Weighted-residual methods for the solution of two-particle Lippmann-Schwinger equation without partial-wave decomposition

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Recently there has been a growing interest in computational methods for quantum scattering equations that avoid the traditional decomposition of wave functions and scattering amplitudes into partial waves. The aim of the present work is to show that the weighted-residual approach in combination with local basis functions give rise to convenient computational schemes for the solution of the multi-variable integral equations without the partial wave expansion. The weighted-residual approach provides a unifying framework for various variational and degenerate-kernel methods for integral equations of scattering theory. Using a direct-product basis of localized quadratic interpolation polynomials, Galerkin, collocation and Schwinger variational realizations of the weighted-residual approach have been implemented for a model potential. It is demonstrated that, for a given expansion basis, Schwinger variational method exhibits better convergence with basis size than Galerkin and collocation methods. A novel hybrid-collocation method is implemented with promising results as well.

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I. INTRODUCTION

The standard approach to two-body scattering problem has been through angular momentum decomposition. This is advantageous for central potentials as the equations for partial waves decouple. However, for non-central potentials, partial waves are coupled and advantages of partial wave expansion dispappear to a large extent. Recently there has been a growing interest in computational methods for quantum scattering equations that avoid the traditional decomposition of wave functions and scattering amplitudes into partial waves [1-11]. The reasons for this interest are many fold: At intermediate and high collision energies partial wave expansion are known to converge very slowly. For example, in ion-atom collisions number of partial waves necessary for convergence in the high energy regime may run up to several thousand [6, 10]. It appears that for most potentials, the scattering amplitudes are smooth, but partial wave amplitudes may show oscillatory behavior. Similarly, the off-shell two-body T-matrix has usually simple structure whereas partial wave components might strongly oscillate. Under such circumstances, the partial wave expansion may be inadequate or even unreliable. In the context of three and four particle problems to which the two-particle T-matrices are the input, two-particle T-matrices requiring an excessively large number of partial waves would render even the angular momentum algebra too complicated and computationally difficult to perform [2].

These observations suggest that, to treat two-particle scattering at high energies and within the context of few-particle dynamics, one should work directly with vector momenta without resorting to expansions over angular momentum states. Significant progress has been reported on the formal and computational aspects of solving the three-particle Faddeev equations directly in terms of vector momenta [2, 13, 14].

Thanks to the present day computing power, direct numerical solution of three-dimensional Lippmann-Schwinger (LS) equation for two-particle T-matrix without recourse to partial wave expansion is within reach. The most straight forward approach is the so-called Nystrom method[15] in which the integral equation is converted to a system of linear equations by approximating the multi-dimensional integral by a quadrature. Denoting with (q, θ, ϕ) the spherical components of the momentum vector $\mathbf{q}$, the dimension of the matrix problem would be $N_q N_\theta N_\phi$, if a direct-product quadrature scheme is used. Here N_q , N_θ and N_ϕ are the number of quadrature points for the variables q, θ and ϕ, respectively. The matrix

size of this three-dimensional Nystrom method, however, might quickly get prohibitive and may require special computational environment. Fortunately, however, for central potentials, dependence on the azimuthal angle ϕ can be eliminated from the three-dimensional LS equation [1]. This leads to an integral equation in two variables, solution of which can be carried out via the Nystrom method routinely in commonly available computational platforms.

In three- and four-particle contexts, the two-particle T-matrix $< \mathbf{q}|T(E)|\mathbf{q}' >$ is needed at very many different two-particle energies E and for a great many different off-shell momenta $\mathbf{q}$ and $\mathbf{q}'$. Nystrom solutions may not be the most economical ways of generating the needed T-matrix elements. The aim of the present work is to show that the weighted-residual approach [17-20] in combination with a direct-product basis of local functions provide efficient computational schemes for the two-particle transition matrix elements $< \mathbf{q}|T|\mathbf{q}' >$ in the form of separable expansions. Generation of off-shell T-matrix elements via these separable expansions involves a matrix inversion problem of much smaller order than the one encountered in the Nystrom method.

The weighted-residual idea (also known as the Petrov-Galerkin approach) [17-20] provides a unifying framework for basis-set expansion methods for the solution of differential and integral equations. It involves two function spaces: a finite-dimensional approximation subspace (of trial solutions) and a subspace of test (or weight) functions. The coefficients of the expansion of the unknown function over the approximation subspace are determined by requiring the residual (i.e., the difference between the exact and approximate solutions) to be orthogonal to the test space. For the two-particle LS equation this leads to a separable expansion of the T-operator. We discuss the connections of this separable expansion with oblique projections [21,22,23] and inner projections [24,25]. Depending on the choices made for the approximation and test spaces, the weighted-residual approach give rise to a wide range of methods. Galerkin method, collocation method and method of moments are the well-known examples.

Schwinger variational (SV) method represents another instance of the weighted-residual approach. Of course, the Schwinger variational principle is well known and has been widely used to solve partial-wave (single-variable) LS equations. Reference [16] gives a comprehensive review of (and an extensive list of references for) the formal and computational aspects of Schwinger variational methods. The present paper demonstrates that Schwinger varia-

tional method (SVM) is a versatile tool for the solution of the vector-variable LS equations without the partial wave expansion as well. In particular, we show that, for the potential considered in this work, SVM exhibits better convergence with basis size than the Galerkin and collocation methods.

We note that Galerkin method in conjunction with a direct-product basis of wavelets has been used in Ref.[5] to solve the two-dimensional LS equation with a model two-nucleon potential. It is likely that the two-dimensional wavelets will also prove efficient if used as the expansion basis in SVM. Another application of the Galerkin method without partial wave expansion has been made in Ref. [3] to solve the two-variable Schrodinger equation subject to scattering boundary conditions using a direct-product basis of local fifth degree polynomials.

Plan of this article is as follows: In Sec. II, we discuss the reduction of the three-dimensional Lippmann-Schwinger equation into a two-dimensional integral equation. Some features of the reduced T-matrix is noted. Sec. III gives an exposition of the general weighted-residual approach in the context of the Lippmann-Schwinger equation. The connection between the weighted residual method and a projection approximation of the potential is established using the concept of *oblique* projector. Sec. IV discusses the various choices for the expansion and test spaces that lead to Galerkin, collocation and Schwinger variational methods. A novel version of the collocation method (termed as it hybrid-collocation) that combines the advantages of collocation and SV methods is formulated. Details of the computational construction of the expansion and test bases are described in Sec. V. The subtraction procedure to handle the singular integrals that come up in Petrov-Galerkin and Nystrom methods are discussed in this section as well. In Sec. VI the results of calculations for a model potential are discussed and compared for different bases and methods. In Sec.VII we summarize our conclusions.

II. LIPPMANN-SCHWINGER EQUATION

Basic equation for the description of two-particle scattering is the Lippman-Schwinger equation for the two-particle transition operator $T(z)$:

$$T(z) \;=\; V \;+ V\, G_0(z)\, T(z)\;, \tag{1}$$

where V is the interaction potential between two particles, $G_0 = (z - H_0)^{-1}$, with z being the (complex) energy of the two-particle system. For on-shell scattering, $z = E + i0$ with

$E = q_0^2/2\mu$. Working in the center-of-mass frame, the eigenstates of the free Hamiltonian H_0 are the relative momentum states $|\mathbf{q}>$. The matrix elements $T(\mathbf{q}, \mathbf{q}_0\,; z) =< \mathbf{q}|T(z)|\mathbf{q}_0 >$ satisfy the three-dimensional integral equation

$$T(\mathbf{q},\, \mathbf{q}_0\,; z) \;=\; V\,(\mathbf{q},\, \mathbf{q}_0) \,+\, \int \mathrm{d}\mathbf{q}'\, \frac{V\,(\mathbf{q}, \mathbf{q}')\; T(\mathbf{q}', \mathbf{q}_0\,; z)}{z \,-\, q'^2/2\mu} \tag{2}$$

where μ is the reduced mass. Atomic units will be used throughout this article. The z-dependence of T-matrix elements $T(\mathbf{q},\, \mathbf{q}_0\,; z)$ will be suppressed in the rest of this article. The momentum-space matrix elements $V\,(\mathbf{q},\, \mathbf{q}')$ of the potential V are given as

$$V(\mathbf{q},\, \mathbf{q}') \,=< \mathbf{q}|V|\mathbf{q}' > = \int d\mathbf{r} \;< \mathbf{q}|\mathbf{r} > \; V(\mathbf{r}) \;< \mathbf{r}|\mathbf{q}' >\,, \tag{3}$$

with $< \mathbf{r}|\mathbf{q} >= \, e^{i\mathbf{r}\cdot\mathbf{q}}/(2\pi)^{3/2}$.

As first noted in Ref. [1], the azimuthal-angle dependence in Eq. (2) can be integrated out to obtain a two-dimensional integral equation. This is possible because $V(\mathbf{q},\, \mathbf{q}')$ and $T(\mathbf{q},\, \mathbf{q}')$ in the case of central potentials depend only on q, q' and $x_{qq'} = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}' = \, cos\,\theta_{qq'}$. Here $\theta_{qq'}$ is the angle between $\mathbf{q}$ and $\mathbf{q}'$ vectors. Denoting the polar and azimuthal angles of the momentum vector $\mathbf{q}$ by θ and ϕ, respectively, we have $x_{qq'} = xx' + ss'\, cos\,(\phi - \phi')$, where $x = cos\,\theta$ and $s = \sqrt{1-x^2}$. Whenever we want to make the functional dependence explicit, the notation $T(q, q', x_{qq'})$ will be used in place of $T(\mathbf{q}, \mathbf{q}') \;=\; T(q, \theta, \phi,\, q', \theta', \phi')$.

We now introduce the reduced quantities

$$V(q, x; q', x') \;=\; \int_0^{2\pi} d\phi\; V(\mathbf{q}, \mathbf{q}') \;=\; \int_0^{2\pi} d\phi\; V(q, q', x_{qq'})\,, \tag{4}$$

$$T(q, x; q', x') \;=\; \int_0^{2\pi} d\phi\; T(\mathbf{q}, \mathbf{q}') \;=\; \int_0^{2\pi} d\phi\; T(q, q', x_{qq'})\,. \tag{5}$$

The crucial observation [1] is that the above integrals are independent of the value of the azimuthal angle ϕ'. In fact, if we define an averaged momentum state $|qx>$ as

$$|qx> \,=\, (2\pi)^{-1/2} \int_0^{2\pi} d\phi\; |\mathbf{q}> \tag{6}$$

one can easily verify that $V(q, x; q', x') \;=< qx|V|q'x' >$ and $T(q, x; q', x') \;=$ $< qx|T|q'x' >$. This observation allows us to integrate Eq. (2) over ϕ and obtain the two-dimensional Lippmann-Schwinger (LS2D) equation:

$$T(q, x; q_0, x_0) \;=\; V(q, x; q_0, x_0) \;+\; \int_0^{\infty} dq'\, q'^2 \int_{-1}^{1} dx'\; \frac{V(q, x; q', x')\; T(q', x'; q_0, x_0)}{z - q'^2/(2\mu)}\;. \tag{7}$$

For an initial momentum vector $\mathbf{q}_0$ along the z axis and a general final momentum vector $\mathbf{q}$, we have $x_0 = 1$ and $x_{qq_0} = x$. Using this in Eq.(5), we find that

$$< \mathbf{q}|T|q_0\hat{\mathbf{z}} >= T(q, q_0, x) \; = \; (2\pi)^{-1}\, T(q, x\,; q_0, 1)\,.$$

Note also that, when $x_0 = -1$, we have $x_{qq_0} = -x$ and $< \mathbf{q}|T|q_0\,\widehat{-\mathbf{z}} >= T(q, q', -x) \; = \; (2\pi)^{-1}\, T(q, x\,; q_0, -1)\,.$ It also follows from Eq.(5) that

$$T(q, x; q_0, x_0) \; = \; (2\pi)^{-1} \int_0^{2\pi} d\phi \; T(q, x_{qq_0}; q_0, 1), \tag{8}$$

a relationship that might be useful in testing the adequacy of numerical procedures employed to obtain $T(q, x; q_0, x_0)\,.$

The LS2D equation can be solved by the Nystrom method in which the integrals over q' and x' are approximated by suitable quadrature rules and then x and q variables are collocated at the quadrature points. We use the Nystrom method to obtain benchmark results against which the performance of the weighted-residual methods for different choices of expansion and test bases are tested. Computational implementation of the Nystrom method is outlined in Sec. V.

III. WEIGHTED-RESIDUAL APPROACH

The weighted-residual methods (also known as the Petrov-Galerkin approach) involve a finite dimensional approximation subspace $\mathcal{S}_\mathcal{A}$ (of trial solutions) and a subspace $\mathcal{S}_\mathcal{T}$ of test (or weight) functions. These two spaces are in general different, but are usually taken to have the same dimension. (The possibility exist, however, for using $\mathcal{S}_\mathcal{A}$ and $\mathcal{S}_\mathcal{T}$ that have have different dimensions, but the solution of the ensuing weighted-residual equations would then require the use of generalized-inverses. This is a possibility that we do not pursue in this article). If $\mathcal{S}_\mathcal{A}$ and $\mathcal{S}_\mathcal{T}$ are taken to coincide, the resulting methods are referred to as Galerkin methods. Use of different test subpaces $\mathcal{S}_\mathcal{T}$ with a given approximation space $\mathcal{S}_\mathcal{A}$ gives rise to a wide range of Petrov-Galerkin methods (such as collocation , method of subdomains, least squares, and method of moments)[17-20]. The only compatibility requirement on the $(\mathcal{S}_\mathcal{A}, \mathcal{S}_\mathcal{T})$ pairs is that no member of $\mathcal{S}_\mathcal{A}$ be orthogonal to $\mathcal{S}_\mathcal{T}$.

The basis set for the approximation subspace $\mathcal{S}_\mathcal{A}$ will be denoted as $\{\varphi_k(q, x)\,,\, k \; = \; 1, 2, ..., K\,\}$. The basis functions are linearly independent, but not necessarily orthonormal. The projection operator onto the approximation subspace $\mathcal{S}_\mathcal{A}$ is given as

$$\mathcal{P}_\mathcal{A} \; = \; \Sigma_{k=1}^{K} \Sigma_{k'=1}^{K} \, |\varphi_k > \, (\mathbf{\Delta}_\mathcal{A}^{-1})_{k,k'} \, < \varphi_{k'}|\,, \tag{9}$$

where $\mathbf{\Delta}_{\mathcal{A}}$ is the overlap matrix, viz., $(\mathbf{\Delta}_{\mathcal{A}})_{k,k'} =< \varphi_k|\varphi_{k'} >$.

The test subspace $\mathcal{S}_{\mathcal{T}}$ is similarly spanned by a set of linearly independent functions $\{\chi_k(q,x)\,,\, k=1,2,...,K\}$. The projection operator onto the test space is given as

$$\mathcal{P}_{\mathcal{T}} \,=\, \Sigma_{k=1}^{K}\,\Sigma_{k'=1}^{K}\,|\chi_k > (\mathbf{\Delta}_{\mathcal{T}}^{-1})_{k,k'} \,< \chi_{k'}|\,, \tag{10}$$

where $\mathbf{\Delta}_{\mathcal{T}}$ is the overlap matrix of the test functions viz., $(\mathbf{\Delta}_{\mathcal{T}})_{k,k'} =< \chi_k|\chi_{k'} >$. The overlap matrix of the two bases is denoted by $\mathbf{\Lambda}$, viz.,

$$(\mathbf{\Lambda})_{k,k'} \equiv < \chi_k|\varphi_{k'} > \,. \tag{11}$$

The compatibility condition for the subspaces $\mathcal{S}_{\mathcal{A}}$ and $\mathcal{S}_{\mathcal{T}}$ is that $\mathbf{\Lambda}$ be non-singular.

It will be convenient to introduce a primitive basis $\{\xi_k(q,x)\,, k=1,2,...,K\}$, and to generate various choices of expansion and test functions by transforming the primitive basis under the action of appropriate operators (like V and G_0) from the scattering theory. This idea is similar in spirit to the concept of *Riesz Bases* used in the theory of approximations [26]. Denoting with $\mathcal{S}_{\pi}$ the subspace spanned by the primitive basis $\{\xi_k(q,x)\}$, possibilities for the approximation space include choices like $\mathcal{S}_{\mathcal{A}} = U\mathcal{S}_{\pi}$ where U can be taken as I, or V, or even VG_0, depending on the nature of the primitive basis. Similarly, the test space can be generated via $\mathcal{S}_{\mathcal{T}} = U'\mathcal{S}_{\pi}$, where possible choices for U' include operators I and V.

We next define an operator Γ by

$$\Gamma \,=\, \Sigma_{k=1}^{K}\,\Sigma_{k'=1}^{K}\,|\varphi_k > (\mathbf{\Lambda}^{-1})_{k,k'} \,< \chi_{k'}|\,. \tag{12}$$

Note that $\Gamma|\varphi_k >= |\varphi_k >$, and $< \chi_k|\Gamma =< \chi_k|$. Since Γ has the idempotency property $\Gamma^2 = \Gamma$, it is a projector. However, $\Gamma \neq \Gamma^{\dagger}$, in general. Such projection operators are referred to as *oblique* projectors [21]. Oblique projections have received less attention in the past than the orthogonal projections, but are recently becoming an important tool in, e.g., numerical linear algebra [21, 22] and signal processing [23].

The weighted-residual approach to the LS2D equation seeks an approximate solution T^{WR} in $\mathcal{S}_{\mathcal{A}}$:

$$< qx|\,T^{WR}\,|q_0x_0 >= \Sigma_k \,< qx|\varphi_k > \,c_k(q_0,x_0)\,, \tag{13}$$

where $c_k(q_0,x_0)$ are the unknown expansion coefficients. In operator form, $T^{WR} = \mathcal{P}_{\mathcal{A}}T$. Use of T^{WR} in the LS equation $T - VG_0T - V = 0$ gives rise to a non-zero residual (or

error) function $\varepsilon(q,x)$:

$$\varepsilon(q,x) \;=\; \Sigma_n \Sigma_m \;\; < qx| \left(I - VG_0\right) |\varphi_k > \;\; c_k(q_0,x_0) - \; < qx|V|q_0x_0 > \;\; . \tag{14}$$

In weighted residual methods, one demands that the residual error function $\varepsilon(q,x)$ be orthogonal to the space of test functions:

$$< \chi_k|\varepsilon > = \; 0 \, , \quad k = 1,2,...,K \, . \tag{15}$$

In operator form, this requirement corresponds to

$$P_T \left(P_A T - V - VG_0 P_A T\right) \; = 0 \, .$$

This leads the following system of linear equations for the expansion coefficients

$$\Sigma_{k'} \left(\mathbf{D}^{-1}\right)_{k,k'} c_{k'}(q_0,x_0) \; = < \chi_k|V|q_0x_0 >$$

where

$$\left(\mathbf{D}^{-1}\right)_{k,k'} \; = < \chi_k|I - VG_0|\varphi_{k'} > \, . \tag{16}$$

Upon solving for expansion coefficients $\{c_k\}$ and using them in Eq.(7), we obtain

$$< qx|T^{WR}|q_0x_0 > = \; \Sigma_k \, \Sigma_{k'} \;\; < qx|\varphi_k > \; \mathbf{D}_{k,k'} \;\; < \chi_{k'}|V|q_0x_0 > \, , \tag{17}$$

which represents a separable expansion of rank K. We can easily verify that T^{WR} is the exact T-operator for the approximate (left-projected)potential $V^L \; = \; \Gamma V$, which reads in explicit notation

$$< qx|V^L|q'x' > = \; \sum_k \sum_{k'} \;\; < qx|\varphi_k > \left(\mathbf{\Lambda}^{-1}\right)_{kk'} \;\; < \chi_{k'}|V|q'x' > \;\; . \tag{18}$$

Note that, $< \chi_k|V^L \; = < \chi_k|V \;\; .$ That is, V^L is approximate only as far as the left off-shell behaviour of V is concerned.

We note in passing that this procedure could be carried out in exactly the same manner for the three dimensional LS equation, Eq. (2). Taking the approximation and test bases as functions of the full momentum vector (i.e., $\varphi_k(q,x,\phi)$ and $\chi_k(q,x,\phi)$, we would obtain

$$< qx\phi|T^{WR}|q'x'\phi' > = \; \Sigma_k \, \Sigma_{k'} \;\; < qx\phi|\varphi_k > \; \mathbf{D}_{k,k'} \;\; < \chi_{k'}|V|q'x'\phi' > \, , \tag{19}$$

where the matrix elements involving T, V and G_0 are now to be understood in the original three-dimensional sense. Although in this article we will not pursue this version of the

method any further, it is conceivable that this separable form might provide a convenient way to generate the fully three-dimensional T-matrix elements $< \mathbf{q}|T(E)|\mathbf{q}' >$ (rather than the reduced elements) as needed in the context of three-particle calculations employing Jacobi momenta vectors directly [2,13].

IV. GALERKIN, COLLOCATION and SCHWINGER-VARIATIONAL METHODS

There are a multitude of possibilities for choosing the expansion and test bases of the weighted residual method. In this article, we will explore and computationally test only a few of these possibilities. The primitive basis in our work is taken as local low-order (in fact, quadratic) piecewise polynomials (of the type used, e.g., in finite element methods)[18,19]. The (orthogonal) projector onto the subspace $\mathcal{S}_\pi$ spanned by the primitive basis is given as

$$\mathcal{P}_\pi \; = \; \Sigma_{k=1}^{K} \, \Sigma_{k'=1}^{K} \, |\xi_k > \, (\mathbf{\Delta}_\pi^{-1})_{k,k'} \, < \xi_{k'}| \, . \tag{20}$$

Here $\mathbf{\Delta}_\pi$ is the overlap matrix of the primitive basis, i.e., $(\mathbf{\Delta}_\pi)_{kk'} \, =< \xi_k|\xi_{k'} > .$

The Galerkin method follows from taking both expansion and test bases as the primitive basis: $\varphi_k(q,x) \; = \; \xi_k(q,x)$ and $\chi_k(q,x) \; = \; \xi_k(q,x)$. The Galerkin approximation T^G for T reads

$$< qx|T^G|q_0x_0 >= \; \Sigma_k \, \Sigma_{k'} \; < qx|\xi_k > \; (\mathbf{D}^G)_{k,k'} \; < \xi_{k'}|V|q_0x_0 > , \tag{21}$$

where

$$[(\mathbf{D}^G)^{-1}]_{k,k'} \, =< \xi_k|1 - VG_0|\xi_{k'} > .$$

We note that T^G is the exact T-operator for the projected potential $V^G \; \equiv \; \mathcal{P}_\pi V$, which may be termed as the left-sided projection of the operator V. We note in passing that another version of the Galerkin method follows from the right-sided projection $V\mathcal{P}_\pi$. Yet another approximation scheme can be based on the two-sided projection $\mathcal{P}_\pi V \mathcal{P}_\pi$. (In the terminology of Ref. [25], this represents an *outer*-projection approximation.)

For the collocation method, we take $\varphi_k(q,x) \; = \; \xi_k(q,x)$ and require that the error function $< qx|\varepsilon >$ of Eq.(14) vanish on a set of K collocation points on the computational q-x domain. Let $\{ q_{Cn} \, , \, n \; = \; 1,2,3,...,N \}$ and $\{ x_{Cm} \, , \, m \; = \; 1,2,3,...,M \}$ be the sets of collocation points for the q and x variables, respectively. Here N and M are such that $K = NM$. A natural choice of for these collocation points for a primitive basis of piecewise

quadratic polynomials is discussed in Sec. V. Test functions $\chi_k(q,x)$ of the collocation method are the delta functions located at the collocation points, viz.,

$$\chi_k(q,x) \,=\, \delta(q-q_{Cn})\,\delta(x-x_{Cm})\,,$$

where index k stands for (n,m). The collocation approximation T^C for T reads

$$< qx|T^C|q_0x_0 >= \,\Sigma_k\,\Sigma_{k'}\, < qx|\xi_k > \,(\mathbf{D}^C)_{k,k'}\, < \chi_{k'}|V|q_0x_0 >\,, \tag{22}$$

where

$$[(\mathbf{D}^C)^{-1}]_{k,k'} \,=< \chi_k|1-VG_0|\xi_{k'} > \,.$$

The collocation method has the advantage that the numerical construction of the matrix $\mathbf{D}^C$ is considerably easier than than that of $\mathbf{D}^G$.

The Schwinger variational result for the T-operator follows from the choices $\varphi_k(q,x) \,=\, < qx|V|\xi_k >$ and $\chi_k(q,x) \,=\, \xi_k(q,x)$. Employing these choices in Eq. (16), we obtain

$$< qx|T^{SV}|q_0x_0 >= \,\Sigma_k\,\Sigma_{k'}\, < qx|V|\xi_k > \,(\mathbf{D}^{SV})_{k,k'}\, < \xi_{k'}|V|q_0x_0 >\,, \tag{23}$$

where

$$[(\mathbf{D}^{SV})^{-1}]_{k,k'} \,=< \xi_k|V-VG_0V|\xi_{k'} > \,.$$

It is a well known fact that T^{SV} is the exact T-operator for the finite-rank approximate potential

$$V^{IP} \equiv V\,\mathcal{P}_\pi\,(\mathcal{P}_\pi V\mathcal{P}_\pi)^{-1}\,\mathcal{P}_\pi V.$$

Such operator approximations are known as *inner-projection* approximations in the Quantum Chemistry literature [25, 26]. In explicit notation,

$$V^{IP}(q,x;q',x') \,=\, \Sigma_{k=1}^K\,\Sigma_{k'=1}^K\, < qx|V|\xi_k > \,(\mathbf{V^{-1}})_{k,k'}\, < \xi_{k'}|V|q'x' > \,. \tag{24}$$

The inner-projection approximation has the interesting property that $V^{IP}\mathcal{P}_\pi \,=\, V\mathcal{P}_\pi$ and $\mathcal{P}_\pi V^{IP} \,=\, \mathcal{P}_\pi V$. That is, V^{IP} is not restricted to the approximation space $\mathcal{S}_\pi$. Inner projection approximation can also be viewed as an oblique projection. Defining the oblique projector $\Gamma^V \,=\, \Sigma_{k=1}^K\,\Sigma_{k'=1}^K\,|\xi_k > \,(\mathbf{V^{-1}})_{k,k'}\, < \xi_{k'}|V$, we have $V^{IP} \,=\, V\,\Gamma^V \,=\, \Gamma^{V\dagger}\,V$.

A variant of the Schwinger variational method can be obtained by taking $\chi_k(q,x) \,=\, < qx|G_0|\xi_k >$ and $\varphi_k(q,x) \,=< qx|VG_0|\xi_k >$. We will refer to this scheme as Schwinger

Variational method with a G_0-weighted basis (in short, $SVG0$ method). The resulting expression for the T-matrix is

$$< qx|T^{SVG0}|q_0x_0 >= \Sigma_k \Sigma_{k'} < qx|VG_0|\xi_k > (\mathbf{D}^{SVG0})_{k,k'} < \xi_{k'}|G_0V|q_0x_0 > , \qquad (25)$$

where

$$[(\mathbf{D}^{SVG0})^{-1}]_{k,k'} =< \xi_k|G_0VG_0 - G_0VG_0VG_0|\xi_{k'} > .$$

Another choice for the expansion and test bases would be $\varphi_k(q,x) =< qx|V|\xi_k >$ and $\chi_k(q,x) = \delta(q-q_{Cn})\,\delta(x-x_{Cm})$, respectively. The ensuing approximation will be referred to as the *hybrid collocation (HC)* method. The expression for T^{HC} reads

$$< qx|T^{HC}|q_0x_0 >= \Sigma_k \Sigma_{k'} < qx|V|\xi_k > (\mathbf{D}^{SV})_{k,k'} < q_{Cn'}x_{Cm'}|V|q_0x_0 > ,$$

where

$$[(\mathbf{D}^{HC})^{-1}]_{k,k'} =< q_{Cn}x_{Cm}|V - VG_0V|\xi_{k'} > ,$$

where $k = (n,m)$ and $k' = (n',m')$ whenever k and k' enumerate the collocation points. This method stands to the SV method in the same way as collocation method stands to the Galerkin method. Construction of $\mathbf{D}^{HC}$ involves one integration (over q-x domain) less than the construction of $\mathbf{D}^{SV}$.

V. FINITE ELEMENT BASES AND COMPUTATIONAL IMPLEMENTATION

The primitive approximation space $\mathcal{S}_\pi$ is constructed as a direct product space: $\mathcal{S}_\pi = \mathcal{S}_{\pi q} \otimes \mathcal{S}_{\pi x}$. The basis for the N-dimensional space $\mathcal{S}_{\pi q}$ is denoted as $\{ f_n(q)\,,\, n = 1,2,...,N \}$, whereas $\mathcal{S}_{\pi x}$ is M-dimensional and spanned by $\{ h_m(x)\,,\, m = 1,2,...,M \}$. Hence, $\mathcal{S}_\pi$ is of dimension $K = NM$, and spanned by the direct-product basis $\{ \xi_{nm}(q,x) \equiv f_n(q)h_m(x) \}$. The basis sets in the q and x variables are linearly independent, but not necessarily orthonormal. The overlap matrix is a direct-product matrix: $\mathbf{\Delta}_\pi = \mathbf{\Delta}_{\pi q} \otimes \mathbf{\Delta}_{\pi x}$, where $(\mathbf{\Delta}_{\pi q})_{n,n'} =< f_n|f_{n'} >$ and $(\mathbf{\Delta}_{\pi x})_{m,m'} =< h_m|h_{m'} >$. The inner products are taken as $< f_n|f_{n'} >= \int_0^\infty q^2\,dq\, f_n^*(q)\, f_{n'}(q)$ and $< h_m|h_{m'} >= \int_{-1}^1 dx\, h_m^*(x)\, h_{m'}(x)$.

The primitive basis functions will be taken as local piecewise quadratic polynomials [19] defined over a grid, as in the finite element method. For our purposes, quadratic interpolates are found to provide sufficient flexibility, although higher order interpolates like cubic

hermites or cubic splines [19] could also be used. Interestingly, in Ref.[27], piecewise constant functions (the so-called *hat* functions) over a grid has been shown to be quite efficient to solve partial-wave (single-variable) scattering integral equations via a projection method (similar to the outer-projection method mentioned in the previous section).

To define the q-grid over which piecewise polynomials are constructed, we divide the domain into two intervals: $[0,\, 2q_0]$, and $[2q_0, \infty)$. This scheme is adopted to treat the singularity at q_0 as symmetrically as possible, and to use a denser grid for q in the vicinity of q_0. To this end, the first interval $[0,\, 2q_0]$, is subdivided into I_1 (equal) subintervals (finite elements).

On the other hand, the second interval $[2q_0, \infty)$ is mapped to $[-1, +1]$ via the transformation

$$u \,=\, \frac{q - 2q_0 - f}{q - 2q_0 + f}\,, \quad \text{or} \quad q \,=\, 2q_0 \,+\, f\,\frac{1+u}{1-u}\,, \tag{26}$$

where f is a scale factor. By setting an upper limit $u_{max}\,(< 1)$ to the u variable, the q-variable is cut off at some large but finite value q_{max}. Depending on the values used for u_{max} and the scale factor f, momentum cutoff in our calculations ran into several thousand atomic units. This scheme paves the way for a discretization of the semi-infinite interval $[0, \infty)$ with relatively few finite elements. The interval $[-1, u_{max}]$ is divided into I_2 equal finite elements (which, however, correspond to a non-uniform partitioning in the q-variable.)

Let $\{Q_1,\, Q_2,\, ...,\, Q_{I_1+1}\}$ be the set of break points for a partition of the interval $[0, 2q_0]$ into I_1 finite elements. Here $Q_1 \,=\, 0$ and $Q_{I_1+1} \,=\, 2q_0$. The midpoint of the ith finite element $[Q_i, Q_{i+1}]$ is denoted $Q_{i+1/2}$, $i = 1, 2, ..., I_1$. For the second interval $[2q_0, q_{max}]$, let $\{u_1,\, u_2,\, ...,\, u_{I_2+1}\}$ be the break points for a partition of the corresponding interval $[-1, u_{max}]$ of the transformed variable u. Here $u_1 = -1$, and $u_{I_2+1} = u_{max}$. The breakpoints $\{u_{i'}\}$ and mid-points $\{u_{i'+1/2}\}$, $i' = 1, 2, ..., I_2$, of this partition are mapped via Eq. (26), respectively, to $\{Q_i\}$ and $\{Q_{i+1/2)}\}$, where $i = i' + I_1$.

The total number of finite elements covering the computational interval $[0, q_{max}]$ is I ($\equiv I_1 + I_2$). For the calculations reported in the next section, the choice $I_2 = 3I_1$ (hence $I = 4I_1$) was found adequate after some experimentation. Collecting and ordering the break-points and mid-points of all the finite elements together, we form the set $\{q_1, q_2, ..., q_N\}$ of grid points, where $N = 2I + 1$, $q_N \,=\, q_{max}$, and $q_{2i-1} \,=\, Q_i$, $q_{2i} \,=\, Q_{i+1/2}$, for $i = 1, ..., I$. This set (to be referred to as the *grid*) provides the setting for the definition of the q-basis $\{f_n\}$. Each basis function $f_n(q)$ will be centered at its corresponding grid point q_n and will

satify the cardinal property $f_n(q_m) = \delta_{nm}\,,\ n,m = 1,2,...,N\,.$ This set of grid points also provide a natural choice as the collocation points q_{Cn} for the q-variable.

The basis functions associated with the first $2I_1 + 1$ grid points are taken as piecewise quadratic functions of q, while the ones associated with the grid points in the in the interval $[2q_0, q_{max}]$ are taken as piecewise quadratic polynomials in the transformed variable u. These local piecewise polynomials are best described in terms of a local variable s, defined separately for each finite element. For the finite elements covering $[0, 2q_0]$, the finite-element interval $[Q_i, Q_{i+1}]$ is mapped to $[-1, 1]$ via $s = (2q - Q_i - Q_{i+1})/(Q_{i+1} - Q_i)\,.$ For finite elements in $[2q_0, q_{max}]$, we map the u-variable finite element $[u_i, u_{i+1}]$ into $[-1, +1]$ via the map $s = (2u - u_i - u_{i+1})/(u_{i+1} - u_i)\,.$

In terms of the local variable s, the basis functions associated with the breakpoints read

$$f_{2i-1}(q) \;=\; \begin{cases} -s(1-s)/2 \;\text{ for }\; Q_i \,<\, q \,<\, Q_{i+1} \\ s(1+s)/2 \;\;\text{ for }\; Q_{i-1} \,<\, q \,<\, Q_i \\ \qquad 0 \qquad\qquad\quad \text{otherwise} \end{cases} \tag{27}$$

for $i = 1, 2, ..., I + 1\,;$ while the functions associated with the midpoints of finite elements have the form

$$f_{2i}(q) \;=\; \begin{cases} 1 - s^2 \;\text{ for }\; Q_i \,<\, q \,<\, Q_{i+1} \\ \qquad 0 \qquad\qquad\quad \text{otherwise}\ , \end{cases} \tag{28}$$

for $i = 1, 2, ..., I\,.$ These functions are depicted, e.g., in Ref. [28] where they have been used to discretize the momentum space in the context of a time-dependent wave-packet calculation of partial-wave S-matrix elements.

We note that each basis function has a finite support: two finite elements for functions associated with breakpoints, and one finite element for functions corresponding to the midpoints. A characteristic (cardinal) property of these finite-element basis functions is that $f_n(q)$ vanishes at all grid points except at $q = q_n$ where it has the value of unity: $f_n(q_{n'}) = \delta_{nn'}\,.$

The discretization of the x-variable proceeds similarly to that of the q-variable. The interval $[-1, 1]$ is partitioned into J subintervals (elements) by specifying breakpoints $\{X_1, X_2, ..., X_{J+1}\}\,.$ Here, $X_1 = -1$ and $X_{J+1} = 1\,.$ In contrast to q-variable, the placement of the breakpoints for the x-partition is uniform. (A non-uniform x-grid is of course possible and may be more appropriate in some cases.) The midpoint of the ith interval

$[X_i, X_{i+1}]$ is denoted $X_{i+1/2}$. Collecting the breakpoints and midpoints together, we define the set of grid points $\{x_1, x_2, ..., x_M\}$, where $M = 2J+1$, $x_M = 1$, with $x_{2i-1} = X_i$ and $x_{2i} = X_{i+1/2}$ for $i = 1, ..., J$. The x-basis $\{h_m(x)\}$ consists of M piecewise quadratic functions defined on this grid. Again, there is one quadratic function associated with each grid point and, in terms of the local variable s, defined by $s = (2x - X_i - X_{i+1})/(X_{i+1} - X_i)$, they have exactly the same functional form as in Eqs. (26) and (27) (with of course q and Q replaced by x and X, respectively) .

Of course, other basis functions than piecewise quadratic polynomials could be used for the variables q and x. Use of global bases (like gaussians on the grid, or sinc functions) in place of localized bases for q and/or x is a possibility. For instance, the use of Legendre polynomials for x would be equivalent to the partial wave expansion. Another possibility is to employ more sophisticated finite-element bases, such as the higher order piecewise polynomials adopted to more complicated grids (such as decomposition into triangles) of the computational domain on the $q - x$ plane. For example, Ref. [3] used fifth-degree polynomials in radial coordinate r and polar angle θ over a rectangular grid on the $r - \theta$ plane to solve the two-dimensional Schrodinger equation in coordinate space.

Collision energies used in our calculations correspond to the on-shell momentum q_0 having values 0.5 and 2.0. For each finite-element $[Q_i, Q_{i+1}]$, a set of n_q Gauss-Legendre quadrature points are chosen by transforming to the local variable s defined earlier. The Gauss-Legendre quadrature points for all elements are then combined and ordered to form a composite quadrature rule with the set of quadrature points $\{q_\alpha, \alpha = 1, 2, ..., N_q\}$, where $N_q = I\, n_q$. The quadrature weights are similarly collected in the set $\{w_\alpha, \alpha = 1, 2, ..., N_q\}$. In the calculations reported in the next section, n_q was typically taken as 8. For the x-variable, in each finite element $[X_j, X_{j+1}]$, we take n_x Gauss-Legendre quadrature points. The quadrature points and their weights are collected, respectively, in the sets $\{x_\beta, \beta = 1, 2, ..., N_x\}$, and $\{\rho_\beta, \beta = 1, 2, ..., N_x\}$, where $N_x = J\, n_x$. In our calculations, typically $n_x = 8$ (and $N_x = 80$) was sufficient to obtain 6 digit accuracy.

Singular integrals involved in matrix elements like $< \xi_k|VG_0V|\xi_{k'} >$, $< \xi_k|G_0VG_0|\xi_{k'} >$, and $< \xi_k|G_0VG_0VG_0|\xi_{k'} >$ are handled by the well-known subtraction technique. For instance, the matrix element $< f_n h_m|VG_0V|f_{n'}h_{m'} >$ is first written as

$$< f_n h_m|VG_0V|f_{n'}h_{m'} > = 2\mu\, A_{nm,n'm'} - i\pi\mu q_0\, B_{nm,n'm'}(q_0)$$

where

$$A_{nm,n'm'} \;=\; \mathcal{P}\int_0^{q_{max}} dq\,\frac{q^2\,B_{nm,n'm'}(q)}{q_0^2-q^2}$$
$$B_{nm,n'm'}(q) \;=\; \int_{-1}^{1} dx\;<f_n h_m|V|qx><qx|V|f_{n'}h_{m'}>$$

where $\mathcal{P}$ denotes principle-value integral. The matrix element $A_{nm,n'm'}$ is then rewritten as the sum of non-singular and singular parts:

$$A_{nm,n'm'} \;=\; A^{(ns)}_{nm,n'm'} \;+\; A^{(s)}_{nm,n'm'}\;,$$

where

$$A^{(ns)}_{nm,n'm'} \;=\; \int_0^{q_{max}} dq\;\frac{q^2\,B_{nm,n'm'}(q)\;-\;q_0^2\,B_{nm,n'm'}(q_0)}{q_0^2-q^2}\,,$$
$$A^{(s)}_{nm,n'm'} \;=\; B_{nm,n'm'}(q_0)\int_0^{q_{max}} dq\;\frac{q_0^2}{q_0^2-q^2} \;=\; B_{nm,n'm'}(q_0)\,\frac{q_0}{2}\ln\frac{q_{max}+q_0}{q_{max}-q_0}\;.$$

The integrals involved in $B_{nm,n'm'}(q)$ and $A^{(ns)}_{nm,n'm'}$ are approximated by quadrature:

$$B_{nm,n'm'}(q) \;\approx\; \Sigma_{\beta=1}^{N_x}\,\rho_\beta\;<f_n h_m|V|qx_\beta><qx_\beta|V|f_{n'}h_{m'}>$$
$$A_{nm,n'm'} \;\approx\; \Sigma_{\alpha=1}^{N_q}\;w_\alpha\,q_\alpha^2\,\frac{B_{nm,n'm'}(q_\alpha}{q_0^2-q_\alpha^2} \;+\; C_{sing}\,q_0^2\,B_{nm,n'm'}(q_0)$$

where C_{sing} represents the difference between exact and quadrature evaluations of the singular integral $\mathcal{P}\int_0^{q_{max}} dq/(q_0^2-q^2)$:

$$C_{sing} \;=\; \frac{1}{2q_0}\ln\frac{q_{max}+q_0}{q_{max}-q_0} \;-\; \sum_{\alpha=1}^{N_q}\;\frac{w_\alpha}{q_0^2-q_\alpha^2}$$

The reference results against which the results of weighted-residual methods will be compared are obtained by solving the two-variable integral equation via the Nystrom method (i.e., the quadrature discretization method). To prepare for the quadrature discretization, we define

$$\mathcal{K}(q,x;q'x'|q_0) \;=\; q'^2\,V(q,x;q',x') \;-\; q_0^2\,V(q,x;q_0,x') \tag{29}$$

and rewrite Eq. (7) as

$$\begin{aligned} T(q,x;q_0,x_0) \;&=\; V(q,x;q_0,x_0) \\ &+\; 2\mu\int_0^{q_{max}} dq'\int_{-1}^{1} dx'\;\frac{\mathcal{K}(q,x;q'x'|q_0)}{q_0^2-q'^2}\;T(q',x';q_0,x_0) \\ &+\; 2\mu q_0^2\int_{-1}^{1} dx' V(q,x;q_0,x')T(q_0,x';q_0,x_0)\int_0^{q_{max}} dq'\;\frac{1}{q_0^2-q'^2+i0}\;, \end{aligned} \tag{30}$$

where a term involving the singular integral $\int_0^{q_{max}} dq' \, (q_0^2 - q'^2 + i0)^{-1}$ has been added and subtracted. The first term on the right hand side with the subtracted kernel is now non-singular and can be approximated by quadrature. The second integral is to be evaluated analytically. This scheme has been tested and verified against other subtraction methods. For example, a three-dimensional generalization of Kowalski-Noyes method [16] has also been used and will be described elsewhere.

The same set of quadrature points used in the implementation of the weighted-residual methods are used to discretize Eq. (30). Replacing the integral by the quadrature sum and collocating at $q' = q_\alpha$, $x' = x_\beta$, and $q' = q_0$, we obtain a set of $(N_q + 1)N_x$ linear equations for $T(q_\alpha, x_\beta; q_0, x_0)$ and $T(q_0, x_\beta; q_0, x_0)$ as

$$\begin{aligned} T(q_\alpha, x_\beta; q_0, x_0) \;&=\; V(q_\alpha, x_\beta; q_0, x_0) \\ &+\; 2\mu \, \Sigma_{\alpha'=1}^{N_q} \Sigma_{\beta'=1}^{N_x} \, {q_{\alpha'}}^2 w_{\alpha'} \, \rho_{\beta'} \, \frac{V(q_\alpha, x_\beta; q_{\alpha'}, x_{\beta'}) \, T(q_{\alpha'}, x_{\beta'}; q_0, x_0)}{{q_0}^2 \;-\; {q_{\alpha'}}^2} \\ &+\; C_{pole} \, \Sigma_{\beta'=1}^{N_x} \rho_{\beta'} \; V(q_\alpha, x_\beta; q_0, x_{\beta'}) \, T(q_0, x_{\beta'}; q_0, x_0) \, , \end{aligned} \tag{31}$$

and

$$\begin{aligned} T(q_0, x_\beta; q_0, x_0) \;&=\; V(q_0, x_\beta; q_0, x_0) \\ &+\; 2\mu \, \Sigma_{\alpha'=1}^{N_q} \Sigma_{\beta'=1}^{N_x} \, {q_{\alpha'}}^2 \, w_{\alpha'} \, \rho_{\beta'} \, \frac{V(q_0, x_\beta; q_{\alpha'}, x_{\beta'}) \, T(q_{\alpha'}, x_{\beta'}; q_0, x_0)}{{q_0}^2 \;-\; {q_{\alpha'}}^2} \\ &+\; C_{pole} \, \Sigma_{\beta'=1}^{N_x} \rho_{\beta'} \; V(q_0, x_\beta; q_0, x_{\beta'}) \, T(q_0, x_{\beta'}; q_0, x_0) \, . \end{aligned} \tag{32}$$

where $C_{pole} \;=\; 2\mu q_0^2 \, C_{sing} \;-\; i\pi\mu \, q_0 \, .$

Once $T(q_\alpha, x_\beta; q_0, x_0)$ and $T(q_0, x_\beta; q_0, x_0)$ are obtained by solving the above set of linear equations, the matrix elements $T(q, x; q_0, x_0)$ for arbitrary values of q and x can now be obtained from

$$\begin{aligned} T(q, x; q_0, x_0) \;&=\; V(q, x; q_0, x_0) \\ &+\; 2\mu \, \Sigma_{\alpha=1}^{N_q} \Sigma_{\beta=1}^{N_x} \, {q_\alpha}^2 \, w_\alpha \, \rho_\beta \, \frac{V(q, x; q_\alpha, x_\beta) \, T(q_\alpha, x_\beta; q_0, x_0)}{{q_0}^2 \;-\; {q_\alpha}^2} \\ &+\; C_{pole} \, \Sigma_{\beta=1}^{N_x} \rho_\beta \; V(q, x; q_0, x_\beta) \, T(q_0, x_\beta; q_0, x_0) \, . \end{aligned} \tag{33}$$

VI. RESULTS

For our calculations, we use the Hartree potential

$$V(r) \;=\; V_0 \, e^{-\lambda r} \, \left(1 + \frac{1}{r} \right) \, .$$

The values used for the potential parameters are $V_0 = -2.0$ and $\lambda = -2.0$, and the reduced mass is $\mu = 0.5$.

The momentum-space representation of this potential is given as

$$V(\mathbf{q}, \mathbf{q}') \;=\; \frac{\lambda V_0}{\pi^2}\,\frac{1}{[\,(\mathbf{q}-\mathbf{q}')^2 + \lambda^2\,]^2} \;-\; \frac{V_0}{2\pi^2}\,\frac{1}{(\mathbf{q}-\mathbf{q}')^2 + \lambda^2}$$

For this potential the azimuthal integration in Eq. (4) can be carried out analytically to give

$$\begin{aligned} V(q,x;q',x') \;=\; & \frac{2\lambda V_0}{\pi}\,\frac{(q^2+q'^2-2qq'xx'+\lambda^2)}{[\,(q^2+q'^2-2qq'xx'+\lambda^2)^2 - 4q^2q'^2(1-x^2)(1-x'^2)\,]^{3/2}} \\ & -\frac{V_0}{\pi}\,\frac{1}{[\,(q^2+q'^2-2qq'xx'+\lambda^2)^2 \;-\; 4q^2q'^2(1-x^2)(1-x'^2)\,]^{1/2}} \end{aligned}$$

The availability of analytical form for $V(q,x;q',x')$ is not crucial. The reduced potential $V(q,x;q',x')$ can be generated numerically by applying an appropriate quadrature rule to the ϕ integral. In fact, for the present model, a composite 64-point Gauss-Legendre rule for $\phi-$integral produces results that are indistinguishable within 7-8 digits from those of the analytical reduced potential.

Table I shows results of Nystrom calculations at E=0.25 and 4.0 for two values of momentum cutoff q_{max}. Shown are the real and imaginary parts of the scattering amplitude

$$A(x;E) \;\equiv\; -4\pi^2\mu\, T(q_0, x; q_0, x_0 = 1.0; E)$$

for three values of x. Also shown is the average of the scattering amplitude over x (which is the s-wave component of the scattering amplitude).

The computational parameters for the Nystrom calculations with $q_{max} = 30$ are as follows: the computational q-interval $[0, 30]$ was partitioned into 20 finite elements and a composite quadrature rule constructed by taking 8 quadrature points per finite element. For the x-variable, the interval $[-1, +1]$ divided into 10 finite elements and 8 quadrature points were used per finite element. Thus, 160 points have been used to discretize the q-variable over the computational interval $[0, 30]$, and 80 quadrature points for the x-variable. The order of the coefficient matrix of the Nystrom method is 12880. Such systems of equations have been solved by a direct out-of-core equation solver (described earlier in [28]). For even larger dimensions, Pade re-summation of the Born series generated from Eq. (29) turns out to be

very efficient. Direct and Pade solutions agree to 8 digits. The results are also converged to at least 6 digits with respect to further variations of the computational parameters like number of quadrature points and their distribution.

The case indicated as $q_{max} > 1000$ in Table I involve mapping of the interval $[30, \infty]$ by the transformation (27) to $[-1, +1]$. Momentum cutoff is introduced by truncating $[-1, +1]$ as $[-1, u_{max}]$, with u_{max} taken typically as 0.99. With scale factor $f = 30$, this gives $q_{max} \approx 6000$. In calculations of Table I, the interval $[-1, 0.99]$ was divided into 10 finite-elements (i.e., $I_2 = 10$) and an 8-point quadrature used over each finite element. That is, 80 additional quadrature points have been used for the interval $[30, q_{max}]$. Thus the total number of quadrature points for the full computational q-interval $[0, q_{max}]$ is 240. With 80 quadrature points used to discretize the x integral, the number of equations to be solved comes out as 19280. The results obtained with either the out-of-core direct solver or Pade resummation are converged at least within the number of digits shown in the table (or better) to further variations of computational parameters.

Table I demonstrates that results accurate to within 3 or 4 digits can be obtained if q-integration is cut off at 30 atomic units. To obtain results stable at 6 digit level one needs to extend the cut off beyond 1000 atomic units. If one attempts to discretize the the interval $[30, q_{max}]$ directly in the variable q, this could lead to enormous number of quadrature points and to an intractable computational task. Fortunately, however, the mapping of Eq. (25) makes this task tractable with relatively few finite elements and quadrature points. Similar transformations are applied, e.g., in Refs. [1],[5],and [8], to map the full interval $[0, \infty]$ to $[-1, +1]$ or $[0, 1]$. However, such maps do not treat the singularity at $q = q_0$ with sufficient care. In our scheme, we separate out the low-momentum region for direct and careful treatment, and apply the mapping to the high-momentum region.

Tables II and III shows the results of SVM calculations at $E = 0.25$ and $E = 4.0$ for various basis sizes. In these tables, N and M are the number of basis piecewise quadratic polynomials for the q and x variables, respectively. The orders of the linear equation systems that result from SVM are significantly smaller than that of the Nystrom method. The dimension of the $\mathbf{D}^{SV}$ matrix of Eq. (21) ranges from 99 to 861 for calculations reported in Table II, and from 357 to 1271 in Table III. Also shown on these tables are the results of Shertzer and Temkin who have solved the two-dimensional Schrodinger equation for the same potential with the finite element approach [3]. The agreement between their results

and ours is excellent. Their results, however, are reported to within 3 digits after the decimal point. Our Nystrom results are stable to within at least 6 digits after the decimal point to further variations of all computational parameters.

Table IV shows the results obtained with the Galerkin method at $E = 0.25$ using piecewise quadratic polynomials as the basis. Comparison of these results with those of Table II demonstrates that SVM exhibits better convergence than the Galerkin method. To obtain 6 digit accuracy, Galerkin method requires a finer partitioning of the computational domain. Table V shows that results obtained with the collocation method are very similar to those of the Galerkin method.

Table VI gives the results of calculations employing the Schwinger Variational method with a G_0-weighted basis based on Eq. (23). These are to be compared with those of Table II. The transformation of the primitive q-basis under G_0 is especially effective for small bases. For instance, at the $N = 19$ level, the quality of the results of the weighted basis are superior to those of the (primitive) piecewise quadratic basis. However, the additional G_0 factors in various matrix elements make this approach numerically more involved.

Table VII shows the results obtained with the hybrid-collocation method. Quality of results are very similar to that of SVM (listed in Table II). As collocation methods require less numerical integration, computational savings could make this hybrid method competitive among the various schemes considered.

Finally, Table VIII shows results obtained with SVM using a primitive basis of Gaussian functions for the q-variable. The basis functions $f_n(q)$ are taken as Gaussian functions centered on the collocation points q_{Cn}:

$$f_n(q) \;=\; e^{-a_n(q-q_{Cn})^2}$$

The width parameters a_n were adjusted so that the effective support of the Gaussians extended over only a few finite elements around q_{Cn}. The choice $a_n = 3/(q_{Cn+1} - q_{Cn})$ was used in calculations reported in Table VIII. It is interesting to see that convergence pattern for this Gaussian basis is nearly the same as in the case of piecewise quadratics.

VII. DISCUSSION and CONCLUSIONS

We have shown that versatile computational schemes can be constructed via the the weighted-residual approach to directly calculate the full three-dimensional momentum rep-

resentation of the two-particle transition operator without invoking angular momentum decomposition. With these methods, the accuracy of the Nystrom method with a fine quadrature mesh can be reached with relatively small bases, reducing the order of equations to be solved by at least an order of magnitude. We have demonstrated that SVM converges faster than the Galerkin and collocation methods. Of the various versions considered, Schwinger-variational and hybrid-collocation methods appear more promising. Especially, the hybrid collocation method combines the advantages of Schwinger-variational and collocation methods. The separable form of the T-operator and the relative ease with which arbitrary off-shell T-matrix elements can be generated should make such methods quite attractive for use in direct momentum-vector approach to three-particle Faddeev equations without employing partial-wave decomposition [13,14].

We have discussed the generation of expansion and test bases via transformation of a primitive basis under some (invertible) operator. Such bases can be termed as the Riesz bases, following the terminology of the frame theory [26]. We have shown that employment of $\{G_0|f_n h_m>\}$ as the basis in SVM leads to improved convergence. However, the appearance of additional $G0$ factors in various matrix elements means more numerical work to evaluate them. The use of other Riesz-like bases, such as $\{G_0 V|f_n h_m>\}$, as expansion and/or test functions in the general weighted-residual expression (17) for T^{WR} might be explored.

The use of local finite-element bases in weighted-residual methods is not an inherent requirement of such methods. Other localized bases (like Gaussians on a grid or sinc functions [30]) or global functions may also be considered. Another possibility is to give up the direct-product bases and instead use bases that entangle q and x variables.

We have discussed the SVM , Galerkin and collocation methods in the spirit of the weighted-residual idea (or Petrov-Galerkin ansatz). This paves the way to view these well known approaches in a new light. For example, the Nystrom method can itself be viewed as a collocation-type weighted-residual method. In our implementation of Nystrom and various weighted-residual methods the same quadrature scheme has been used to evaluate the integrals involved. With this caveat in mind, the (smaller) systems of linear equations that result from the weighted-residual methods can be viewed as contractions (or projections) of the (larger) set of equations of the Nystrom method. In effect, the set of equations over the $N_q M_x$-dimensional vector space (stemming from the Nystrom discretization) is replaced by an (approximate) smaller set of equations on a sub-

space of dimension NM. For example, one can show that the contraction from Nystrom to Galerkin is affected by the $(N_q M_x \times NM)$-dimensional direct-product matrix $\mathbf{U}$, defined as $\mathbf{U}_{nm,\alpha\beta} = \xi_k(q_\alpha, x_\beta)\, w_\alpha \rho_\beta = f_n(q_\alpha) h_m(x_\beta)\, w_\alpha \rho_\beta$. This is similar, e.g., to the well-known connection between (orthogonal) collocation and Galerkin methods [19]. In fact, this type of contraction is common place in numerical linear algebra. Although the weighted-residual idea is usually employed in the context of differential and integral equations, its use in numerical linear algebra leads to fruitful results as well [22]. For instance, Krylov subspace methods [22,31] for linear systems use the weighted-residual idea to replace an original large matrix problem by a smaller approximate system of equations.

For the present model, the number of partial waves needed to achieve convergence within 6 digits is about 10 for $E = 0.25$ and is no more than 20 for $E = 4.0$. At these relatively low energies, the use of local interpolation polynomials instead of the usual Legendre polynomials to treat the x-variable does not appear to give any computational advantage. In the context of a model nucleon-nucleon potential, Kessler, Payne and Polyzou [5] had reached a similar conclusion for the use of a wavelet basis in the Galerkin method. Whether other bases (like global functions or more sophisticated local interpolation polynomials in conjunction with more elaborate discretization grids on the $q - x$ plane) might lead to computational benefits at this energy range over Legendre basis remains to be explored. It is conceivable that to beat the Legendre-function representation of the x-variable, one should use bases that are not of simple direct-product type, but entangle q and x variables via, perhaps, a suitable coordinate transformation.

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TABLE I.

Dependence of the scattering amplitudes on the momentum cutoff. Shown are the results of converged Nystrom calculations for the scattering amplitude $A(x;E)$ for $E = 0.25$ and $E = 4.0$.

E	q_{max}	s-wave	$x = -1.0$	$x = 0.0$	$x = 1.0$
		Real part of scattering amplitude			
0.25	30	0.868839	0.725575	0.861919	1.040082
	> 1000	0.868552	0.725289	0.861633	1.039795
4.0	30	0.245902	0.050810	0.162513	0.978586
	> 1000	0.245919	0.050828	0.162530	0.978604
		Imaginary part of scattering amplitude			
0.25	30	1.495095	1.495095	1.495086	1.499179
	> 1000	1.495598	1.491553	1.495589	1.499682
4.0	30	0.204919	0.144448	0.197058	0.299073
	> 1000	0.205014	0.144543	0.197152	0.299168

TABLE II. Convergence with respect to the basis size in the q-variable for the Schwinger variational method (SVM) employing a direct-product basis of piecewise quadratic polynomials. Shown are the scattering amplitudes $A(x;E)$ at $E = 0.25$. Parameters N and M denote the number of basis basis functions in q and x variables, respectively.

N	M	s-wave	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude			
9	11	0.869427	0.726166	0.862508	1.040668
17	11	0.868557	0.725306	0.861650	1.039812
25	11	0.868554	0.725290	0.861635	1.039797
33	11	0.868552	0.725289	0.861633	1.039795
41	11	0.868552	0.725289	0.861633	1.039795
Nystrom		0.868552	0.725289	0.861633	1.039795
Ref.[3]		0.869	0.725	0.862	1.040
		Imaginary part of scattering amplitude			
9	11	1.494061	1.490016	1.494051	1.498145
17	11	1.495568	1.491522	1.495558	1.499652
25	11	1.495595	1.491550	1.495586	1.499679
33	11	1.495598	1.491552	1.495588	1.499681
41	11	1.495598	1.491553	1.495588	1.499682
Nystrom		1.495598	1.491553	1.495589	1.499682
Ref.[3]		1.495	1.491	1.496	1.500

TABLE III. Convergence with respect to the basis size for the Schwinger variational method (SVM) employing a direct-product basis of piecewise quadratic polynomials. Shown are the scattering amplitudes $A(x;E)$ at $E = 4.0$.

N	M	s-wave	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude			
17	21	0.245910	0.0509076	0.162662	0.976805
25	21	0.245919	0.0508297	0.162535	0.978505
33	21	0.245919	0.0508287	0.162530	0.978584
	31	0.245919	0.0508275	0.162530	0.978600
41	21	0.245919	0.0508287	0.162530	0.978588
	31	0.245919	0.0508276	0.162530	0.978604
Nystrom		0.245919	0.0508275	0.162530	0.978604
Ref.[3]		0.246	0.051	0.164	0.979
		Imaginary part of scattering amplitude			
17	21	0.204964	0.144588	0.197135	0.298868
25	21	0.205013	0.144544	0.197152	0.299158
33	21	0.205014	0.144543	0.197152	0.299168
	31	0.205014	0.144543	0.197152	0.299168
41	21	0.205014	0.144543	0.197152	0.299168
	31	0.205014	0.144543	0.197152	0.299168
Nystrom		0.205014	0.144543	0.197152	0.299168
Ref. [3]		0.205	0.145	0.197	0.300

TABLE IV.

Calculations with the Galerkin method with the direct-product basis of piecewise quadratic polynomials. Shown are the results for scattering amplitude $A(x;E)$ at $E = 0.25$.

N	M	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude		
9	11	0.729404	0.864266	1.042470
17	11	0.724437	0.861607	1.040121
25	11	0.725323	0.861596	1.039761
33	11	0.725260	0.861655	1.039803
41	11	0.725295	0.861621	1.039770
49	11	0.725292	0.861640	1.039784
	15	0.725287	0.861640	1.039796
	21	0.725285	0.861641	1.039801
	25	0.725284	0.861641	1.039802
81	25	0.725289	0.861635	1.039795
Nystrom		0.725289	0.861633	1.039795
		Imaginary part of scattering amplitude		
9	11	1.486512	1.490502	1.494557
17	11	1.491686	1.495757	1.499885
25	11	1.491595	1.495629	1.499721
33	11	1.491527	1.495564	1.499660
41	11	1.491568	1.495604	1.499697
49	11	1.491542	1.495578	1.499672
	15	1.491542	1.495578	1.499672
	21	1.491542	1.495578	1.499672
	25	1.491542	1.495578	1.499672
81	25	1.491550	1.495586	1.499680
Nystrom		1.491553	1.495589	1.499682

TABLE V.

Calculations with the collocation method using the direct-product basis of piecewise quadratic polynomials. Shown are the results for the scattering amplitude $A(x;E)$ at $E = 0.25$.

N	M	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude		
9	11	0.723380	0.859676	1.037778
17	11	0.725509	0.861862	1.040035
25	11	0.725231	0.861573	1.039734
33	11	0.725319	0.861665	1.039830
41	11	0.725276	0.861621	1.039784
49	11	0.725298	0.861643	1.039807
	21	0.725298	0.861642	1.039805
	25	0.725298	0.861642	1.039805
Nystrom		0.725289	0.861633	1.039795
		Imaginary part of scattering amplitude		
9	11	1.494976	1.499008	1.503099
17	11	1.491153	1.495189	1.499283
25	11	1.491659	1.495695	1.499788
33	11	1.491499	1.495535	1.499628
41	11	1.491576	1.495612	1.499705
49	11	1.491537	1.495573	1.499667
	21	1.491536	1.495572	1.499665
	25	1.491536	1.495572	1.499665
Nystrom		1.491553	1.495589	1.499682

TABLE VI.

Calculations with the hybrid-collocation method using piecewise quadratic polynomials for both q and x variables. Shown are the results for the scattering amplitude $A(x;E)$ at $E = 0.25$.

N	M	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude		
9	11	0.726049	0.862408	1.040588
17	11	0.725288	0.861632	1.039795
25	11	0.725290	0.861534	1.039797
33	11	0.725289	0.861633	1.039795
41	11	0.725289	0.861633	1.039795
Nystrom		0.725289	0.861633	1.039795
		Imaginary part of scattering amplitude		
9	11	1.490365	1.494374	1.498443
17	11	1.491553	1.495589	1.499683
25	11	1.491550	1.495586	1.499679
33	11	1.491552	1.495588	1.499682
41	11	1.491553	1.495589	1.499682
Nystrom		1.491553	1.495589	1.499682

TABLE VII. Scattering amplitude $A(x;E)$ for $E = 0.25$ calculated from Schwinger variational method using a basis constructed from piecewise quadratic polynomials under the action of G_0 . In these calculations $M = 11$.

N	x=-1.0	x=0.0	x=1.0
	Real part of scattering amplitude		
9	0.725287	0.861630	1.039792
17	0.725288	0.861632	1.039795
25	0.725288	0.861633	1.039795
	Imaginary part of scattering amplitude		
9	1.491554	1.495589	1.499681
17	1.491553	1.495589	1.499683
25	1.491553	1.495589	1.499682

TABLE VIII.

Calculations with SVM using N Gaussians as the q-basis. The x-basis consists of M piecewise quadratic polynomials. Shown are the results for the scattering amplitude $A(x;E)$ at $E = 0.25$.

N	M	x=-1.0	x=0.0	x=1.0
		Real part of scattering amplitude		
9	11	0.725429	0.861771	1.039932
17	11	0.725298	0.861642	1.039805
25	11	0.725292	0.861636	1.039798
33	11	0.725280	0.861634	1.039797
41	11	0.725289	0.861633	1.039796
Nystrom		0.725289	0.861633	1.039795
		Imaginary part of scattering amplitude		
9	11	1.491310	1.495345	1.499439
17	11	1.491536	1.495572	1.499665
25	11	1.491547	1.495583	1.499676
33	11	1.491550	1.495586	1.499679
41	11	1.491552	1.495587	1.499681
Nystrom		1.491553	1.495589	1.499682