Dynamical basis sets for algebraic variational calculations in quantum-mechanical scattering theory

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We propose new basis sets for linear algebraic variational calculations of transition amplitudes for quantum-mechanical scattering problems. These basis sets are hybrids of those that yield the Kohn variational principle (KVP) and those that yield the generalized Newton variational principle (GNVP) when substituted in Schlessinger's stationary expression for the T operator. Trial calculations show that efficiencies almost as great as that of the GNVP and much greater than the KVP can be obtained even for basis sets with the majority of the members independent of energy.

I. INTRODUCTION

Recent work on linear algebraic approaches for quantum-mechanical scattering problems has made significant progress on the formulation of efficient and computationally advantageous basis-set expansion methods for molecular scattering problems.[1-27] Particularly noteworthy progress has occurred in the treatment of chemically reactive molecular collisions, where new basis-set methods without dimensionality-reducing approximations have been used for accurate calculations on several reactions previously treated only by more approximate methods, in particular, the high-energy D + H_2 reaction (Refs. 4, 22, and 28), and the O + H_2 (Refs. 29 and 30), H + OH (Ref. 30), H + HBr (Ref. 31), O + HD (Refs. 32 and 33), and F + H_2 (Ref. 34) reactions. We have treated these systems by the generalized Newton variational principle[13,22,35] (GNVP) or a method of moments[23] related to it, with either real or complex boundary conditions and with a basis-set expansion of the square-integrable (denoted by the symbol $\mathcal{L}^2$) amplitude density. The GNVP has shown especially rapid convergence as the number of basis functions is increased.[13,14,22] Another promising approach is the Kohn variational principle (KVP) based on an expansion of the (non-$\mathcal{L}^2$) scattering-wave function satisfying complex boundary conditions.[11,12,36] A particularly noteworthy aspect of the KVP is that many of the required matrix elements are independent of energy and need not be recalculated if two or more energies are treated with the same basis set.[37,38]

It has been pointed out[11] that results equivalent to a version of the KVP may be obtained from a scattered-wave variational principle (SWVP), due originally to Schlessinger[39] and discussed further by Schlessinger, Nuttall, Rescigno, and co-workers,[40-45] for a special case of a non-$\mathcal{L}^2$ trial function. In the present work we show that with another choice of non-$\mathcal{L}^2$ trial function this "Kohn-type"[39,41] or "modified Kohn"[40] SWVP yields the GNVP. We then propose a new method in which the SWVP is used with a subset of the basis functions that yield the GNVP and another subset of those that yield the KVP. We choose the subsets to retain the computational advantage that most of the matrix elements are independent of energy, and we present trial calculations for a two-channel problem showing that the efficiency of convergence is comparable to the GNVP. We suggest therefore that this hybrid-basis-set SWVP approach may provide a powerful method for more demanding applications in the future.

For completeness we will also present some calculations using the KVP on the same trial problem.

II. THEORY

We consider a general multichannel scattering problem. For simplicity we consider the case of a single arrangement, although the extension to rearrangement scattering is straightforward.[46] The Hamiltonian is written as

$$H = H^D + V^C , \tag{1}$$

where V^C is a coupling potential, H^D is a distorted-wave reference Hamiltonian

$$H^D = T_{\text{kin}} + V^D , \tag{2}$$

involving the full kinetic energy T_{kin} and a distortion potential V^D, and for use below we define $G^{D\pm}$ as the distorted-wave Green's operators:

$$G^{D\pm} = \left[\frac{-\hbar^2}{2\mu}\right](E - H^D \pm i\epsilon)^{-1} . \tag{3}$$

The transition operator T is defined by

$$T\psi^{+n_0}=U\Psi^{+n_0}\ , \tag{4}$$

where U is the coupling operator defined by

$$U=\left[-\frac{\hbar^2}{2\mu}\right]V^C\ , \tag{5}$$

and μ is the relative translational reduced mass, n_0 denotes the initial channel (the index n is an ordinal channel index), ψ^{+n_0} and Ψ^{+n_0} satisfy the usual[32] T-matrix boundary conditions, the unscattered wave ψ^{+n_0} satisfies a homogeneous Schrödinger equation for the reference problem

$$(E-H^D)\psi^{+n_0}=0\ , \tag{6}$$

and Ψ^{+n_0} is the solution of the full Schrödinger equation

$$(E-H)\Psi^{+n_0}=0\ . \tag{7}$$

The state Ψ^{+n_0} also satisfies the usual Lippmann-Schwinger equation[47]

$$\Psi^{+n_0}=\psi^{+n_0}+G^{D+}U\Psi^{+n_0}\ . \tag{8}$$

The stationary T functional of Schlessinger[39] may be written

$$T_{nn_0}=T^B_{nn_0}+\langle\psi^{-n}|U|\Psi^{+n_0}_{\rm SW}\rangle+\langle\Psi^{-n}_{\rm SW}|U|\psi^{+n_0}\rangle -\left\langle\Psi^{-n}_{\rm SW}\left|\left[\frac{-2\mu}{\hbar^2}\right](E-H)\right|\Psi^{+n_0}_{\rm SW}\right\rangle\ , \tag{9}$$

where $T^B_{nn_0}$ is the Born approximation to the amplitude, and $\Psi^{+n_0}_{\rm SW}$ is the scattered wave given by the last term of Eq. (8), and $\Psi^{-n_0}_{\rm SW}$ is its complex conjugate. Equation (9) is accurate to second order in the scattered waves $\Psi^{+n_0}_{\rm SW}$ and $\Psi^{-n_0}_{\rm SW}$, hence we sometimes call it the scattered-wave variational principle.

To use Eq. (9) for practical calculations one writes[39,41]

$$\Psi^{+n_0}_{\rm SW}=\sum_{\beta=1}^{M}A_{\beta n_0}\Phi_\beta\ , \tag{10}$$

where Φ_β is a basis-set function, and one determines the coefficients to make T_{nn_0} stationary. We now consider two choices of basis functions that yield known methods and a third (new) choice that appears to have an interesting combination of advantages.

The first choice is to take $\{\Phi_\beta\}_{\beta=1}^{n_{\rm open}}$ as a set of functions satisfying energy-dependent scattered-wave boundary conditions in $n_{\rm open}$ open channels and $\{\Phi_\beta\}_{n_{\rm open}+1}^{M}$ as a set of $\mathcal{L}^2$ functions. For this choice of trial functions the stationary T expression (9) yields a version of the Kohn[11,12,36] variational principle in which the non-$\mathcal{L}^2$ function with incoming wave boundary conditions satisfies (6). One advantage of this approach is that most of the basis-set functions are independent of energy.

The second choice of basis set is based on writing the scattered wave as

$$\Psi^{\pm n_0}_{\rm SW}=G^{D\pm}\zeta^{\pm n_0}\ , \tag{11}$$

where $\zeta^{\pm n_0}$ is the $\mathcal{L}^2$ amplitude density defined as either side of Eq. (4). Substituting Eq. (11) into the stationary T functional (9) and using Eqs. (1), (3), (5), and (8) results in

$$T_{nn_0}=T^B_{nn_0}+\left\langle\psi^{-n}\left|UG^{D+}\right|\zeta^{+n_0}\right\rangle+\left\langle\zeta^{-n}\left|G^{D+}U\right|\psi^{+n_0}\right\rangle -\left\langle\zeta^{-n}\left|G^{D+}-G^{D+}UG^{D+}\right|\zeta^{+n_0}\right\rangle\ , \tag{12}$$

which is the generalized Newton variational principle for the $\mathcal{L}^2$ amplitude density. To utilize the GNVP as a linear algebraic method we write[13,22,27]

$$\zeta^{+n_0}=\sum_{\beta=1}^{M}A_{\beta n_0}\Phi_\beta\ , \tag{13}$$

where the $\{\Phi_\beta\}$ are now all $\mathcal{L}^2$ functions. The equivalent procedure for the SWVP is obtained by substituting (13) into (11), which yields

$$\Psi^{\pm n_0}_{\rm SW}=\sum_\beta A_{\beta n_0}\grave{G}^{\pm}_\beta\ , \tag{14}$$

where $\grave{G}^{\pm}_\beta$ is a quantity introduced previously[13,22,27] for computational efficiency and called a half-integrated Green's function (HIGF):

$$\grave{G}^{\pm}_\beta=G^{D\pm}\Phi_\beta\ . \tag{15}$$

Notice that in this case all the scattered-wave basis functions in (9) are non-$\mathcal{L}^2$ and depend on energy. In addition, they are complex, and this lessens the likelihood of spurious singularities. Finally we note that the asymptotic behavior of (11) is governed by $G^{D\pm}$. Outside the interaction region $G^{D\pm}\zeta^{\pm n_0}$ and $G^{D\pm}\Phi_\beta$ only differ by a constant factor. Therefore, using even one HIGF as the non-$\mathcal{L}^2$ basis-set function may be sufficient to give rapid convergence. $G^{D\pm}\zeta^{\pm n_0}$ and $G^{D\pm}\Phi_\beta$ are regular at the origin.

The main point of the present paper is to propose a third possibility for the basis, motivated by both the GNVP and the KVP. In particular, we suggest

$$\Psi^{+n_0}_{\rm SW}=\sum_{\beta=1}^{M_1}A_{\beta n_0}G^{D+}\Phi_\beta+\sum_{\beta=M_1+1}^{M_1+M_2}A_{\beta n_0}\Phi_\beta\ , \tag{16}$$

where the first M_1 functions are of the GNVP type used in (14) and the next M_2 functions are $\mathcal{L}^2$. If $M_2>M_1$, then most of the matrix elements will be independent of energy. The questions to be determined computationally then are whether the new hybrid basis set leads to rapid convergence comparable to that of the GNVP and—if so—how small can we make M_1? In addition, we will compare the rate of convergence to Kohn variational calculations for the same problem.

The premise for suggesting Eq. (16) as a trial function is based on interpreting the HIGF as a "prepared" or "dynamical" basis-set function. The operation of the Green's function on the basis has a similar effect to iterating the Lippmann-Schwinger equation, i.e., it leads to a higher-order trial function. This effect was observed

clearly in earlier comparisons of variational principles, where each action of Green's function led to a general improvement in accuracy.[14] We propose then that the optimum basis may involve a compromise between the most efficient basis set, in which all basis-set functions contain a Green's function, as in the GNVP, and a basis set leading to simpler and more energy-independent integrations. The choice of one "prepared" basis-set function per open channel is particularly interesting for further investigation since it involves the same number of energy-dependent basis-set functions as the KVP but a greater number of prepared basis-set functions.

III. CALCULATIONS

For a computational test of the efficiency of the new kind of hybrid basis set, we consider a two-channel test problem corresponding to nonreactive scattering of I by H_2. This problem has been used as a test case in previous work[22,27] as well, and we consider the same potential energy surface,[48] total energy (0.045 hartree), total angular momentum ($J=0$), and vibrational-rotational-orbital functions ϕ_n as previously. The channels included are

$$n=1:\ v=0,\ j=l=0$$

$$n=2:\ v=0,\ j=l=2$$

where v, j, and l are vibrational, rotational, and orbital quantum numbers, respectively. We use a single-channel distortion potential, which is also defined in previous work.[22,27] The results are well converged with respect to all numerical parameters except those associated with the basis set, and we concentrate our attention in particular on the size of the radial translational basis required for convergence with each type of basis set.

For convenience, we use wave functions $\psi^{(\pm)n_0}$ and $\Psi^{(\pm)n}$ satisfying S-matrix boundary conditions[27] rather than those above, $\psi^{\pm n}$ and $\Psi^{\pm n}$, satisfying T-matrix boundary conditions.[32] Analogous to (8) we write

$$\Psi^{(+)n_0}=\psi^{(+)n_0}+\Psi_{\rm OW}^{(+)n_0}\ , \tag{17}$$

where $\psi^{(+)n_0}$ satisfies (6) with unit amplitude for the incoming wave, $\Psi^{(+)n_0}$ satisfies (7) with unit amplitude for the incoming wave, and $\Psi_{\rm OW}^{(+)n_0}$ is the outgoing wave due to scattering by U. We consider three types of expansion:

$$\Psi^{(+)n_0}=\sum_{n=1}^{2} R^{-1}\phi_n\left[f(R)Rh_{l_n}^{(2)}(k_nR)+c_{1nn_0}\lambda_n^{(+)}+\sum_{\mu=2}^{m} c_{\mu nn_0}\lambda_\mu\right],\quad \text{KVP} \tag{18}$$

$$\Psi_{\rm OW}^{(+)n_0}=\sum_{n=1}^{2} R^{-1}\phi_n\sum_{\mu=1}^{m} c_{\mu nn_0}\dot{g}_{n\mu}^{N},\quad \text{GNVP} \tag{19}$$

$$\Psi_{\rm OW}^{(+)n_0}=\sum_{n=1}^{2} R^{-1}\phi_n\left[\sum_{\mu=1}^{m_1} c_{\mu nn_0}\dot{g}_{n\mu}^{N}+\sum_{\mu=m_1+1}^{m} c_{\mu mn_0}\lambda_\mu\right],\quad \text{HBS} \tag{20}$$

which yield the KVP, GNVP, and hybrid-basis-set (HBS) methods when the coefficients $c_{\mu nn_0}$ are found variationally. In all cases the λ_μ will be taken as distributed Gaussians in the radial scattering coordinate R, and the other functions are explained in the next two paragraphs.

Equation (18) also involves $f(R)$, which is a cutoff function:

$$f(R)\underset{R\to 0}{\longrightarrow} 0\ , \tag{21}$$

$$f(R)\underset{R\to\infty}{\longrightarrow} 1\ , \tag{22}$$

and it involves $h_{l_n}^{(2)}(k_nR)$, which is the incoming spherical Hankel function, and $\lambda_n^{(+)}$, which is taken as an outgoing wave basis function of the form

$$\lambda_n^{(+)}=f(R)Rh_{l_n}^{(1)}(k_nR)\ , \tag{23}$$

where $h_{l_n}^{(1)}(k_nR)$ is the outgoing spherical Hankel function. The parameters l_n and k_n are the orbital angular momentum quantum number and wave number in channel n. Notice that both kinds of non-$\mathcal{L}^2$ functions in (18) contain the same regularizing function $f(R)$, as in the improved S-matrix KVP of Zhang, Chu, and Miller.[24] However, even though $V^D=0$, the non-$\mathcal{L}^2$ functions in (18) do not satisfy (6), and so we cannot use the SWVP, Eq. (9) [or its S-matrix analog, Eq. (24) below]. Thus the KVP equations for the trial function (18) must be obtained from the Kohn variational functional.[24,36]

Equations (19) and (20) also involve $\dot{g}_{n\mu}^{N}$ which is the radial half-integrated Green's function[22,27] associated with $\mathcal{L}^2$ function λ_μ in channel n. The distortion potential for generating the Green's function is taken in this study to be the diagonal element of the potential matrix. When Eq. (19) is inserted into

$$S_{nn_0}=S_{nn_0}^{B}+\langle\psi^{(-)n}|U|\Psi_{\rm OW}^{(+)n_0}\rangle+\langle\Psi_{\rm OW}^{(-)n_0}|U|\psi^{+n_0}\rangle-\left\langle\Psi_{\rm OW}^{(-)n}\left|\left[-\frac{2\mu}{\hbar^2}\right](E-H)\right|\Psi_{\rm OW}^{(+)n_o}\right\rangle\ , \tag{24}$$

which is the S-matrix version of Eq. (9), the results are equivalent to the complex Green's function version[27,32] of the GNVP.

The transition probabilities are related to scattering-matrix elements in the usual way:

$$P_{n_0 n} = |S_{nn_0} - \delta_{nn_0}|^2 \ . \tag{25}$$

Since we use complex boundary conditions, the scattering matrix is not automatically unitary. Therefore we monitor both P_{11} and P_{12} as measures of convergence. We also monitor the eigenphase sum η_{sum}, defined in the standard[49] way.

For the efficiency tests we always used equally spaced Gaussians with widths determined such that the overlap parameter[22,24,50] c is 1.0. The Gaussians used to generate the dynamical basis functions are located at

$$R_\alpha^G = R_1^G + (\alpha - 1)\Delta, \quad \alpha = 1, \ldots, m_1 \tag{26}$$

in the mass-scaled coordinate system,[22,23] and the centers of the $\mathcal{L}^2$ Gaussian basis functions are located at

$$R_\alpha^G = R_{m_1+1}^G + (\alpha - m_1 - 1)\Delta \ , \quad \alpha = m_1 + 1, \ldots, m \ . \tag{27}$$

Thus the parameters that need to be specified are m, R_2^G, R_m^G, and the parameters R_0 and β (see below) in $f(R)$ for the KVP; m, R_1^G, and R_m^G for the GNVP; and m, m_1, R_1^G, and $R_{m_1}^G$ for the Gaussians used to generate the HIGF's, and $R_{m_1+1}^G$ and R_m^G for the $\mathcal{L}^2$ basis for the HBS calculations.

IV. RESULTS AND DISCUSSION

Converged values for P_{11} and P_{12} and for the eigenphase sum η_{sum} were calculated by the finite-difference boundary-value method[22] and confirmed by the GNVP with 30 narrowly spaced Gaussians. The converged results are given in the first row of Table I. Table I also gives examples of the results for all three types of basis sets in the Schlessinger outgoing-wave variational principle, and the Kohn variational principle.

For all the basis-set methods we define m_1 as the number of energy-dependent basis functions per channel, excluding $f(R)Rh_l^{(2)}(k_n R)$ in the KVP, and m is the *total*

TABLE I. Comparison of results of calculations for quantum-mechanical scattering problems using different algebraic methods.

Basis	m	m_1	HIGF's $R_1^G - R_{m_1}^G$	$\mathcal{L}^2$ functions $R_{m_1+1}^G - R_m^G$	P_{11}	P_{12}	η_{sum}
Converged					0.593	0.407	0.237
GNVP	20	20	4.65–9.40		0.593	0.407	0.237
	13	13	5.25–8.85		0.604	0.412	0.232
	12	12	5.55–8.85		0.604	0.412	0.231
	11	11	5.85–8.85		0.603	0.411	0.228
	12	12	5.65–8.95		0.591	0.411	0.236
	10	10	5.95–8.65		0.593	0.409	0.216
HBS	18	9	5.50–7.90	5.50–7.90	0.592	0.409	0.238
	14	7	5.50–7.30	5.50–7.30	0.592	0.411	0.238
	10	5	5.50–6.70	5.50–6.70	0.589	0.416	0.241
	8	4	5.50–6.40	6.40–7.30	0.602	0.415	0.241
	8	4	5.50–6.40	5.95–6.85	0.592	0.419	0.238
	11	2	5.85–6.15	6.15–7.90	0.593	0.412	0.239
	10	2	5.85–6.15	6.15–7.60	0.595	0.413	0.241
	10	1[a]	5.95	5.50–7.90	0.593	0.411	0.238
	13	1[a]	5.65	5.50–8.80	0.592	0.410	0.233
	12	1[a]	5.65	5.50–8.50	0.592	0.410	0.234
	11	1[a]	5.65	5.50–8.20	0.592	0.411	0.235
	10	1[a]	5.65	5.50–7.90	0.592	0.412	0.236
	9	1[a]	5.65	5.80–7.90	0.593	0.413	0.226
KVP	53	1[b]		5.35–13.00	0.594	0.407	0.215
	45	1[b]		5.05–11.50	0.602	0.409	0.217
	43	1[b]		5.35–11.50	0.602	0.409	0.212
	41	1[b]		5.65–11.50	0.628	0.385	-0.059
	40	1[b]		5.35–12.95	0.603	0.416	-0.052
	32	1[b]		5.35–12.85	9.568	2.863	0.071
	31	1[b]		5.65–10.00	0.637	0.412	-0.040
	21	1[b]		5.65–8.50	0.734	0.609	0.038
	16	1[b]		5.65–8.45	0.980	0.854	0.097

[a] When $m_1 = 1$, the width of the Gaussian for the HIGF is the same as for the $\mathcal{L}^2$ Gaussian basis functions.

[b] $\beta = 30$, $R_0 = 6.81 a_0$.

number of basis functions per channel for the outgoing wave, as specified in Eqs. (18)–(20).

We will use 1–2 % in the probabilities and 0.01–0.02 in the absolute eigenphase sum as a criterion of "good" convergence in the present discussion. The GNVP section of the table shows that we can achieve this with 10–11 basis functions per channel. In this method all basis functions are energy dependent ($m_1 = m$).

The next section of Table I, based on the hybrid basis set, shows we can obtain good convergence with a comparable number of basis-set functions (8–11) as the GNVP, even when only one basis function is energy dependent.

The final section of Table I shows results obtained with the KVP. Using either the conventional cutoff function[12,51]

$$f(R) = 1 - e^{-\alpha R} , \tag{28}$$

or the channel-dependent cutoff function

$$f_n(R) = 1 - e^{-(\alpha R)^{l_n+1}} , \tag{29}$$

which removes the singularity near the origin even when some channels have $l_n \neq 0$ (in the present two-channel example, $l_1 = 0$ and $l_2 = 2$), we were unable to get reasonable results for any values of α, and we attribute this to the fact that neither cutoff procedure is sharp enough to simultaneously remove the unphysical behaviors of $h_{l_n}^{(1)}(k_n R)$ and $h_{l_n}^{(2)}(k_n R)$ at small R and yet reach its large-R limiting form at a distance which is not significantly larger than where the potential becomes negligible. (Similar difficulties may explain the difficulties in converging the KVP for some test problems in Ref. 18.) We obtained much better results with

$$f(R) = 1 - e^{-(R/R_0)^{\beta}} , \tag{30}$$

with $\beta = 30$ and $R_0 = 6.81 a_0$, and these results are shown in Table I.

We found that the KVP needed much more closely spaced Gaussians than either the GNVP or the new HBS approach and that, very critically, the KVP needs the Gaussians to extend to much larger R than with the GNVP or hybrid basis set. Good convergence requires 45 basis-set functions. Although it is hard to be completely systematic in choosing nonlinear parameters for cutoff functions, we experimented with various forms of non-$\mathcal{L}^2$ functions for the KVP basis set and convinced ourselves that we cannot obtain efficiencies close to those obtained with the GNVP or hybrid basis set.

V. CONCLUDING REMARKS

We have proposed a different approach to basis-set selection in linear-algebraic quantum-mechanical-scattering calculations based on the stationary T functional of Schlessinger, which is employed as a scattered-wave or outgoing-wave variational principle. We propose a hybrid basis set approach, illustrated by Eq. (20) and motivated by the generalized Newton and Kohn variational principles (GNVP and KVP). This approach appears to offer a promising combination of computational advantages, as demonstrated by calculations on a two-channel test problem which was also solved by the GNVP and KVP for comparison.

Further work to explore the computational efficiency of other hybrid-type basis functions in the Schlessinger-type variational principle would be very interesting. For example, we have carried out calculations for potential scattering problems ($n_0 = 1$) without introducing a distortion potential and using basis sets of the form

$$\Psi_{\mathrm{SW}}^{+1} = A_{11} G^{+D} V \psi^{+1} + \sum_{\beta=1}^{M-1} A_{\beta 1} \Phi_{\beta} . \tag{31}$$

This is like (20) except the first basis-set function is obtained by approximating Ψ^{+1} in (4) by its Born approximation ψ^{+1} and inserting the resulting amplitude density in (11) to make a basis function for (14). Although only one basis-set function depends on energy we found (for three different cases tested) very similar convergence rates to those obtained with the Newton variational principle where all basis-set functions depend on energy. The implication is the same as for the two-channel studies presented above, namely, that hybrid basis sets containing a few dynamical basis functions augmented by a convenient $\mathcal{L}^2$ basis can provide a very efficient computational approach to linear-algebraic basis-set calculations of quantum-mechanical scattering amplitudes.

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