Direct numerical solution of the two-particle Lippmann-Schwinger equation in coordinate space using the multi-variable Nystrom method

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Abstract Direct numerical solution of the coordinate-space integral-equation version of the two-particle Lippmann Schwinger (LS) equation is considered as a means of avoiding the shortcomings of partial-wave expansion at high energies and in the context of few-body problems. Upon the regularization of the singular kernel of the three-dimensional LS equation by a subtraction technique, a three-variate quadrature rule is used to solve the resulting nonsingular integral equation. To avoid the computational burden of discretizing three variables, advantage is taken of the fact that, for central potentials, azimuthal angle can be integrated out leaving a two-variable reduced integral equation. Although the singularity in the kernel of the two-variable integral equation is weaker than that of the three-dimensional equation, it nevertheless requires careful handling for quadrature discretization to be applicable. A regularization method for the kernel of the two-variable integral equation is derived from the treatment of the singularity in the three-dimensional equation. A quadrature rule constructed as the direct-product of single-variable quadrature rules for radial distance and polar angle is used to discretize the two-variable integral equation. These two- and three-variable methods are tested on a model nucleon-nucleon potential. The results show that Nystrom method for the coordinate-space LS equation compares favorably in terms of its ease of implementation and effectiveness with the Nystrom method for the momentum-space version of the LS equation.

1 Introduction

Expansion in angular-momentum states has hitherto been the usual ansatz for computational approaches to quantum-mechanical scattering problems. However, a critical re-assessment of this strategy has occurred during recent years, especially for high-energy collisions [1] and within the context of few-body problems [2]. It has been realized that even for two-body problems involving central
potentials, where the advantage due to the decoupling of partial wave equations is manifest, the partial wave expansion might lose its practical edge in high energies and for use in few-body calculations employing Faddeev-Yakubovsky-type equations. Although the scattering amplitudes for most potentials are rather smooth, 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 involving an excessively large number of partial waves may be computationally impractical or even unreliable.

These observations suggest that, to treat two-particle scattering at high energies and within the context of few-particle dynamics, direct multi-variable methods without recourse to expansions over angular momentum states might be more appropriate. Towards this end, multivariable methods have been investigated for the solution of the multi-variable LS equation in the momentum space [3-13]. For example in Refs. [11, 12], we have considered multivariable implementations of Schwinger variational and Bateman methods for two-body LS equation in momentum space. Significant progress has also been reported on the formal and computational aspects of solving the three-particle momentum-space Faddeev equations directly as 5-variable problems without invoking angular momentum decomposition [2, 14, 15].

Calculational schemes based on momentum-space LS equations dominate the literature for two-body scattering computations, as exemplified in [3, 5-13]. Coordinate-space version of the LS equation have received relatively less attention as a computational vehicle, although the coordinate-space partial-wave LS equation has been employed in connection with various types of Schwinger variational methods [16-17]. As far as the present author is able to ascertain, the direct numerical solution of the three-dimensional coordinate-space LS equation for the transition operator does not appear to have been reported before. Presumably this is due to the singularity of the free Green's function $G_0(r, r')$ in the kernel of the LS equation. The most straightforward approach to solve an integral equation is the so-called Nystrom method[18] in which the integral equation is converted to a system of linear equations by approximating the integral by a quadrature. However, as the Green's function $G_0(r, r')$ in the kernel of the LS equation becomes singular as $r \rightarrow r'$, the Nystrom method can be applied only after the kernel of the LS equation is regularized. Similar singularities also occur in integral-equation formulations of electromagnetic scattering. In this article, a subtraction technique commonly used in computational electromagnetics [19,20] is adopted to the three-dimensional LS equation. This subtraction scheme regularizes the singular kernel of the three-dimensional LS equation and brings it into a form appropriate for the application of the Nystrom method.

Employing a direct-product quadrature rule with a quadrature mesh \( \{r_\alpha, \alpha = 1, 2, ..., N_Q\} \) for integration over the computational domain in coordinate space, Nystrom method yields a system of $N_Q$ linear equations for the (mixed representation) matrix elements $<r_\alpha | T(E^+) | q_0>$, where $|q_0>$ is the initial state.
with relative momentum \( q_0 \) and energy \( E = |q_0|^2/2\mu \). The momentum-space representation \( < q|T(E+)|q_0 > \) is then obtained from \( < r|T(E+)|q_0 > \) by the same three-dimensional quadrature used in the Nyström method.

In our implementation of the three-dimensional Nyström method for model potentials, 3-4 digit accuracy for scattering amplitude could be obtained with \( N_Q \) in the order of 30–40 thousand quadrature points (involving 60-100 points in \( r \), and 16–20 points in \( \theta \) and \( \phi \) each. As usual with direct-product approaches to multi-variable problems, the curse of dimensionality makes reaching higher level of accuracy a formidable task. Fortunately, however, for central potentials, number of variables can be reduced by one. Using the fact that \( G_0(r,r') \), and \( < r|T(E+)|q + 0 > \) for central potentials, depend on azimuthal angles only via the cosine of the difference of the azimuthal angles of the vectors involved, the azimuthal-angle dependence in the LS equation can be eliminated. By integration over the azimuthal angle, the three-dimensional equation reduces to a two-variable LS equation for the reduced matrix element \( < r\theta|T(E)|q_0\theta_0 > \), where \( r = |r| \), \( q_0 = |q_0| \) and \( \theta \) and \( \theta_0 \) are the polar angles associated with vectors \( r \) and \( q_0 \), respectively. This reduced integral equation can be considered as the integral-equation counterpart of the two-variable differential equation that was solved in Ref. [4] using the finite-element method to avoid partial wave expansion.

Integration over the azimuthal angle weakens the singularity of the original Green’s function, but the new reduced kernel still requires careful handling. We show that the regularized non-singular three-dimensional integral equation can be reduced to obtain a regularized two-variable equation which is in a form ready for the quadrature discretization. Constructing a direct-product quadrature scheme by using \( N_r \) points in \( r \) and \( N_\theta \) points in \( \theta \), Nyström solution of the reduced LS equation yield a linear system of \( N_r N_\theta \) equations which can be solved routinely in commonly available computational platforms.

Plan of this article is as follows: In Sect. 2, we discuss the reduction of the three-dimensional LS equation into a two-variable integral equation. Sect. 3 discusses the subtraction scheme for the removal of the singularity from the kernels of the three dimensional and reduced forms of the LS equation. In Sect. 4, the details of the computational implementation and results of calculations for the model potential are presented. In Sect. 5 we summarize our conclusions.

2 Lippmann-Schwinger Equation

We consider the two-particle scattering problem for a central interparticle potential. Working in the center-of-mass frame, the relative momentum states are denoted by \( |q > \) and the relative position states by \( |r > \), with the normalizations \( < r|r' > = \delta(r - r') \), \( < q|q' > = \delta(q - q') \), and \( < r|q > = e^{i r \cdot q}/(2\pi)^{3/2} \). We will set \( \hbar = 1 \) throughout this article.

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

$$T(z) = V + V G_0(z) T(z),$$

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 $E = q_0^2/2\mu$, where $\mu$ is the reduced mass. Using Eq. 5 for the wave function, the matrix elements $T(r, q_0) (\equiv < r|T(E + i0)|q_0 >)$ satisfy the three-dimensional integral equation

$$T(r, q_0) = V(r) < r|q_0 > + V(r) \int dr' G_0(r, r') T(r', q_0),$$

where $G_0(r, r')$ is the free Green’s function, viz.,

$$G_0(r, r') = < r|G_0(E + i0)|r' > = \frac{\mu}{2\pi} e^{i(r-r')} \equiv \frac{1}{r-r'},$$

Note that the $T(r, q_0)$ is closely related to the scattering wave function $\psi_{q_0}(r)$, viz.,

$$T(r, q_0) = V(r) \psi_{q_0}(r),$$

where $\psi_{q_0}$ is the solution of the LS equation for the wave function

$$\psi_{q_0}(r) = < r|q_0 > + \int dr' G_0(r, r') V(r') \psi_{q_0}(r').$$

Since $V(r)$ vanishes as $r$ gets sufficiently large, solving Eq.2 for the amplitude $T(r, q_0)$ proves to be much more convenient computationally than directly working with Eq. 5 for the wave function. The momentum-space matrix elements $T(q, q_0) (\equiv < q|T(E + i0)|q_0 >)$ of the transition operator can be calculated from the solution of Eq.2 via a quadrature:

$$T(q, q_0) = \int dr < q|r > T(r, q_0).$$

We will denote the polar and azimuthal angles of the position vector $r$ by $\theta$ and $\phi$, and those of the momentum vector $q$ by $\theta_q$ and $\phi_q$, respectively. We will also use the notation $x$ for $\cos \theta$, $s$ for $\sin \theta$, $x_q$ for $\cos \theta_q$, and $s_q$ for $\sin \theta_q$. Since $|r-r'| = \sqrt{x^2 + r'^2 - 2rr'x_{rr'}}$ with $x_{rr'} = xx' + ss' \cos (\phi - \phi')$, dependence of $G_0(r, r')$ on azimuthal angles is only through the difference $\phi - \phi'$. Similarly $T(r, q_0)$ for central potentials depend on $r$, $q_0$, and $r_{xq}$. Here $x_{xq}$ is the cosine of the angle between vectors $r$ and $q_0$, i.e., $x_{r_{xq}} = \hat{r} \cdot q_0$.

Towards the elimination of the azimuthal angles, we introduce the states $|rx >$ and $|qx_q >$ via

$$|rx > = (2\pi)^{-1/2} \int_0^{2\pi} d\phi |r > = (2\pi)^{-1/2} \int_0^{2\pi} d\phi |r\theta\phi >, \quad (7)$$

$$|qx_q > = (2\pi)^{-1/2} \int_0^{2\pi} d\phi_q |q > = (2\pi)^{-1/2} \int_0^{2\pi} d\phi_q |q\theta_q\phi_q >. \quad (8)$$
We next introduce reduced matrix elements of $G_0$ and $T$ via

$$\hat{G}_0(r,x; r', x') = \langle rx | G_0 | r' x' \rangle = (2\pi)^{-1} \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi' G_0(r, r'),$$  \hspace{1cm} (9)

$$\hat{T}(r,x; q_0, x_{q_0}) = \langle rx | T | q_0 x_{q_0} \rangle = (2\pi)^{-1} \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi_{q_0} T(r, q_0).$$  \hspace{1cm} (10)

Note that operators, matrix elements and other quantities associated with the two-variable representation will be distinguished from those of three-dimensional representation by a caret over the symbol.

Since $G_0(r, r')$ and $T(r, q_0)$ depend on azimuthal angles only through the differences $\phi - \phi'$ and $\phi - \phi_{q_0}$, respectively, integration over one of the azimuthal angles can be carried out to obtain

$$\hat{G}_0(r,x; r', x') = \int_0^{2\pi} d\phi G_0(r, r'),$$ \hspace{1cm} (11)

$$\hat{T}(r,x; q_0, x_{q_0}) = \int_0^{2\pi} d\phi T(r, q_0).$$ \hspace{1cm} (12)

Note that, in Eq. 11, the first integral on the right-hand side is independent of the azimuthal angle $\phi'$ of $r'$, while the second integral is independent of $\phi_{q_0}$. Integrating both sides of Eq. (2) over $\phi$ and $\phi_{q_0}$, interchanging the order of integration over $\phi$ and $\phi'$ and then making use of Eqs. 11 and 12, we obtain the reduced two-variable LS equation

$$\hat{T}(r,x; q_0, x_{q_0}) = V(r) < rx | q_0 x_{q_0} > + V(r) \int_0^{\infty} r'^2 dr' \int_{-1}^{1} dx' \hat{G}_0(r,x; r', x') \hat{T}(r', x'; q_0, x_{q_0}),$$ \hspace{1cm} (13)

where

$$< rx | q_0 x_{q_0} > = \int_0^{2\pi} d\phi < r | q_0 > = (2\pi)^{-1/2} e^{i q_0 r x_{q_0}} J_0(q_0 r x_{q_0}),$$ \hspace{1cm} (14)

with $J_0$ denoting the zeroth order Bessel function. We write Eq. 7 in operator form as

$$\hat{T} = \hat{V} + \hat{V} \hat{G}_0 \hat{T},$$ \hspace{1cm} (15)

which is to be understood as an operator equation in the space of two-variable functions (of $r$ and $x$). On the other hand, the reduced version of Eq. 5 reads

$$\hat{T}(q, x_q; q_0, x_{q_0}) = \int r^2 dr \int_{-1}^{1} dx < q x_q | r x > \hat{T}(r, x; q_0, x_{q_0}).$$ \hspace{1cm} (16)
As discussed in [11], for an initial momentum vector $q_0$ along the $z$ axis and a general final momentum vector $q$, the transition matrix element $q|T|q_0 \hat{z}$ is given by

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

2 Regularization of the singular kernels and the Nystrom method

The standard method for the numerical solution of non-singular integral equations is the Nystrom method, in which the integrals are replaced by sums via suitable quadrature rules and the resulting equations are collocated at the quadrature points. However, singular nature of $G_0(r, r')$ does not allow the direct application of Nystrom method to Eq. (2) in full three-dimensional approach or Eq. (7) in two-variable version. We first recast the singular Green’s function as a sum of non-singular and singular parts by subtracting and adding an (analytically) integrable singular term:

$$G_0(r, r') = -\frac{\mu}{2\pi} \left\{ e^{iq_0|r-r'|} - \frac{1}{|r-r'|} \right\} - \frac{\mu}{2\pi} \frac{1}{|r-r'|} \quad (17)$$

where the term within curly brackets is no longer singular as $r' \to r$, while the last term is analytically integrable over $r'$ for fixed $r$.

Using this splitting in Eq. (2), we obtain

$$T(r, q_0) = V(r) < r | q_0 > - \frac{\mu}{2\pi} V(r) I_e(r) T(r, q_0)$$

$$- \frac{\mu}{2\pi} V(r) \int dr' \frac{e^{iq_0|r-r'|} T(r', q_0) - T(r, q_0)}{|r-r'|}, \quad (18)$$

where

$$I_e(r) = \int dr' \frac{1}{|r-r'|}. \quad (19)$$

The integral over $r'$ in Eq. (18) can now be approximated by a quadrature rule. It is understood that the term $I_e$ is to be calculated analytically over the computational domain. Introducing a cutoff $r_{max}$ for the radial variable $r$, we find that

$$I_e(r) = \int_0^{r_{max}} r^2 dr' \int_{-1}^{+1} dx' \int_0^{2\pi} d\phi' |r-r'|^{-1} = 4\pi \left( \frac{r_{max}^2}{2} - \frac{r^2}{6} \right) \quad (20)$$

Note that $I_e(r)$ is in fact independent of the orientation of $r$. The same integral

$$\int_0^{r_{max}} r^2 dr' \int_{-1}^{+1} dx' \int_0^{2\pi} d\phi' |r-r'|^{-1}$$

also occurs as part of the second term in the right hand side of Eq. (18), where however it is to be evaluated via the quadrature rule chosen for the discretization of the integral equation.
Let \( r_\alpha, \alpha = 1, 2, ..., N_Q \) be a set of quadrature points over the computational \( r \)–domain with corresponding weights denoted by \( w_\alpha \). We will construct this three-dimensional quadrature rule as the direct product of single-variable quadrature rules for \( r, x \) and \( \phi \). Let \( \{ r_i, i = 1, ..., N_r \}, \{ x_j, j = 1, ..., N_x \} \) and \( \{ \phi_k, k = 1, ..., N_\phi \} \) be the sets of quadrature points chosen for \( r, x \) and \( \phi \) over the intervals \([0, r_{\text{max}}], [-1, +1]\) and \([0, 2\pi]\), with corresponding weights \( \{ w_r \}, \{ w_x \} \) and \( \{ w_\phi \} \), respectively. Using the composite index \( \alpha \) for the index combination \((ijk)\), the position vector whose spherical components are \( r, x, \phi \) is denoted as \( \mathbf{r}_\alpha, \alpha = 1, 2, ..., N_Q \), where \( N_Q = N_r N_x N_\phi \). With this notation, the weights of the three-dimensional quadrature rule are \( w_\alpha = r_x^2 w_r w_x w_\phi \).

Approximating the integral over \( \mathbf{r}' \) in Eq. (18) by the quadrature rule chosen and collocating \( \mathbf{r} \) at the quadrature points, we obtain

\[
T(\mathbf{r}_\alpha, \mathbf{q}_0) = V(|r_\alpha|) < \mathbf{r}_\alpha, \mathbf{q}_0 > + V(|r_\alpha|) C(\mathbf{r}_\alpha) T(\mathbf{r}_\alpha, \mathbf{q}_0) + V(|r_\alpha|) \sum_{\alpha'}^{N_Q} \delta_{\alpha \alpha'} G_0(\mathbf{r}_\alpha, \mathbf{r}_{\alpha'}) w_{\alpha'} T(\mathbf{r}_{\alpha'}, \mathbf{q}_0),
\]

(21)

where \( \alpha = 1, 2, ..., N_Q \), \( \delta_{\alpha \alpha'} = 1 - \delta_{\alpha \alpha'} \), and

\[
C(\mathbf{r}_\alpha) = -\frac{\mu}{2\pi} [I_\epsilon(\mathbf{r}_\alpha) - I_\alpha(\mathbf{r}_\alpha)].
\]

(22)

Here \( I_\epsilon \) is as defined in Eq. (20) and

\[
I_\alpha(\mathbf{r}_\alpha) = \sum_{\alpha'}^{N_Q} \delta_{\alpha \alpha'} w_{\alpha'}/|\mathbf{r}_\alpha - \mathbf{r}_{\alpha'}|.
\]

(23)

For a given initial momentum vector \( \mathbf{q}_0 \), Eq. (22) represents a system of \( N_Q \) linear equations.

Although computations with small to moderate values of \( N_r, N_x, \) and \( N_\phi \) (say, with 20-30 points in each variable) can be carried out in commonly available computational platforms, more realistic computations would require sophisticated programming techniques and computational environments. Therefore, the two-variable equation with azimuthal angle eliminated is of practical interest. Although the integration over \( \phi \) and/or \( \phi' \) implicit in the definition of \( G_0(\mathbf{r}, \mathbf{r}'; x, x') \) weakens the singularity of the Green’s function \( G_0(\mathbf{r}, \mathbf{r}') \), the numerical treatment of the two-variable LS equation requires a careful handling of the kernel. By application to Eq. (13) of the subtraction trick used for the handling of the kernel singularity in the full three-dimensional equation, Eq. (13) can be recast as

\[
\tilde{T}(r, x; q_0, x_0) = V(r) < r x | q_0, x_0 > - (\mu/2\pi) V(r) I_\epsilon(r) T(r, x; q_0, x_0)
\]

\[
+ V(r) \int_0^\infty r^2 dr' \int_{-1}^1 dx' \int d\phi' \left\{ G_0(\mathbf{r}, \mathbf{r}') T(r', x'; q_0, x_0)
\right.
\]

\[
+ (\mu/2\pi) | \mathbf{r} - \mathbf{r}' |^{-1} T(r, x; q_0, x_0) \right\}.
\]

(24)

In Eq. (24), the azimuthal angle \( \phi \) of the vector \( \mathbf{r} \) has been set to zero. This choice can be made because integrals \( \int d\phi' G_0(\mathbf{r}, \mathbf{r}') \) and \( \int d\phi' | \mathbf{r} - \mathbf{r}' |^{-1} \) are
I composite quadrature rule of \( N \) element. By combining the quadrature points and weights for all elements, a Gauss-Legendre points and their corresponding weights are generated for each \( i \), \( j \), sub-intervals: \([0, V] \).

The parameters for MT-III potential are taken from Ref. [6]: \( V \) MeV fm, as the unit of length. The nucleon mass adopted yields the conversion factor \( 8 \) fm

$$ T(r_i, x_j; q_0, x_0) = V(r_i) < r_i x_j | q_0 x_0 > - V(r_i) \hat{C}(r_i, x_j) \hat{T}(r_i, x_j; q_0, x_0) + V(r_i) \sum_{i'=1}^{N_{r'}} \sum_{j'=1}^{N_{x'}} \hat{G}_0(r_i, x_j; r_{i'}, x_{j'}) r_{i}^2 \rho_{i} w_{i}, w_{x}, \hat{T}(r_{i'}, x_{j'}; q_0, x_{q_0}), $$

(25)

where

$$ \hat{G}_0(r_i, x_j; r_{i'}, x_{j'}) = -(\mu / 2 \pi) \sum_{k=1}^{N_{k}} w_{\phi k} e^{i q_0 d(ij, i'j'; k) / d(ij, i'j'; k),} $$
$$ d(ij, i'j'; k) = [r_{i}^2 + r_{i'}^2 - 2r_{i} r_{i'} (x_j x_{j'} + s_j s_{j'} \cos \phi_{k})]^{1/2}, $$
$$ \hat{C}(r_i, x_j) = -(\mu / 2 \pi) [I(c)(r_i) - I(a)(r_i, x_j)] $$
$$ I(c)(r_i, x_j) = \sum_{k=1}^{N_{k}} w_{\phi k} / d(ij, i'j'; k). $$

The singularity-correction term \( \hat{C}(r_i, x_j) \) turns out to be crucial for the success of the Nyström method.

4 Computational Implementation and Results

To test the two- and three-variable implementations of the Nyström method discussed in the previous section, Malfliet-Tjon III (MT-III) model for the two-nucleon potential has been used:

$$ V(r) = V_R e^{-\mu_R r} - V_A e^{-\mu_A r} $$

The parameters for MT-III potential are taken from Ref. [6]: \( V_A = 626.8932 \) MeV fm, \( V_R = 1438.723 \) MeV fm, \( \mu_A = 1.55 \) fm\(^{-1}\) and \( \mu_R = 3.11 \) fm\(^{-1}\). For the two-nucleon calculations, we set nucleon mass and \( \hbar \) to unity and take \( fm \) as the unit of length. The nucleon mass adopted yields the conversion factor \( 1 fm^{-2} = 41.47 \) MeV.

The cut-off \( r_{\text{max}} \) for the \( r \)-variable is taken as \( 15 fm \), although a value of \( 8 fm \) is sufficient for about 4 digit accuracy. Quadrature grid for \( r \) is uneven: denser for small \( r \), coarser for large \( r \). The interval \([0, r_{\text{max}}]\) is divided into 4 sub-intervals: \([0, 0.5], [0.5, 2], [2, 10], [10, 15]\), which are in turn subdivided into \( I_i \)-elements, \( i = 1, 2, 3, 4 \). Each element is mapped to \([-1, +1]\), and a set of \( n_r \) Gauss-Legendre points and their corresponding weights are generated for each element. By combining the quadrature points and weights for all elements, a composite quadrature rule of \( N_r \) points is generated. Here \( N_r = I_r n_r \), with \( I_r = I_1 + I_2 + I_3 + I_4 \) denoting the total number of \( r \)-elements. Similarly, the
interval $[-1, +1]$ for the $x$-variable was divided into $I_x$ equal elements, with $n_x$ Gauss-Legendre points chosen in each element. Thus, a composite quadrature rule with $N_x = I_x n_x$ was generated. For doing the $\phi$ integrals, the interval $[0, 2\pi]$ was divided into $I_\phi$ equal elements, with $n_\phi$ Gauss-Legendre points in each element, yielding a composite quadrature rule with $N_\phi = I_\phi n_\phi$.

Reference results for the MT-III potential were obtained with momentum-space Nystrom calculations, as reported in Ref. [13], and are stable within seven digits after the decimal point to further variations in computational parameters.

4.1 Results of three-dimensional calculations

Tables 1 and 2 report results of Nystrom calculations with different values of $N_r$, $N_x$, and $N_\phi$. Table 1 probes the convergence with respect to $N_r$ with fixed $N_x$ and $N_\phi$, while Table 2 with respect to $N_x$ and $N_\phi$ with fixed $N_r$.

The largest calculation in Table 1 is for $N_r = 100$ and corresponds to the following distribution of quadrature points for $r$: $I_1 = 6, I_2 = 6, I_3 = 9, I_4 = 4$, and $n_r = 4$. With $N_x = 20$ and $N_\phi = 20$, this corresponds to $N_Q = 40000$. As the matrices of this size can not be kept in the fast memory, they are stored in the disk space in a block-by-block fashion. The system of equations is solved either by a direct out-of-core equation solver (a block-by-block scheme of Gaussian elimination with partial pivoting that was described earlier in [21]) or by Padé re-summation of the Born series generated from Eq. (21). Typically, $[8, 7]$-approximant is sufficient for convergence. It is reassuring that direct and Padé solutions agree within at least 8 significant digits for a given set of computational parameters.

As we were restricted to use rather modest values (12 to 20) for $N_x$ and $N_\phi$ to avoid excessively large $N_Q$, accuracy of the results of three-dimensional calculations is limited to 3-4 significant figures. For the largest three-dimensional calculation in Table 1 (namely, the run with $N_r = 100, N_x = N_\phi = 20$ and hence $N_Q = 40000$), the largest relative error among the transition matrix elements reported in Table 1 is about 0.3 percent. Although the value of $N_r = 80 - 100$ may be close to being adequate for the $r$-variable, Table 2 shows that the values of $N_x$ and $N_\phi$ are far from being sufficient. Indeed, two-dimensional calculations of next section suggest that $N_x$ and $N_\phi$ must be in the order of 60 to 80 if we ask for results accurate to within 5-6 significant figures. However, going beyond $N_Q = 40000$ is a formidable task, requiring special programming and hardware, and has not been attempted. Instead, two-dimensional reduced equations were solved to obtain results with 7-8 significant figures.

4.2 Results of two-variable calculations

Tables 3 and 4 report convergence of the Nystrom method for the two-variable LS equation with respect to $N_r$ and $N_x$. Integration over $\phi$ implicit in the
calculation of $\hat{G}(r,x; r', x')$ is done with $N_\phi = 64$, which is sufficient for the stability of results to the number of digits shown in these tables. For the most refined calculation (with $N_r = 440$ and $N_x = 96$) in Table 3, the largest absolute deviation (from the reference solution) is $1.4 \times 10^{-6}$ for the imaginary part of the forward amplitude at 400 MeV. This corresponds to a relative error of about $2.3 \times 10^{-5}$ percent. For the other values of $x$ in the same calculation, the absolute value of the difference between momentum-space and coordinate-space calculations is less than $5 \times 10^{-7}$, while relative errors are less than $5 \times 10^{-4}$ percent.

The relatively high values of $N_r$ and $N_x$ were needed to achieve agreement within 7-8 significant figure. However, more moderate values like $N_r = 176$ and $N_x = 60$ would be sufficient to obtain agreement within 5-6 significant figures. We note in passing that, reference results obtained from momentum-space Nystrom method [11,13] involves about the same level of computational effort as the coordinate-space Nystrom method for comparable levels of convergence.

Finally we would like to point out the role that the singularity correction term $\hat{C}(r_i, x_j)$ plays in the performance of the coordinate-space Nystrom method for the reduced LS equation. Table 5 gives the results obtained by setting $\hat{C}(r_i, x_j) = 0$ in Eq. (25), which corresponds to pretending as if the kernel has no singularity. As the singularity of the reduced kernel is in fact weaker, ignoring it does not lead to a catastrophe, but results are of low accuracy. Note, however, that the correction term $C(r_\alpha)$ in (21) for the three-dimensional case plays a much more crucial role, for without it Nystrom idea is totally inapplicable.

5 Conclusions

As part of our continuing interest in multi-variable methods for solving scattering integral equations without invoking expansions over angular-momentum states, we have considered the LS integral equation in coordinate space. Both the original three-dimensional and the reduced two-variable versions have been considered. To apply the Nystrom method (which combines quadrature discretization with collocation), a suitable scheme for handling the (moving-type) singularity of the free Green’s function has been implemented. The basic idea is to cancel out the Green’s function singularity by subtracting a known singularity (namely $|r - r'|^{-1}$) which can be integrated in closed form, leaving a smoother kernel that can be integrated by quadrature. Of course, the kernel of the momentum-space LS equation is also singular, but the singularity occurs at a fixed value of the integration variable and is somewhat easier to treat by a similar subtraction scheme as discussed, e.g., in [11]. Apart from this small difference in handling the kernel singularities, momentum-space and coordinate-space Nystrom methods involve about the same level of computational effort. For local potentials, however, coordinate-space approach may be more natural,
as the need for the (possibly numerical) calculation of the momentum-space representation is avoided. For instance, in the context of a Faddeev-equations approach to three-atom problems [24–25], calculation of the atom-atom transition matrices (for numerically available diatomic potentials) would be more practical in coordinate space.

Calculations presented in this article have been done with complex arithmetic. The K-matrix version of the present approach is possible and could lead to some computational savings (in computation time and memory needs) by allowing to work in real arithmetic. However, obtaining T-matrix from K-matrix would involve the solution of an additional integral equation in the angular variables. This possibility is currently under investigation.

The present calculations show that the Nystrom method coupled with the particular singularity removal scheme adopted is a viable procedure that is capable of producing accurate solutions of the LS equation. However, matrix dimensions in the Nystrom method implemented with direct-product quadrature schemes quickly becomes computationally prohibitive. In fact, both coordinate- and momentum-space versions suffer from this problem. Variational methods based on multivariate bases may provide the alternative to the multivariate Nystrom method. The singularity subtraction scheme used in the present article would also be applicable in calculating the matrix elements that come up in the variational approaches and in other Galerkin-Petrov methods. However, the so-called "curse of dimensionality" hampers all methods that make use of direct-product bases. The radial basis function (rbf) approach (which is nearly dimension independent) has emerged during recent years as an alternative to direct-product bases [22,23]. In a recent article [13] we explored the use of rbf’s (in momentum space) in relation to momentum-space LS equation with promising results (for both three-dimensional and two-dimensional versions). A logical continuation of the present work would be to consider rbf expansions (in coordinate space) as a means of solving the coordinate-space LS equation and of obtaining separable expansions of the multivariable T-matrix. Separable expansions (of manageable rank) in multivariate bases for the two-particle T-matrix would be particularly useful for three-body calculations without angular momentum decomposition [2,14,15].

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Table 1: Convergence study for the three-dimensional Nystrom method with respect to the number of quadrature points $N_r$ for the $r$-variable. Listed are the on-shell T-matrix elements $\langle q_0 x \phi | T(E) | q_0 x_0 \phi_0 \rangle$ with $x_0 = 1.0$ and $\phi = \phi_0 = 0$ at $E = 150$ and $E = 400$ MeV obtained with different values of $N_r$. The number of quadrature points used for the angular variables are $N_x = 20$ and $N_\phi = 20$.

| $N_r$ | $x=1.0$ | $x=0.0$ | $x=-1.0$ | $x=1.0$ | $x=0.0$ | $x=-1.0$ |
|------|---------|---------|---------|---------|---------|---------|
|      | Re $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ | Im $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ | Re $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ | Im $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ | Re $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ | Im $\langle q_0 x \phi | T | q_0 x_0 \phi_0 \rangle$ |
|      | $E = 150$ MeV | | | | | |
| 64   | -6.0976 | 0.4923 | 0.2351 | -1.9294 | 0.2864 | 0.3656 |
| 72   | -6.0963 | 0.4923 | 0.2349 | -1.9305 | 0.2864 | 0.3656 |
| 80   | -6.0955 | 0.4922 | 0.2347 | -1.9312 | 0.2864 | 0.3656 |
| 88   | -6.0954 | 0.4922 | 0.2347 | -1.9315 | 0.2864 | 0.3656 |
| 100  | -6.0949 | 0.4922 | 0.2346 | -1.9319 | 0.2864 | 0.3655 |
| Ref. [11] | -6.0928 | 0.4918 | 0.2340 | -1.9373 | 0.2861 | 0.3657 |
|      | $E = 400$ MeV | | | | | |
| 64   | -6.1699 | 0.4556 | 0.2498 | -1.2982 | 0.1110 | -0.0785 |
| 72   | -6.1685 | 0.4554 | 0.2496 | -1.3005 | 0.1108 | -0.0784 |
| 80   | -6.1677 | 0.4553 | 0.2495 | -1.3018 | 0.1108 | -0.0783 |
| 88   | -6.1675 | 0.4553 | 0.2495 | -1.3022 | 0.1108 | -0.0783 |
| 100  | -6.1670 | 0.4552 | 0.2495 | -1.3031 | 0.1108 | -0.0782 |
| Ref. [11] | -6.1638 | 0.4549 | 0.2491 | -1.3116 | 0.1108 | -0.0776 |
Table 2 Convergence study for the three-dimensional Nystrom method with respect to the number of quadrature points $N_x$ and $N_\phi$ in the $x$ and $\phi$ variables, respectively. Listed are the on-shell T-matrix elements $< q_0 x \phi | T(E) | q_0 x_0 \phi_0 >$ with $x_0 = 1.0$ and $\phi = \phi_0 = 0$ at $E = 150$ and $E = 400$ MeV. For calculations of this table, $N_{r} = 100$.

| $N_x$ | $N_\phi$ | $x=1.0$ | $x=0.0$ | $x=-1.0$ | $x=1.0$ | $x=0.0$ | $x=-1.0$ |
|-------|----------|---------|---------|---------|---------|---------|---------|
|       |          | Re $< q_0 x \phi | T | q_0 x_0 \phi_0 >$ | Im $< q_0 x \phi | T | q_0 x_0 \phi_0 >$ |       |       |       |
| 12    | 12       | -6.0939 | 0.4982  | 0.2357  | -1.9198 | 0.2870  | 0.3648  |
| 16    | 16       | -6.0951 | 0.4931  | 0.2352  | -1.9284 | 0.2865  | 0.3654  |
| 20    | 20       | -6.0949 | 0.4922  | 0.2346  | -1.9319 | 0.2864  | 0.3655  |
| Ref. [11] | -6.0928 | 0.4918  | 0.2340  | -1.9373 | 0.2861  | 0.3657  |
|       |          |         |         |         |         |         |         |
|       |          | $E = 150$ MeV |       |       |       |       |       |
| 12    | 12       | -6.1722 | 0.4565  | 0.2593  | -1.2893 | 0.1089  | -0.0793 |
| 16    | 16       | -6.1685 | 0.4579  | 0.2490  | -1.2985 | 0.1108  | -0.0785 |
| 20    | 20       | -6.1670 | 0.4552  | 0.2495  | -1.3031 | 0.1108  | -0.0782 |
| Ref. [11] | -6.1638 | 0.4549  | 0.2491  | -1.3116 | 0.1108  | -0.0776 |
Table 3 Convergence study for the two-variable Nystrom method with respect to the number of quadrature points $N_r$ for the $r$-variable. Listed are the on-shell T-matrix elements $< q_0 x | \hat{T}(E) | q_0 x_0 >$ with $x_0 = 1.0$ at $E = 150$ and $E = 400$ MeV for different values of $N_r$. For calculations reported in this table, the number $N_x$ of quadrature points for the $x$-variable is 96.

| $N_r$ | $E = 150$ MeV | $E = 400$ MeV |
|-------|---------------|---------------|
|       | Re $< q_0 x | \hat{T} | q_0 x_0 >$ | Im $< q_0 x | \hat{T} | q_0 x_0 >$ | Re $< q_0 x | \hat{T} | q_0 x_0 >$ | Im $< q_0 x | \hat{T} | q_0 x_0 >$ |
|       | $x = +1.0$ | $x = 0.0$ | $x = -1.0$ | $x = +1.0$ | $x = 0.0$ | $x = -1.0$ | $x = +1.0$ | $x = 0.0$ | $x = -1.0$ |
| 44    | -6.0934081  | 0.4929036  | 0.2316417  | -1.935842  | 0.2869646  | 0.3608944  | -6.1645448  | 0.4540738  | 0.2350731  | -1.3147435  | 0.1087639  | -0.0891877  |
| 88    | -6.0928178  | 0.4917631  | 0.2339522  | -1.937208  | 0.2860977  | 0.3656473  | -6.1638597  | 0.4549345  | 0.2490815  | -1.3116644  | 0.1107539  | -0.0776850  |
| 132   | -6.0927905  | 0.4917664  | 0.2339563  | -1.937253  | 0.2860970  | 0.3656480  | -6.1638233  | 0.4549285  | 0.2491381  | -1.3116431  | 0.1107532  | -0.0776415  |
| 176   | -6.0927853  | 0.4917668  | 0.2339572  | -1.937248  | 0.2860967  | 0.3656485  | -6.1638145  | 0.4549285  | 0.2491381  | -1.3116420  | 0.1107529  | -0.0776417  |
| 220   | -6.0927834  | 0.4917670  | 0.2339575  | -1.937247  | 0.2860966  | 0.3656485  | -6.1638105  | 0.4549287  | 0.2491384  | -1.3116416  | 0.1107528  | -0.0776418  |
| 264   | -6.0927826  | 0.4917669  | 0.2339575  | -1.937246  | 0.2860966  | 0.3656485  | -6.1638097  | 0.4549285  | 0.2491384  | -1.3116413  | 0.1107528  | -0.0776417  |
| 308   | -6.0927825  | 0.4917669  | 0.2339575  | -1.937246  | 0.2860966  | 0.3656485  | -6.1638094  | 0.4549288  | 0.2491385  | -1.3116411  | 0.1107532  | -0.0776420  |
| 352   | -6.0927823  | 0.4917669  | 0.2339575  | -1.937246  | 0.2860966  | 0.3656485  | -6.1638080  | 0.4549298  | 0.2491389  | -1.3116411  | 0.1107532  | -0.0776420  |
|       | Ref. [11]  | -6.0927820  | 0.4917677  | 0.2339576  | -1.937247  | 0.2860968  | 0.3656489  | -6.1638080  | 0.4549298  | 0.2491389  | -1.3116411  | 0.1107532  | -0.0776420  |
Table 4 Convergence of the Nystrom solution of the two-variable LS equation with respect to $N_x$, the number of quadrature points in $x$-variable. Listed are the on-shell T-matrix elements $< q_0 x | T(E) | q_0 x_0 >$ with $x_0 = 1.0$ at $E = 150$ and $E = 400$ MeV for different values of $N_x$. For calculations reported in this table, the number $N_r$ of quadrature points for the $r$-variable is 352.

| $N_x$ | Re $< q_0 x | T | q_0 x_0 >$ | Im $< q_0 x | T | q_0 x_0 >$ |
|-------|-------------------------------|-------------------------------|
|       | $x=+1.0$ | $x=0.0$ | $x=-1.0$ | $x=+1.0$ | $x=0.0$ | $x=-1.0$ |
| 40    | -6.0927853 | 0.4917625 | 0.2339612 | -1.9372358 | 0.2860970 | 0.3656424 |
| 60    | -6.0927823 | 0.4917658 | 0.2339585 | -1.9372437 | 0.2860958 | 0.3656472 |
| 80    | -6.0927823 | 0.4917666 | 0.2339578 | -1.9372460 | 0.2860965 | 0.3656482 |
| 96    | -6.0927825 | 0.4917669 | 0.2339575 | -1.9372468 | 0.2860965 | 0.3656485 |
| 108   | -6.0927825 | 0.4917670 | 0.2339574 | -1.9372471 | 0.2860966 | 0.3656486 |
| 120   | -6.0927826 | 0.4917671 | 0.2339574 | -1.9372473 | 0.2860966 | 0.3656487 |
| Ref. [11] | -6.0927820 | 0.4917677 | 0.2339576 | -1.9372472 | 0.2860968 | 0.3656489 |
|       | $E = 150$ MeV | | | |
| 40    | -6.1638379 | 0.4549246 | 0.2491048 | -1.3116480 | 0.1107446 | -0.0776408 |
| 60    | -6.1638144 | 0.4549259 | 0.2491388 | -1.3116420 | 0.1107508 | -0.0776415 |
| 80    | -6.1638106 | 0.4549281 | 0.2491383 | -1.3116414 | 0.1107523 | -0.0776417 |
| 96    | -6.1638097 | 0.4549287 | 0.2491384 | -1.3116413 | 0.1107528 | -0.0776417 |
| 108   | -6.1638095 | 0.4549290 | 0.2491385 | -1.3116413 | 0.1107530 | -0.0776417 |
| 120   | -6.1638093 | 0.4549291 | 0.2491385 | -1.3116413 | 0.1107531 | -0.0776418 |
| ref. [11] | -6.1638080 | 0.4549298 | 0.2491389 | -1.3116411 | 0.1107532 | -0.0776420 |
|       | $E = 400$ MeV | | | | | |
Table 5 Comparison of two-variable Nystrom calculations with and without the singularity correction term. Listed are the on-shell T-matrix elements $\langle q_0 x | \hat{T}(E) | q_0 x_0 \rangle$ with $x_0 = 1.0$ at $E = 150$ and $E = 400$ MeV. For calculations in this table, $N_r = 176$, $N_x = 80$.

|        | $E = 150$ MeV |        | $E = 400$ MeV |
|--------|---------------|--------|---------------|
|        | Re $\langle q_0 x | \hat{T}(E) | q_0 x_0 \rangle$ |        |         |
|        | Im $\langle q_0 x | \hat{T}(E) | q_0 x_0 \rangle$ |        |         |
| $x = +1.0$ | -6.092514 0.492374 0.233732 | $x = +1.0$ | -6.166331 0.455116 0.249336 |
| $x = 0.0$  | -1.940060 0.286935 0.365925 | $x = 0.0$  | -1.313334 0.111257 -0.077629 |
| $x = -1.0$ | -1.311641 0.110753 -0.077642 | $x = -1.0$ | -1.311641 0.110753 -0.077642 |
|         | $\hat{C}$   |        |         |
| $x = +1.0$ | -6.092785 0.491767 0.233957 | $x = +1.0$ | -6.163816 0.454928 0.249138 |
| $x = 0.0$  | -1.937248 0.286097 0.365648 | $x = 0.0$  | -1.311644 0.110753 -0.077642 |
| $x = -1.0$ | -1.311641 0.110753 -0.077642 | $x = -1.0$ | -1.311641 0.110753 -0.077642 |
|         | Ref. [11]   |        |         |
| $x = +1.0$ | -6.092782 0.491768 0.233958 | $x = +1.0$ | -6.163808 0.454930 0.249139 |
| $x = 0.0$  | -1.937247 0.286097 0.365649 | $x = 0.0$  | -1.311644 0.110753 -0.077642 |
| $x = -1.0$ | -1.311641 0.110753 -0.077642 | $x = -1.0$ | -1.311641 0.110753 -0.077642 |