Discrete-basis-set approach to nonspherical scattering. II.†

Thomas N. Rescigno, Clyde W. McCurdy, Jr., and Vincent McKoy
Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91109*
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A method is described for computing scattering amplitudes for a cylindrically symmetric potential using square-integrable basis functions. The addition of variational corrections using the Kato formula is also outlined. Results for a two-center Gaussian potential are presented.

I. INTRODUCTION

In a previous article, hereafter referred to as I, we outlined a method for computing scattering amplitudes for a nonspherical potential.[1] The approach involves representing the potential in a discrete set of Gaussian basis functions and solving the Lippmann-Schwinger equation for the full scattering amplitude as a matrix equation in this subspace. In this paper we present a more complete discussion of the details of the method. We also show that improved results may be obtained by a variational correction of the calculated scattering amplitudes. We report numerical results for a two-center Gaussian potential at several energies and scattering angles.

The outline of this paper is as follows. In Sec. II A the details of the calculation, in particular the choice of basis functions and computation of the necessary matrix elements, are examined. Section II B discusses a method for obtaining variationally stable results, and in Sec. II C we comment briefly on an alternative approach to the problem of scattering from nonspherical potentials. Our numerical results are reported in Sec. III. Section IV contains a brief discussion.

II. THEORY

A. Use of Gaussian functions in solving the Lippmann-Schwinger equation

As discussed in I, the *ansatz* which forms the basis for the approach used here is the approximate representation of the potential in a finite, discrete basis. We denote this truncated potential as V^t:

$$V^t = \sum_{\alpha,\beta} |\alpha\rangle\langle\alpha|V|\beta\rangle\langle\beta| . \tag{1}$$

If this approximation seems severe, it should be noted that whenever the Schrödinger equation is solved by diagonalization of the Hamiltonian in a basis set, the same approximation for the potential (as well as for the kinetic energy) is being used. The advantage of this truncation of the potential in scattering problems is that it leads to a separable kernel[2] in the Lippmann-Schwinger equation which may then be written as a finite matrix problem. Denoting the truncated transition operator as T^t, its matrix elements in the finite basis satisfy the equation

$$\langle\alpha|T^t(E)|\beta\rangle = \langle\alpha|U|\beta\rangle + \sum_{\gamma,\delta} \langle\alpha|U|\gamma\rangle \times \langle\gamma|G_0(E)|\delta\rangle\langle\delta|T^t(E)|\beta\rangle , \tag{2}$$

where $U = 2V$ in atomic units. The solution of this equation yields the exact scattering amplitude for the truncated potential V^t via the transformation

$$f(\vec{k}_{out} \leftarrow \vec{k}_{in}) = -\frac{1}{4\pi}\langle\vec{k}_{out}|T^t(E)|\vec{k}_{in}\rangle = -\frac{1}{4\pi}\sum_{\alpha,\beta}\langle\vec{k}_{out}|\alpha\rangle\langle\alpha|T^t(E)|\beta\rangle\langle\beta|\vec{k}_{in}\rangle , \tag{3}$$

where

$$\langle\alpha|\vec{k}\rangle = \int e^{i\vec{k}\cdot\vec{r}}\langle\vec{r}|\alpha\rangle\, d^3r . \tag{4}$$

The solution of Eq. (2) requires only matrix elements of the potential and the free-particle Green's function.

As in I, we restrict our attention to cylindrically symmetric potentials which possess a center of inversion. If one chooses basis functions which transform with the irreducible representations of the point group $D_{\infty h}$, then Eq. (2) may be solved separately for each symmetry ($\Sigma_g^+, \Sigma_u^+, \Pi_g$, etc.). This is an extremely important consideration, since it greatly reduces the size of the matrices that must be handled at any point in the calculation. The basis $\{|\alpha\rangle\}$ can then be obtained by orthonormalization of a set of functions of the form

$$\varphi_\alpha = g_\alpha(\vec{r} - \vec{A}) \pm g_\alpha(\vec{r} + \vec{A}) , \tag{5}$$

where $\pm$ determines the symmetry under inversion (g or u).

In multicenter problems, it is normal to choose $g_\alpha(\vec{r})$ to be a Gaussian function.[3] This choice is particularly convenient here since it leads to great simplification in the calculation of matrix elements

of the free-particle Green's function. Specifically, we choose

$$g_\alpha(\vec{r}-\vec{A}) = x^l y^m (z-A)^n e^{-\alpha[x^2+y^2+(z-A)^2]}. \quad (6)$$

A matrix element of $G_0(E)$ can be written as

$$\langle\alpha|G_0(E)|\beta\rangle = \lim_{\epsilon\to 0^+}\frac{1}{(2\pi)^3}\left(\int \frac{\langle\alpha|\vec{k}\rangle\langle\vec{k}|\beta\rangle}{k_0^2-k^2+i\epsilon}\,d^3k\right) \quad (7)$$

where $E=\frac{1}{2}k_0^2$. The required Fourier transform of φ_α [Eq. (5)] can be done in closed form[4]:

$$\int e^{i\vec{k}\cdot\vec{r}}\varphi_\alpha(\vec{r})\,d^3r = (e^{ik_zA}\pm e^{-ik_zA})\left(\frac{\pi}{\alpha}\right)^{3/2}\frac{1}{(2i\sqrt{\alpha})^{l+m+n}}e^{-k^2/4\alpha}H_l\left(-\frac{k_x}{2\sqrt{\alpha}}\right)H_m\left(-\frac{k_y}{2\sqrt{\alpha}}\right)H_n\left(-\frac{k_z}{2\sqrt{\alpha}}\right), \quad (8)$$

where H_l is a Hermite polynomial.

In performing the triple integration over $\vec{k}$ in Eq. (7) we choose the z direction of $\vec{k}$ to lie along the symmetry axis. The θ integration to be performed is then of the form

$$\int_{-1}^{1} dx\, P(x)Q(x).$$

$P(x)$ is a polynomial in x where $x=\cos\theta$, and $Q(x)$ is either $\cos^2(kAx)$, $\sin^2(kAx)$, or $\sin(kAx)\cos(kAx)$ depending on the symmetry of the basis functions. This integration was performed analytically. Analytic integration over θ is important since numerical quadrature of the θ integration would be made difficult by oscillations of $\sin(kAx)$ and $\cos(kAx)$ for large values of the integration variable k. The ϕ integration is simply that of a polynomial in even powers of $\cos\phi$ and $\sin\phi$; hence a low-order Chebyschev quadrature of the first kind[5] can be employed to perform this integration *exactly*. The remaining integration over k requires more care, since the integrand possesses a simple pole at the point $k=k_0$. Before numerical quadrature can be used, the singularity must be subtracted off. Specifically, an integral of the form

$$\lim_{\epsilon\to 0^+}\int_0^\infty \frac{f(k)k^2\,dk}{k_0^2-k^2+i\epsilon}$$

can be approximated with little resulting error by the expression[6]

$$\sum_i \frac{f(k_i)k_i^2\omega_i}{k_0^2-k_i^2}+\frac{f(k_0)k_0}{2} \times\left(\mathrm{P}\int_0^{k_{\max}}\frac{dk}{k_0-k}-\sum_i\frac{\omega_i}{k_0-k_i}-i\pi\right), \quad (9)$$

where k_i and ω_i denote quadrature weights and points, respectively, and $k_{\max}=\sum_i\omega_i$. In performing the k quadrature in Eq. (7), it was found that 20 to 30 Gauss-Legendre points were sufficient to perform the integration to better than five significant figures.

After the matrix representations of $G_0(E)$ and U have been constructed, the discrete matrix $\underline{T}^t(E)$ can be obtained by a single matrix inversion:

$$\underline{T}^t(E) = [\underline{1}-\underline{U}^t\underline{G}_0(E)]^{-1}\underline{U}^t. \quad (10)$$

The scattering amplitude for any relative orientation of the incoming and outgoing wave vectors is obtained by the transformation of Eq. (3). $\underline{T}^t(E)$ of course only depends on the magnitude of the energy and not on the directions of $\vec{k}_{\text{in}}$ and $\vec{k}_{\text{out}}$. This is an important consideration, since in any molecular problem an average over target orientations would have to be performed in order to obtain physical results. The transformation of Eq. (3) can be done quite rapidly when compared with the recomputation of $\underline{T}^t(E)$. If the energy is changed, $\underline{T}^t(E)$ must be recomputed.

B. Variational corrections

The method we have outlined provides a solution for the exact scattering amplitude corresponding to the truncated potential V^t. This amplitude, however, will generally contain errors that are first-order in the difference $(V-V^t)$ when compared with the amplitude for the exact potential V. Variational stability may be obtained by solving for the wave function corresponding to $T^t(E)$, which we denote by ψ_t, and employing it in a generalization of the Kato formula.[7] The stationary amplitude is then given by the prescription

$$\langle\vec{k}_{\text{out}}|T^s(E)|\vec{k}_{\text{in}}\rangle = \langle\vec{k}_{\text{out}}|T^t(E)|\vec{k}_{\text{in}}\rangle + 2\langle\psi_t^{\text{out}}|H-E|\psi_t^{\text{in}}\rangle; \quad (11)$$

$\psi_t^{\text{in, out}}$ is easily expressed in terms of $\underline{T}^t(E)$ as

$$\psi_t^{\text{in, out}} = \varphi_0^{\text{in, out}} + G_0(E)\underline{T}^t(E)\varphi_0^{\text{in, out}}, \quad (12)$$

where $\varphi_0^{\text{in, out}}$ is the incoming, outgoing plane wave. It is important to notice that while ψ_t certainly has components outside the truncated L^2 space employed here, only its L^2 components are needed in defining the trial scattering amplitude, as can be readily seen from the identity

$$\langle\vec{k}_{\text{out}}|T^t(E)|\vec{k}_{\text{in}}\rangle = \langle\vec{k}_{\text{out}}|U^t|\psi_t^{\text{in}}\rangle. \quad (13)$$

Bearing this in mind we can write $\psi_t^{\text{in, out}}$ in the form

$$\psi_t^{\text{in, out}} = \varphi_0^{\text{in, out}} + \sum_\alpha c_\alpha^{\text{in,out}}|\alpha\rangle, \quad (14)$$

and this form will be perfectly consistent with $\underline{T}^t(E)$. It is easily verified that the coefficients $c_\alpha^{\text{in, out}}$ are obtained as

$$c_\alpha^{\text{in, out}} = \langle \alpha | \underline{G}_0(E) \underline{T}^t(E) | \varphi_0^{\text{in, out}} \rangle = \sum_{\rho,\gamma} \langle \alpha | G_0(E) | \beta \rangle \langle \beta | T^t(E) | \gamma \rangle \langle \gamma | \varphi_0^{\text{in, out}} \rangle , \tag{15}$$

i.e., in computing $\underline{T}^t(E)$, we have already done all the work necessary to compute the coefficients $c_\alpha^{\text{in,out}}$. If on substituting $\psi_t^{\text{in,out}}$ into the Kato formula, we assume that $(H_0 + V^t - E)\psi_t^{\text{in,out}} = 0$ [which is not strictly true in this case since the scattered wave in Eq. (12) has been truncated], then the Kato formula, as Heller and Yamani pointed out,[8] reduces to the distorted-wave Born formula, with U^t as the unperturbed distorting potential:

$$\langle \vec{k}_{\text{out}} | T^s(E) | \vec{k}_{\text{in}} \rangle = \langle \vec{k}_{\text{out}} | T^t(E) | \vec{k}_{\text{in}} \rangle + \langle \psi_t^{\text{out}} | U - U^t | \psi_t^{\text{in}} \rangle . \tag{16}$$

The price for variational stability is that bound-free and free-free matrix elements of V are now required.

C. Comment on the direct quadrature of the Lippmann-Schwinger equation

Several authors have suggested calculating $\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle$ by direct quadrature of the Lippmann-Schwinger equation in momentum space.[9,10] This approach was first carried out successfully for the full amplitude by Walters[9] for the case of spherical potentials. Quite recently, Schneider[10] showed that this technique could be simplified by employing the same L^2 truncation of the potential used here. In momentum space, the Lippmann-Schwinger equation for the scattering amplitude reads

$$\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle = \langle \vec{k}_{\text{out}} | U | \vec{k}_{\text{in}} \rangle + \frac{1}{(2\pi)^3} \int \frac{\langle \vec{k}_{\text{out}} | U | \vec{k} \rangle \langle \vec{k} | T(E) | \vec{k}_{\text{in}} \rangle}{k_0^2 - k^2 + i\epsilon} d^3k . \tag{17}$$

If V has spherical symmetry and if one uses spherical coordinates to perform the above integration, letting the z axis coincide with the direction of $\vec{k}_{\text{in}}$, the ϕ integration drops out of the above integral since $\langle \vec{k} | T(E) | \vec{k}_{\text{in}} \rangle$ is independent of the azimuthal angle that $\vec{k}$ makes with $\vec{k}_{\text{in}}$. A finite matrix equation for $\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle$ is then obtained by subtracting the singularity in the integrand at $k = k_0$ and approximating the two-dimensional integral by numerical quadrature. If the potential is energy independent, this approach can lead to an efficient algorithm for computing the scattering amplitude at any energy after a single prediagonalization of a (possibly large) matrix is carried out. If the potential has an energy dependence, this diagonalization must be done at each energy.

If V does not possess spherical symmetry, then $\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle$ is not independent of the azimuthal angle between $\vec{k}_{\text{out}}$ and $\vec{k}_{\text{in}}$. However for a cylindrically symmetric potential, a simplification can be found. Since the L^2 truncation of V allows one to solve the Lippmann-Schwinger equation one symmetry (Σ_g^+, Σ_u^+, etc.) at a time, $\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle$ can be written as (for one symmetry)

$$\langle \vec{k}_{\text{out}} | T(E) | \vec{k}_{\text{in}} \rangle = \langle \vec{k}_{\text{out}} | T^\Gamma(E) | \vec{k}_{\text{in}} \rangle e^{im(\phi_{\text{in}} - \phi_{\text{out}})} , \tag{19}$$

where m is the component of the angular momentum along the symmetry axis and $\langle \vec{k}_{\text{out}} | T^\Gamma(E) | \vec{k}_{\text{in}} \rangle$ is independent of ϕ_{in} and ϕ_{out}. Thus the Lippmann-Schwinger equation for $\langle \vec{k}_{\text{out}} | T^\Gamma(E) | \vec{k}_{\text{in}} \rangle$ can again be reduced to a two-dimensional equation. We should like to stress the point that this approach would lead to matrices of much larger dimensionality than those used in the present work and that such a quadrature, even if carried out to arbitrary accuracy, would only yield the result obtainable by solving the equation for $\underline{T}^t$ as outlined in Sec. II A.

III. NUMERICAL RESULTS

As a model application of the method outlined in Secs. II A and II B we have computed amplitudes for scattering from an attractive, two-center Gaussian potential:

$$U(\vec{r}) = -\tfrac{1}{2}(e^{-(\vec{r}-\vec{A})^2} + e^{-(\vec{r}+\vec{A})^2}) . \tag{20}$$

For these computations, we took $|\vec{A}| = 1.0$. The matrix elements of this potential between the basis functions of Eq. (5) can be written in terms of one- and two-center overlap integrals of Gaussians which are well known.[3] In this paper we report results for choices of the incoming wave vector $\vec{k}_{\text{in}}$ along the symmetry axis of the potential and perpendicular to it.

For $\vec{k}_{\text{in}}$ along the axis of the potential, nonzero matrix elements of $\underline{T}^t(E)$ exist only for basis functions of Σ_g^+ and Σ_u^+ symmetries, and, as noted earlier, $\langle \alpha | T^t(E) | \beta \rangle$ is diagonal in these symmetries. The contributions of functions transforming with other irreducible representations of $D_{\infty h}$ vanish because their Fourier transforms $\langle \alpha | \vec{k}_{\text{in}} \rangle$, with $\vec{k}_{\text{in}}$ along the axis of V, are zero. It was found that, although basis functions of Σ_g^+ and Σ_u^+ symmetry may be constructed with g_α in Eq. (5) chosen to be a z-type Gaussian [$l = m = 0$, $n = 1$ in Eq. (6)], the contribution of such functions is negligible at the energies considered here. Table I compares results at $k = 0.447$ a.u. for basis sets of 14 and 20 functions with g_α of S symmetry. The exponents

TABLE I. Comparison of scattering amplitudes at $k = 0.447$ a.u. for sets of 14 and 20 basis functions. Incident wave vector is along the symmetry axis of the potential.

No. basis functions	θ	Exact Born $(\Sigma_g^+ + \Sigma_u^+)$	Born (Σ_g^+)	Born (Σ_u^+)	$f(\theta)(\Sigma_g^+)$	$f(\theta)(\Sigma_u^+)$
14	0	0.443	0.336	0.112	0.405+0.088i	0.125+0.0024i
	$\frac{1}{4}\pi$	0.427	0.354	0.080	0.427+0.093i	0.089+0.0017i
	$\frac{1}{2}\pi$	0.362	0.373	0.0	0.449+0.098i	0.0
	$\frac{3}{4}\pi$	0.270	0.354	−0.080	0.427+0.093i	−0.089−0.0017i
	π	0.227	0.336	−0.112	0.405+0.088i	−0.125−0.0024i
20	0	0.443	0.328	0.115	0.399+0.086i	0.127+0.0025i
	$\frac{1}{4}\pi$	0.427	0.346	0.082	0.421+0.090i	0.091+0.0018i
	$\frac{1}{2}\pi$	0.362	0.364	0.0	0.443+0.095i	0.0
	$\frac{3}{4}\pi$	0.270	0.346	−0.082	0.421+0.090i	−0.091−0.0018i
	π	0.227	0.328	−0.115	0.399+0.086i	−0.127−0.0025i

of the Gaussian functions were chosen in geometric series over a range of values between 6×10^{-4} and 5. Studies of convergence showed that results converged to within less than 1% could be obtained for each symmetry with 15 to 20 basis functions.

For $\vec{k}_{in}$ perpendicular to the axis of the potential, $T^t(E)$ has nonzero matrix elements for functions of Σ_g^+, Π_u and symmetries of higher angular momentum projections. The contributions of Σ_u^+ and Π_g symmetries vanish, as do the contributions of certain other symmetries, because their Fourier transforms evaluated at $\vec{k}_{in}$ are zero. A simplification involved in calculations of Π contributions should be noted. In computing the scattering amplitude we made use of the fact that the L^2-matrix representation of $T^t(E)$ is the same for basis functions of Π symmetry chosen with g_α as x-type or y-type Gaussians. However the Fourier transforms of x and y Gaussian functions are not identical. In Table II we give the contributions of Σ_g^+ and Π_u symmetries for $\vec{k}_{in}$ perpendicular to the axis of the potential for $k = 0.447$ and 1.0 a.u.

As a check on the efficacy of our numerical codes, several tests were performed. The separation of the two-center potential was made vanishingly small, and it was found that the results so obtained agreed with those of Holt and Santoso[11] for a one-center Gaussian potential at $k = 0.447$ a.u. In addition, it was also verified [by integrating $\langle \vec{k}_{out} | T^t(E) | \vec{k}_{in} \rangle$ over all orientations of $\vec{k}_{out}$] that the optical theorem holds exactly for contributions to the scattering amplitude from each symmetry. It should be expected that the optical theorem is satisfied exactly, because solution of the matrix equation (2) should yield, as we have stated, the exact T matrix for the particular choice of truncated potential V^t.

The application of the variational correction described in Sec. IIB permits the use of much smaller basis sets than those employed in the above calculations. Using Eqs. (14) and (15) we may write the second term on the right-hand side of Eq. (16) for the Kato correction as

TABLE II. Scattering amplitudes with 20 basis functions per symmetry. The incident wave vector is perpendicular to the axis of the potential, and the outgoing wave lies in the plane of the incident wave vector and the axis of the potential.

k (a.u.)	θ	Exact Born	Born (Σ_g^+)	Born (Π_u)	$f(\theta)(\Sigma_g^+)$	$f(\theta)(\Pi_u)$
0.447	0	0.443	0.403	0.044	0.491+0.105i	0.046+0.0003i
	$\frac{1}{4}\pi$	0.409	0.383	0.030	0.467+0.100i	0.031+0.0002i
	$\frac{1}{2}\pi$	0.362	0.364	0.0	0.423+0.095i	0.0
	$\frac{3}{4}\pi$	0.355	0.383	−0.030	0.467+0.100i	−0.031−0.0002i
	π	0.363	0.403	−0.044	0.491+0.105i	−0.046−0.0003i
1.0	0	0.443	0.295	0.147	0.295+0.066i	0.156+0.0067i
	$\frac{1}{4}\pi$	0.291	0.224	0.079	0.224+0.050i	0.084+0.0036i
	$\frac{1}{2}\pi$	0.145	0.159	0.0	0.159+0.036i	0.0
	$\frac{3}{4}\pi$	0.143	0.224	−0.079	0.224+0.050i	−0.084−0.0036i
	π	0.163	0.295	−0.147	0.295+0.066i	−0.156−0.0067i

TABLE III. Comparison of scattering amplitudes using Kato correction and two basis functions per symmetry with 20 function results. Energies are $k = 0.447$ and $k = 1.0$ a.u. and incident wave as in Table I.

k (a.u.)	θ	$f(\theta)$ Two basis functions uncorrected	$f(\theta)$ Two basis functions + Kato correction	$f(\theta)$ 20 basis functions + Kato correction
0.447	0	0.693 + 0.163i	0.515 + 0.093i	0.528 + 0.089i
	$\frac{1}{4}\pi$	0.677 + 0.170i	0.499 + 0.096i	0.511 + 0.092i
	$\frac{1}{2}\pi$	0.561 + 0.168i	0.431 + 0.098i	0.440 + 0.095i
	$\frac{3}{4}\pi$	0.446 + 0.165i	0.331 + 0.094i	0.336 + 0.089i
	π	0.372 + 0.155i	0.283 + 0.090i	0.287 + 0.084i
1.0	0	0.451 + 0.073i	0.465 + 0.052i	0.473 + 0.057i
	$\frac{1}{4}\pi$	0.407 + 0.071i	0.382 + 0.053i	0.389 + 0.058i
	$\frac{1}{2}\pi$	0.173 + 0.043i	0.141 + 0.038i	0.147 + 0.040i
	$\frac{3}{4}\pi$	−0.145 − 0.018i	−0.049 + 0.008i	−0.045 + 0.008i
	π	−0.264 − 0.027i	−0.097 − 0.005i	−0.094 − 0.005i

$$\langle \psi_t^{\text{out}} | U - U^t | \psi_t^{\text{in}} \rangle = \langle \vec{k}_{\text{out}} | U | \vec{k}_{\text{in}} \rangle - \langle \vec{k}_{\text{out}} | U^t | \vec{k}_{\text{in}} \rangle + \sum_{\alpha,\beta,\gamma} \langle \vec{k}_{\text{out}} | \alpha \rangle \langle \alpha | T^t(E) | \beta \rangle \langle \beta | G_0(E) | \gamma \rangle \langle \gamma | U - U^t | \vec{k}_{\text{in}} \rangle$$
$$+ \sum_{\alpha,\beta,\gamma} \langle \vec{k}_{\text{out}} | U - U^t | \alpha \rangle \langle \alpha | G_0(E) | \beta \rangle \langle \beta | T^t(E) | \gamma \rangle \langle \gamma | \vec{k}_{\text{in}} \rangle . \tag{21}$$

The usual separation of the contributions of different symmetries may be made for all but the first term in Eq. (21). As mentioned earlier, the only matrix elements appearing in (21) which have not been used in the calculation of $\underline{T}^t$ are free-free and bound-free matrix elements of the exact potential V. Due to our choice of a Gaussian potential, the free-free matrix elements may be expressed in terms of the Fourier transform of a Gaussian given in Eq. (8). The bound-free matrix elements reduce to matrix elements of $e^{i\vec{k}\cdot\vec{r}}$ between Gaussians on different centers, and these integrals are known in closed form.[12]

In Tables III and IV we compare the results of Kato corrected calculations using only two basis functions of each symmetry (exponents of 1.0 and 2.0) with 20 function results. The agreement of these calculations suggests that, for potentials for which free-free and bound-free matrix elements can be computed, the Kato correction will allow the use of conveniently small basis sets.

It should be noted that a significant proportion of the variational improvement is carried by the leading term of the Kato correction [first line of Eq. (21)], which is simply the exact matrix element of the Born term. One would generally expect this to be true at intermediate energies, and even at very low energies for potentials without bound states. Furthermore, this leading term automatically adds in the Born contributions from

TABLE IV. Comparison of scattering amplitudes using Kato correction and two basis functions per symmetry with 20 function results. $k = 0.447$ and 1.0 a.u. Orientation of incident and outgoing wave vectors as in Table II.

k (a.u.)	θ	$f(\theta)$ Two basis functions uncorrected	$f(\theta)$ Two basis functions + Kato correction	$f(\theta)$ 20 basis functions + Kato correction
0.447	0	0.724 + 0.191i	0.518 + 0.104i	0.530 + 0.104i
	$\frac{1}{4}\pi$	0.667 + 0.181i	0.481 + 0.100i	0.492 + 0.100i
	$\frac{1}{2}\pi$	0.583 + 0.171i	0.430 + 0.096i	0.440 + 0.095i
	$\frac{3}{4}\pi$	0.561 + 0.180i	0.425 + 0.100i	0.435 + 0.099i
	π	0.568 + 0.189i	0.435 + 0.103i	0.446 + 0.104i
1.0	0	0.558 + 0.094i	0.445 + 0.064i	0.450 + 0.066i
	$\frac{1}{4}\pi$	0.371 + 0.068i	0.290 + 0.051i	0.296 + 0.053i
	$\frac{1}{2}\pi$	0.178 + 0.043i	0.141 + 0.038i	0.147 + 0.040i
	$\frac{3}{4}\pi$	0.115 + 0.051i	0.135 + 0.045i	0.140 + 0.047i
	π	0.081 + 0.063i	0.152 + 0.055i	0.155 + 0.055i

all higher symmetry groups not explicitly treated and one certainly expects these contributions to be Born dominated. As this term only involves calculation of free-free matrix elements, its addition should be quite feasible in molecular applications of this technique.

IV. DISCUSSION

In this paper we have outlined an efficient method for computing scattering amplitudes for cylindrically symmetric potentials and applied it to a model case. Our results indicate that the use of the Kato correction will allow one to obtain accurate answers with very few basis functions.

This method should find application in the area of low-energy electron–diatomic-molecule collisions. In this case, one would probably construct an energy-dependent optical potential[13] to describe the target. In this context, the necessity for reconstructing matrix elements of the transition operator at such energy is not a drawback. A major portion of the computational effort in this work involved construction of matrix elements of the free-particle Green's function. Much of this effort [the θ and ϕ integrations in Eq. (7)] need be done only once. Applications of this technique to electron–diatomic-molecule scattering are presently under study.

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