac{l}{2}) B_l^{(n)}(r),
\]

then we must take

\[
\cos(\Delta_l^{(n)}(k)) = \frac{A_l^{(n)}}{\sqrt{A_l^{(n)2} + B_l^{(n)2}}} \quad \text{and} \quad \sin(\Delta_l^{(n)}(k)) = \frac{B_l^{(n)}}{\sqrt{A_l^{(n)2} + B_l^{(n)2}}},
\]

where \( \Delta_l^{(n)}(k) \) is the total phase shift up to \( n \)-th order,

\[
\Delta_l^{(n)}(k) = \delta_l^{(1)}(k) + \cdots + \delta_l^{(n)}(k).
\]

At first order, we encounter the integrals

\[
A_l^{(1)}(r) = \frac{\pi m}{k} \int_0^r dr' \sqrt{\frac{2}{\pi}} kr' n_l(kr') V(r') \sqrt{\frac{2}{\pi}} kr j_l(kr'),
\]

\[
B_l^{(1)}(r) = \frac{\pi m}{k} \int_0^r dr' \sqrt{\frac{2}{\pi}} kr' j_l(kr') V(r') \sqrt{\frac{2}{\pi}} kr j_l(kr').
\]

We find

\[
\delta_l^{(1)}(k) = -B_l^{(1)}(\infty),
\]

in agreement with Eq. (40). If \( r \) is increased without bound to find \( B_l^{(1)}(\infty) \), the potential must fall off faster than \( 1/r' \) for convergence. Thus this method cannot be applied to the Coulomb potential, as we found for our method. At small \( r \),

\[
A^{(1)}(r) \sim C \int_0^r dr' \frac{1}{r'^{l+1}} V(r') r'^{l+1},
\]

so \( V(r') \) may diverge at the origin provided the divergence is slower than \( 1/r'^2 \).

At second order, we encounter integrals such as

\[
C^{(2)}(\infty) = \frac{\pi^2 m^2}{k^2} \int_0^\infty dr' \tilde{n}_l(kr') V(r') \tilde{n}_l(kr') \int_0^{r'} dr'' \tilde{j}_l(kr'') V(r'') \tilde{j}_l(kr'').
\]

This will converge if the bounds just found are satisfied. This is a nested double integral, unlike what we found with the unitary method.

As a check on the validity of this method, we again considered the spherical well/barrier for \( s \)-wave scattering \( (l = 0) \). The integrals, such as that in Eq. (71), were straightforward to evaluate for this finite range potential. We expect they would pose more difficulty in the general case. The simplicity of the unitary method, where all integrals we encountered contained approximations to the delta function, compared to evaluating such integrals, is clear. We found complete agreement with the results of Eqs. (40) and (47).

VI. CONCLUSIONS

The aim of this paper was to investigate the consequences of relating an interacting Hamiltonian to the corresponding free Hamiltonian by a unitary transformation. Using the example of scattering from a rotationally invariant potential with the radial Schrödinger equation, we demonstrated how to solve for the transformation to second order in the coupling constant.

As a consequence of these results, we were able to formulate a perturbation theory with significant differences from the commonly used Green function method. The steps in the unitary method involve integrals over momentum while those of the Green function method involve integrals over position. We tested the unitary method on the spherical well and barrier, for which exact solutions are known. Obtaining the \( s \)-wave phase shifts in the regime where \( pR \gg 1 \) (\( p \)}
is the momentum under consideration and $R$ is the finite range of the potential), we found agreement with the Green function method and with the exact solution. It is of note that the unitary method gives analytic approximations to the wavefunction, while the Green function method gives piecewise continuous approximations (with continuous first derivatives). The exact solution has this character for this model.

The most significant difference between the unitary method and the Green function method is that the former preserves wavefunction normalization at all orders, while the latter requires renormalization.

The momentum integrals we encountered in the unitary method all contained approximations to delta functions, greatly simplifying the calculation. Of course away from the regime $pR \gg 1$ the integrals would become more involved. The Green function method position integrals are nested at second order. This was not a problem for the finite range example, but would add complication for a general, continuous, potential.

We comment on the Coulomb scattering problem, with solutions not accessible by this unitary perturbation theory or with the Green function method (which is known in this case as the Born approximation [3]). Yet the exact solutions of the Coulomb problem are known. It should be possible to perturb around those solutions, if the perturbing potential is within the class for which perturbation theory is applicable.

So we consider the problem with Hamiltonian

$$H = H_C + V, \quad H_C = -\frac{1}{2m} \frac{d^2}{dr^2} + \frac{l(l + 1)}{2mr^2} + \frac{Z_1 Z_2 \alpha}{r}. \tag{72}$$

Our results carry over with $y_{l}^{(f)}(r, p)$ replaced by $y_{l}^{(C)}(r, p)$, the exact Coulomb solutions. Another Wronskian result can be derived in this case. With the asymptotic forms [4]

$$y_{l}^{(C)}(r, p) \rightarrow \sqrt{\frac{2}{\pi}} \sin(pr - l\pi/2 - \eta_C \ln(2pr) + \sigma_l(p)) \quad \text{and} \quad y_{l}^{(i)}(r, p) \rightarrow \sqrt{\frac{2}{\pi}} \sin(pr - l\pi/2 - \eta_C \ln(2pr) + \delta_l(p)), \tag{73}$$

we have

$$\sin(\delta_l(p) - \sigma_l(p)) = -\frac{\pi m}{p} \int_0^\infty dr y_{l}^{(i)}(r, p)V(r)y_{l}^{(C)}(r, p), \tag{74}$$

where $\sigma_l(p)$ are the Coulomb phase shifts [4] and $\eta_C$ is defined in Eq. [42]. Use of this formula would give a result to all orders in $\eta_C$ and any desired order in the perturbation.

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