Solution of the Chandler-Gibson equations for a three-body test problem

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(Received 28 May 1991)

The Chandler-Gibson (CG) N-body equations are tested by considering the problem of three nonrelativistic particles moving on a line and interacting through attractive delta-function potentials. In particular, the input Born and overlap matrix-valued functions are evaluated analytically, and the CG equations are solved using a B-spline collocation method. The computed scattering matrix elements are within 0.5% of the known exact solutions, and the corresponding scattering probabilities are within 0.001% of the exact probabilities, both below and above the 3-body breakup threshold. These results establish that the CG method is practical, as well as theoretically correct, and may be a valuable approach for solving certain more complicated N-body scattering problems.

I. INTRODUCTION

Over a period of several years Chandler and Gibson (CG) have derived a theory of N-particle scattering which is very general and has many desirable mathematical properties [1, 2]. The unknowns in the equations of this theory may be either transition operators [1, 2] or $\mathcal{K}$ matrices [2, 3]. This theory has been derived with theorem-proof rigor. However, it is still necessary to test the theory by making calculations which can be compared with known results.

It does not suffice to test the CG theory using a 2-body problem, because in this case the CG transition operator equations reduce to the Lippmann-Schwinger equation [4], the CG $\mathcal{K}$-operator equations reduce to the well known 2-body $\mathcal{K}$ equation, and these equations have already been thoroughly tested over the years. On the other hand, the CG equations for a 3-body problem are different, and have unknowns which differ off-shell, from all previous 3-body equations, including the Faddeev [5] and Alt-Grassberger-Sandhas [6] equations. Therefore, a numerical solution for a 3-body test problem will provide an important test of the CG theory.

In addition, we are in the process of developing a computer program which uses B-splines to solve the CG equations for N-body scattering problems. In order to test this program, it is desirable to have a simple 3-body problem which can be solved and compared with known results. Such tests are necessary for the further development of our N-body computer program.

In this paper we consider a simple 3-body system which can be solved and compared with known results. The test problem which we consider is the nonrelativistic one-dimensional system consisting of three particles moving on a line and interacting through attractive delta function potentials. The main reason for using these potentials is that they lead to exactly solvable three-body systems [7–9], and these exact solutions may be used for comparison.

In order to illustrate the general N-body solution strategy developed in Refs. [2] and [3], we shall follow the notation given there. In particular, the on-shell scattering operator is obtained from either an on-shell $\mathcal{K}$-matrix $\mathcal{K}(E)$ or an on-shell transition matrix $\mathcal{M}(E)$. $\mathcal{K}(E)$ is the on-shell value of a half-on-shell $\mathcal{K}$ matrix $\mathcal{K}(\lambda, e)$ whose matrix elements $\mathcal{K}_{\beta j,\alpha i}(\lambda, e_\alpha)$ satisfy the following system of $\mathcal{K}$ equations [2, 3]

$$\mathcal{K}_{\beta j,\alpha i}(\lambda, e_\alpha) = \mathcal{A}_{\beta j,\alpha i}(\lambda, e_\alpha) + \sum_{\gamma k} \int_0^\infty d\eta \frac{\mathcal{A}_{\beta j,\gamma k}(\lambda, \eta)}{e_\gamma - \eta} \mathcal{K}_{\gamma k,\alpha i}(\eta, e_\alpha) \,, \tag{1.1}$$

and $\mathcal{M}(E)$ is the on-shell value of a half-on-shell transition matrix $\mathcal{M}(\lambda, e)$ whose matrix elements $\mathcal{M}_{\beta j,\alpha i}(\lambda, e_\alpha)$ satisfy the following system of $\mathcal{M}$-equations [2, 3]:

$$\mathcal{M}_{\beta j,\alpha i}(\lambda, e_\alpha) = \mathcal{A}_{\beta j,\alpha i}(\lambda, e_\alpha) + \sum_{\gamma k} \left[\int_0^\infty d\eta \frac{\mathcal{A}_{\beta j,\gamma k}(\lambda, \eta)}{e_\gamma - \eta} \mathcal{M}_{\gamma k,\alpha i}(\eta, e_\alpha) - i\pi \mathcal{A}_{\beta j,\gamma k}(\lambda, e_\gamma) \mathcal{M}_{\gamma k,\alpha i}(e_\gamma, e_\alpha) \right] . \tag{1.2}$$

In Eqs. (1.1) and (1.2) α, β, and γ are channel indices which range over the possible partition and bound states of the N particles. The subscripts i, j, and k are indices which label the basis functions for channels α, β, and γ, respectively. The threshold energy for channel α is denoted by ε_α, where $\varepsilon_\alpha \leq 0$. Also, $e_\alpha \equiv E - \varepsilon_\alpha$, the total energy minus the α-channel threshold energy, is the on-shell channel kinetic energy for any open channel α. The

integral with a bar through it denotes a Cauchy principal-value integral.

The kernel functions $\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu)$ in Eqs. (1.1) and (1.2) are of the form

$$\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu) \equiv \mathcal{B}_{\beta j,\alpha i}(\lambda,\mu) - \mathcal{C}_{\beta j,\alpha i}(\lambda,\mu)(e_\alpha - \mu) , \tag{1.3}$$

where $\mathcal{C}_{\beta j,\alpha i}(\lambda,\mu)$ are overlap integrals and $\mathcal{B}_{\beta j,\alpha i}(\lambda,\mu)$ are Born-type integrals. The matrix $\mathcal{A}(\lambda,\mu)$ with matrix elements $\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu)$ is a real-valued symmetric matrix for real-valued potentials. Since

$$\mathcal{A}_{\beta j,\alpha i}(\lambda,e_\alpha) = \mathcal{B}_{\beta j,\alpha i}(\lambda,e_\alpha) , \tag{1.4}$$

the nonhomogeneous terms in Eqs. (1.1) and (1.2) are half-on-shell Born-type integrals. One of the distinguishing features of the CG equations is the inclusion of the overlap integrals $\mathcal{C}_{\beta j,\alpha i}(\lambda,\mu)$. A second is the fact that the projections onto the channel subspaces are included in the unknowns of the equations. A third is the explicit way in which the breakup channels appear.

The general solution procedure consists of three steps [2, 3]: (1) Evaluate the kernel functions $\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu)$. (2) Solve Eq. (1.1) for the matrix elements $\mathcal{K}_{\beta j,\alpha i}(\lambda,e_\alpha)$ or Eq. (1.2) for the matrix elements $\mathcal{M}_{\beta j,\alpha i}(\lambda,e_\alpha)$. (3) Use the identities of Ref. [2] or [3] to calculate the scattering amplitude. Steps (1)–(3) are carried out in Secs. II–IV for our 3-body test problem.

In Sec. II we discuss kinematics and introduce our coordinate systems and basis functions. In Sec. III we describe the numerical solution procedure which we use to solve Eq. (1.1) or (1.2) and compute the scattering matrix. In Sec. IV we summarize the results of our calculations and compare them with the known exact solution. Our conclusions are contained in Sec. V. The paper ends with an appendix containing the detailed evaluation of the matrix elements of $\mathcal{A}(\lambda,\mu)$.

II. KINEMATICS AND COORDINATES

Let the masses of the three particles be denoted by m_1, m_2, and m_3. The possible partitions A of the particles are denoted by 0, 1, 2, 3, where 0 denotes the free partition $1+2+3$, 1 denotes the partition $1+(23)$, 2 denotes $2+(13)$, and 3 denotes $3+(12)$. Here $(\alpha\beta)$ denotes a bound state of the particles α and β. It will be shown that each partition $A = 1,2,3$ has only one bound state for the bound pair. Therefore, there is a one-to-one correspondence between partitions A and channels $\alpha \in A$, and we will use the channel indices α,β,γ to denote the partitions $0,1,2,3$.

We shall use clustered Jacobi coordinates which are defined in terms of the positions r_α and momenta π_α as follows. Let α,β,γ denote a cyclic permutation of 1, 2, 3. Then the two-cluster channel α has internal coordinate x_α and external coordinate y_α defined by

$$x_\alpha \equiv r_\gamma - r_\beta , \quad y_\alpha \equiv r_\alpha - (m_\beta r_\beta + m_\gamma r_\gamma)/(m_\beta + m_\gamma) . \tag{2.1}$$

The center-of-mass coordinate is independent of the partition α and is given by

$$y_{\text{c.m.}} \equiv (m_1 r_1 + m_2 r_2 + m_3 r_3)/m_0 , \quad m_0 \equiv m_1 + m_2 + m_3 . \tag{2.2}$$

The corresponding internal momentum p_α, external momentum q_α, and total momentum $q_{\text{c.m.}}$ are

$$\begin{aligned} p_\alpha &\equiv (m_\beta \pi_\gamma - m_\gamma \pi_\beta)/(m_\beta + m_\gamma) , \\ q_\alpha &\equiv [(m_\beta + m_\gamma)\pi_\alpha - m_\alpha(\pi_\beta + \pi_\gamma)]/m_0 , \\ q_{\text{c.m.}} &\equiv \pi_1 + \pi_2 + \pi_3 . \end{aligned} \tag{2.3}$$

The free partition 0 may be described by $(x_\alpha, y_\alpha, y_{\text{c.m.}})$ or $(p_\alpha, q_\alpha, q_{\text{c.m.}})$ for any $\alpha = 1,2,3$. The reduced mass μ_α for the pair $(\beta\gamma)$ and the reduced mass $\bar{\mu}_\alpha$ for α with respect to $(\beta\gamma)$ are

$$\mu_\alpha \equiv \frac{m_\beta m_\gamma}{m_\beta + m_\gamma} , \qquad \bar{\mu}_\alpha \equiv \frac{m_\alpha(m_\beta + m_\gamma)}{m_0} , \tag{2.4}$$

respectively, where α,β,γ denote a cyclic permutation of 1,2,3.

The natural Hilbert space for three particles in one dimension is $\mathcal{L}^2(\mathbf{R}^3)$. After removing the center of mass motion, the Hilbert space of interest is $\mathcal{H}_N \equiv \mathcal{L}^2(\mathbf{R}^2)$, which may be identified with $\mathcal{L}^2(\mathbf{R}) \otimes \mathcal{L}^2(\mathbf{R})$. The free Hamiltonian H_0 is defined by multiplication by

$$T_0(p_\alpha, q_\alpha) \equiv \frac{p_\alpha^2}{2\mu_\alpha} + \frac{q_\alpha^2}{2\bar{\mu}_\alpha} . \tag{2.5}$$

H_0 is a self-adjoint operator on its domain $\mathcal{D}(H_0) \subset \mathcal{H}_N$.

Let V_α denote the potential for the two-body interaction of particles β and γ. In order to simplify the calculations and compare with known results [7], we define these potentials to be multiplication by the distributions

$$V_\alpha(x_\alpha) \equiv -g_\alpha \delta(x_\alpha) , \tag{2.6}$$

$\alpha = 1,2,3$, where g_α are strength constants and $\delta(\cdot)$ is the Dirac delta function. The total Hamiltonian H_N, defined on its domain in $\mathcal{H}_N$, is of the form

$$H_N = H_0 + \bar{V}_0 \equiv H_0 + (V_1 + V_2 + V_3) . \tag{2.7}$$

The operator H_N is well defined and self-adjoint as a sum of quadratic forms. For each partition α, $\alpha = 1,2,3$, the total Hamiltonian H_N decomposes as

$$H_N = \hat{H}_\alpha + H_\alpha^0 + \bar{V}_\alpha \equiv \left(\frac{p_\alpha^2}{2\mu_\alpha} + V_\alpha\right) + \left(\frac{q_\alpha^2}{2\bar{\mu}_\alpha}\right) + (V_\beta + V_\gamma) . \tag{2.8}$$

The unique solution for $\alpha = 1,2,3$ of the eigenvalue problem

$$\hat{H}_\alpha \phi_\alpha = \varepsilon_\alpha \phi_\alpha \tag{2.9}$$

is easily computed to be

$$\varepsilon_\alpha = -\frac{1}{2}\mu_\alpha g_\alpha^2 , \tag{2.10}$$

with normalized eigenvector $\hat{\phi}_\alpha$ given in coordinate space by

$$\hat{\phi}_\alpha(x_\alpha) = \sqrt{a_\alpha} e^{-a_\alpha |x_\alpha|} , \tag{2.11}$$

and in momentum space by

$$\hat{\phi}_\alpha(p_\alpha) = \frac{(2/\pi)^{1/2}(a_\alpha)^{3/2}}{p_\alpha^2 + a_\alpha^2} , \tag{2.12}$$

where $a_\alpha \equiv \mu_\alpha g_\alpha$.

The transformation from one set of Jacobi momenta (p_α, q_α) to those for a second set (p_β, q_β) is given by [10]

$$p_\beta = -\frac{\mu_\beta}{m_\gamma} p_\alpha + \epsilon_{\alpha\beta} \frac{\mu_\alpha}{\bar{\mu}_\beta} q_\alpha , \quad q_\beta = -\epsilon_{\alpha\beta} p_\alpha - \frac{\mu_\alpha}{m_\gamma} q_\alpha , \tag{2.13}$$

where

$$\epsilon_{\alpha\beta} \equiv \begin{cases} +1 \text{ if } \alpha\beta \text{ is in cyclic order,} \\ -1 \text{ if } \alpha\beta \text{ is not in cyclic order.} \end{cases} \tag{2.14}$$

In other words, $\epsilon_{\alpha\beta}$ is $+1$ for $(\alpha\beta)$ equal to (12), (23), and (31), and -1 for (13), (21), and (32). The Jacobian of the transformation is equal to one.

For each partition $\alpha = 0, 1, 2, 3$ we use kinetic energy hyperspherical (KEHS) coordinates [2]. Suppose α denotes one of the two-cluster partitions 1, 2, or 3. Let $k_\alpha \equiv q_\alpha / \sqrt{2\bar{\mu}_\alpha}$ and decompose k_α as $k_\alpha = \hat{k}_\alpha |k_\alpha|$, where $\hat{k}_\alpha \equiv k_\alpha / |k_\alpha| = \operatorname{sgn} k_\alpha$. Letting $\mu \equiv |k_\alpha|^2$ denote the input kinetic energy, we have

$$q_\alpha = \hat{k}_\alpha \sqrt{2\bar{\mu}_\alpha \mu} . \tag{2.15}$$

The Jacobian $\nu_\alpha^2(\mu)$ of the transformation from q_α to the $(\hat{k}_\alpha, \mu)$ coordinates is (Ref. [2], Lemma 3.1)

$$\nu_\alpha^2(\mu) \equiv \sqrt{\frac{\bar{\mu}_\alpha}{2\mu}} . \tag{2.16}$$

In this case, the surface of the unit kinetic energy hypersphere is zero-dimensional with $\hat{k}_\alpha = \pm 1$. Since $\hat{k}_\alpha$ assume only the values $+1$ and -1, we define the "basis functions"

$$\chi_{\alpha+}(\hat{k}_\alpha) \equiv \delta(\hat{k}_\alpha - 1) , \quad \chi_{\alpha-}(\hat{k}_\alpha) \equiv \delta(\hat{k}_\alpha + 1) , \tag{2.17}$$

where $\delta(\cdot)$ is the Dirac delta function.

Now consider the breakup partition 0. For external coordinates we may use (p_α, q_α) for any $\alpha = 1, 2, 3$. If μ denotes the input kinetic energy, then

$$\mu = \frac{p_\alpha^2}{2\mu_\alpha} + \frac{q_\alpha^2}{2\bar{\mu}_\alpha} . \tag{2.18}$$

Letting

$$p_\alpha = \sqrt{2\mu_\alpha \mu} \sin\theta_\alpha , \quad q_\alpha = \sqrt{2\bar{\mu}_\alpha \mu} \cos\theta_\alpha , \tag{2.19}$$

with $-\pi < \theta_\alpha \leq \pi$, we obtain new KEHS coordinates (θ_α, μ) for any $\alpha = 1, 2, 3$. In this case the surface of the unit kinetic energy hypersphere is one-dimensional and may be parameterized by θ_α for any $\alpha = 1, 2, 3$. However, it is undesirable to have three different angles θ_α describing the same three-cluster partition 0. Therefore, let us fix α and suppose $\beta \neq \alpha$. The following well known lemma shows that $\theta_\beta - \theta_\alpha$ is a constant. We include its proof for completeness.

Lemma 1.—If α, β, γ is any permutation of 1, 2, 3, then the angles θ_α and θ_β are related by

$$\theta_\beta = \theta_\alpha + \tau_{\beta\alpha} , \tag{2.20}$$

where $\tau_{\beta\alpha}$ is defined by

$$\cos\tau_{\beta\alpha} \equiv -\sqrt{\frac{m_\alpha m_\beta}{(m_\alpha + m_\gamma)(m_\beta + m_\gamma)}} , \qquad \sin\tau_{\beta\alpha} \equiv \epsilon_{\alpha\beta} \sqrt{\frac{m_\gamma m_0}{(m_\alpha + m_\gamma)(m_\beta + m_\gamma)}} , \tag{2.21}$$

and $\epsilon_{\alpha\beta}$ is defined in Eq. (2.14).

Proof.—Substituting Eqs. (2.19) into the first of Eqs. (2.13) gives

$$\sqrt{2\mu_\beta \mu} \sin\theta_\beta = -\frac{\mu_\beta}{m_\gamma} \sqrt{2\mu_\alpha \mu} \sin\theta_\alpha + \epsilon_{\alpha\beta} \frac{\mu_\alpha}{\bar{\mu}_\beta} \sqrt{2\bar{\mu}_\alpha \mu} \cos\theta_\alpha . \tag{2.22}$$

Hence,

$$\begin{aligned} \sin\theta_\beta &= -m_\gamma^{-1} \sqrt{\mu_\alpha \mu_\beta} \sin\theta_\alpha + \epsilon_{\alpha\beta} \mu_\alpha \bar{\mu}_\beta^{-1} \sqrt{\bar{\mu}_\alpha \mu_\beta^{-1}} \cos\theta_\alpha \\ &= \cos\tau_{\beta\alpha} \sin\theta_\alpha + \sin\tau_{\beta\alpha} \cos\theta_\alpha \\ &= \sin(\theta_\alpha + \tau_{\beta\alpha}) , \end{aligned} \tag{2.23}$$

where the definitions in Eqs. (2.4) have been used, and $\cos\tau_{\beta\alpha}$ and $\sin\tau_{\beta\alpha}$ are defined in Eqs. (2.21). Similarly, the second of Eqs. (2.13) yields

$$\begin{aligned} \cos\theta_\beta &= -\epsilon_{\alpha\beta} \sqrt{\mu_\alpha \bar{\mu}_\beta^{-1}} \sin\theta_\alpha - \mu_\alpha m_\gamma^{-1} \sqrt{\bar{\mu}_\alpha \bar{\mu}_\beta^{-1}} \cos\theta_\alpha \\ &= -\sin\tau_{\beta\alpha} \sin\theta_\alpha + \cos\tau_{\beta\alpha} \cos\theta_\alpha \\ &= \cos(\theta_\alpha + \tau_{\beta\alpha}) . \end{aligned} \tag{2.24}$$

This proves the lemma.

Corollary 1.—The constant angles $\tau_{\beta\alpha}$, with $\beta \neq \alpha$, are in the interval $\pi/2 < \tau_{\beta\alpha} < 3\pi/2$, and they are given by

$$\tau_{\beta\alpha} = \tan^{-1}\left(-\epsilon_{\alpha\beta} \sqrt{\frac{m_\gamma m_0}{m_\alpha m_\beta}} \right) . \tag{2.25}$$

The angle $\tau_{\alpha\alpha}$ is equal to zero.

In order to be definite, we will use (p_1, q_1) for the external coordinates in the breakup partition 0. Let $\theta \equiv \theta_1$, with $-\pi < \theta \leq \pi$, and let

$$\mathbf{k}_0 = |\mathbf{k}_0| \hat{k}_0 \equiv \sqrt{\mu}(\sin\theta, \cos\theta) = \left(\frac{p_1}{\sqrt{2\mu_1}}, \frac{q_1}{\sqrt{2\bar{\mu}_1}} \right) . \tag{2.26}$$

The next lemma establishes useful formulas for transforming from the (p_α, q_α) momenta to the (θ, μ) KEHS coordinates.

Lemma 2.—Let $\theta \equiv \theta_1$, and let $\tau_{\alpha 1}$ be defined as in Corollary 1, for $\alpha = 1, 2, 3$. The following identities are then valid for $\alpha = 1, 2, 3$:

$$\begin{aligned} p_\alpha &= \sqrt{2\mu_\alpha \mu} \sin\theta_\alpha = \sqrt{2\mu_\alpha \mu} \sin(\theta + \tau_{\alpha 1}) \\ &= \sqrt{2\mu_\alpha \mu} \cos\tau_{\alpha 1} \sin\theta + \sqrt{2\mu_\alpha \mu} \sin\tau_{\alpha 1} \cos\theta , \end{aligned} \tag{2.27}$$

and

$$q_\alpha = \sqrt{2\bar{\mu}_\alpha \mu}\cos\theta_\alpha = \sqrt{2\bar{\mu}_\alpha \mu}\cos(\theta + \tau_{\alpha 1}) = -\sqrt{2\bar{\mu}_\alpha \mu}\sin\tau_{\alpha 1}\sin\theta + \sqrt{2\bar{\mu}_\alpha \mu}\cos\tau_{\alpha 1}\cos\theta \ . \tag{2.28}$$

Furthermore, the Jacobian of the transformation from (p_α, q_α) to the KEHS coordinates (θ, μ) is given by $\nu_0^2(\mu)$, for any $\alpha = 1,2,3$, where

$$\nu_0^2(\mu) \equiv \sqrt{\mu_0 \bar{\mu}_0} = \sqrt{m_1 m_2 m_3 / m_0} \ . \tag{2.29}$$

Proof.—The identities in Eqs. (2.27) and (2.28) follow immediately from Eqs. (2.19), (2.20), (2.23), and (2.24). Eqs. (2.27) and (2.28) directly yield Eq. (2.29).

As a basis set $\{\chi_{0m}\}, m = 0, \pm 1, \pm 2, \ldots$, on the one-dimensional surface of the unit hypersphere (circle) we choose the orthonormal Fourier series basis functions defined by

$$\chi_{00}(\theta) \equiv \frac{1}{\sqrt{2\pi}} \ , \ \chi_{0m}(\theta) \equiv \frac{1}{\sqrt{\pi}}\cos m\theta \ , \quad \chi_{0(-m)}(\theta) \equiv \frac{1}{\sqrt{\pi}}\sin m\theta \ , \tag{2.30}$$

for $-\pi < \theta \leq \pi$, and $m = 1, 2, \ldots$.

III. NUMERICAL SOLUTION PROCEDURE

A. Computational form of the $\mathcal{K}$ and $\mathcal{M}$ equations

The input terms $\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu)$ in Eqs. (1.1) and (1.2) contain the Jacobians $\nu_\beta(\lambda)$ and $\nu_\alpha(\mu)$. These factors may be singular, and the computational characteristics of either of these equations may be improved by removing these factors [3, 11]. Therefore, we multiply Eqs. (1.1) and (1.2) on the left by $\nu_\beta^{-1}(\lambda)$ and on the right by $\nu_\alpha^{-1}(e_\alpha)$, where $e_\alpha \equiv E - \varepsilon_\alpha$ is the on-shell value of the input channel kinetic energy. Letting

$$\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu) \equiv \nu_\beta^{-1}(\lambda)\mathcal{A}_{\beta j,\alpha i}(\lambda,\mu)\nu_\alpha^{-1}(\mu) \ , \tag{3.1}$$

and analogously defining $\widetilde{\mathcal{K}}_{\beta j,\alpha i}(\lambda,\mu)$ and $\widetilde{\mathcal{M}}_{\beta j,\alpha i}(\lambda,\mu)$, the system of equations in Eq. (1.1) becomes the following system of $\widetilde{\mathcal{K}}$ equations,

$$\widetilde{\mathcal{K}}_{\beta j,\alpha i}(\lambda, e_\alpha) = \widetilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda, e_\alpha) + \sum_{\gamma k} \int_0^\infty d\eta \frac{\widetilde{\mathcal{A}}_{\beta j,\gamma k}(\lambda,\eta)}{e_\gamma - \eta}\nu_\gamma^2(\eta)\widetilde{\mathcal{K}}_{\gamma k,\alpha i}(\eta, e_\alpha) \ , \tag{3.2}$$

and the system of equations in Eq. (1.2) becomes the following system of $\widetilde{\mathcal{M}}$ equations,

$$\widetilde{\mathcal{M}}_{\beta j,\alpha i}(\lambda, e_\alpha) = \widetilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda, e_\alpha) + \sum_{\gamma k}\left[\int_0^\infty d\eta \frac{\widetilde{\mathcal{A}}_{\beta j,\gamma k}(\lambda,\eta)}{e_\gamma - \eta}\nu_\gamma^2(\eta)\widetilde{\mathcal{M}}_{\gamma k,\alpha i}(\eta, e_\alpha) - i\pi\widetilde{\mathcal{A}}_{\beta j,\gamma k}(\lambda, e_\gamma)\nu_\gamma^2(e_\gamma)\widetilde{\mathcal{M}}_{\gamma k,\alpha i}(e_\gamma, e_\alpha)\right] \ . \tag{3.3}$$

Specific formulas for the input terms $\widetilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda,\mu)$ in Eqs. (3.2) and (3.3) are given in Appendix A and in Sec. III C.

In Eqs. (1.1), (1.2), (3.2), and (3.3) λ and η are the kinetic energy variables of channels β and γ, respectively. We remark that we could alternatively use the momentum variables $k_\alpha = \sqrt{e_\alpha}$, $k = \sqrt{\lambda}$, and $k' = \sqrt{\eta}$. The resulting equations are equivalent and have the same computational features as the corresponding Eq. (3.2) or (3.3) [3, 11]. The choice is a matter of personal preference. We emphasize, however, that it is the on-shell $\mathcal{K}(E)$ matrix with matrix elements $\mathcal{K}_{\beta j,\alpha i}(e_\beta, e_\alpha)$ that is related to the scattering matrix $\mathcal{S}(E)$ by Cayley transformation [3].

B. Constants

In order to compare our results with a known exact solution [7], we set the masses m_α of all three particles equal to unity,

$$m_1 = m_2 = m_3 = 1 \ , \tag{3.4}$$

and we set the potential strength constants g_α equal to a common constant value g (usually taken to be 3),

$$g_1 = g_2 = g_3 = g \ . \tag{3.5}$$

It follows that $m_0 = 3$, and for all $\alpha = 1,2,3$,

$$\mu_\alpha = \frac{1}{2} \ , \quad \bar{\mu}_\alpha = \frac{2}{3} \ , \tag{3.6}$$

$$\varepsilon_\alpha = -\frac{g^2}{4} \ , \quad a_\alpha = \frac{g}{2} \ . \tag{3.7}$$

The Jacobians are

$$\nu_0^2(\mu) = \frac{1}{\sqrt{3}} \ , \quad \nu_\alpha^2(\mu) = \frac{1}{\sqrt{3\mu}} \tag{3.8}$$

for $\alpha = 1,2,3$. The first equation in Eq. (2.21) gives

$$\cos\tau_{\beta\alpha} = -\frac{1}{2} \ , \tag{3.9}$$

for all $\alpha \neq \beta$, and by Corollary 1 of Lemma 1, the constant angles $\tau_{\alpha 1}$ are

$$\tau_{11} = 0 \ , \quad \tau_{21} = \frac{2\pi}{3} \ , \quad \text{and} \quad \tau_{31} = \frac{4\pi}{3} \ . \tag{3.10}$$

We will need the constants $\xi_{m\alpha}$ defined by

$$\xi_{m\alpha} \equiv \begin{cases} \sqrt{2}/2 \ , & \text{for } m = 0 \\ \cos m\tau_{\alpha 1} \ , & \text{for } m > 0 \\ \sin m\tau_{\alpha 1} \ , & \text{for } m < 0 \end{cases} \ , \tag{3.11}$$

with $\tau_{\alpha 1}$ defined by Eq. (3.10) for $\alpha = 1,2,3$. We will also need the constants $b_{m\alpha}$ defined for $\alpha = 1,2,3$, and $m = 0, \pm 1, \pm 2, \ldots$, by

$$b_{m\alpha} \equiv \sum_{\beta \neq \alpha, 0} \xi_{m\beta} \ . \tag{3.12}$$

The constants $\xi_{m\alpha}$ and $b_{m\alpha}$ are of two types, depending on whether or not m is an integer multiple of 3. Let $\mathbf{I}$ denote the set of all integers. Let $\mathbf{I}_3$ denote the subset of the integers which are multiples of 3, i.e., $\mathbf{I}_3 \equiv \{0, \pm 3, \pm 6, \ldots\}$, and let $\mathbf{I}'_3 \equiv \mathbf{I} \setminus \mathbf{I}_3$ denote the remaining integers. Then for $m \in \mathbf{I}_3$,

$$\xi_{m\alpha} = \frac{b_{m\alpha}}{2} = \begin{cases} \sqrt{2}/2 \ , & \text{for } m = 0 \\ 1 \ , & \text{for } m > 0 \\ 0 \ , & \text{for } m < 0 \end{cases} \tag{3.13}$$

for all $\alpha = 1,2,3$. On the other hand, for $m \in \mathbf{I}'_3$,

$$\xi_{m\alpha} = -b_{m\alpha} = \begin{cases} 1 \ , & \text{for } m > 0 \text{ and } \alpha = 1 \\ -\frac{1}{2} \ , & \text{for } m > 0 \text{ and } \alpha = 2,3 \\ 0 \ , & \text{for } m < 0 \text{ and } \alpha = 1 \\ \pm\frac{\sqrt{3}}{2} \ , & \text{for } m < 0 \text{ and } \alpha = 2 \\ \mp\frac{\sqrt{3}}{2} \ , & \text{for } m < 0 \text{ and } \alpha = 3. \end{cases} \tag{3.14}$$

When $m < 0$ and $\alpha = 2$, the sign of $\xi_{m\alpha}$ in Eq. (3.14) is plus for $m = 1 + 3\bar{m}$ and minus for $m = 2 + 3\bar{m}$, with $\bar{m} \in \mathbf{I}_3$. The sign of $\xi_{m\alpha}$ for $m < 0$ and $\alpha = 3$ is always the negative of the sign for $\alpha = 2$.

C. Kernel functions

General formulas for the kernel functions $\tilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda,\mu)$ are derived in Appendix A. When the constants are chosen as in Sec. III–B, these general formulas simplify. The simplified formulas for the matrix elements of $\tilde{\mathcal{A}}(\lambda,\mu)$ are the following. Eqs. (A1), (A15), and (A25) yield

$$\tilde{\mathcal{A}}_{\alpha+,\alpha\pm}(\lambda,\mu) = \tilde{\mathcal{A}}_{\alpha-,\alpha\mp}(\lambda,\mu) = \frac{-3g^3/\pi}{(\sqrt{\lambda} \mp \sqrt{\mu})^2 + 3g^2} \ , \tag{3.15}$$

for all $\alpha \neq 0$. In Eq. (3.15) and the following, all equations written with a choice of + or − signs are to be read with either all upper signs or all lower signs. Using Eqs. (A1), (A8), and (A23), we obtain

$$\begin{aligned} \tilde{\mathcal{A}}_{\beta+,\alpha\pm}(\lambda,\mu) &= \tilde{\mathcal{A}}_{\beta-,\alpha\mp}(\lambda,\mu) \\ &= \frac{-3g^3}{4\pi}\left[\frac{1}{4\lambda+\mu\pm4\sqrt{\lambda\mu}+3g^2/4} + \frac{2}{\lambda+\mu\mp2\sqrt{\lambda\mu}+3g^2}\right] \\ &\quad - \frac{9g^3(4\pi)^{-1}(e_\alpha-\mu)}{(\lambda+4\mu\pm4\sqrt{\lambda\mu}+3g^2/4)(4\lambda+\mu\pm4\sqrt{\lambda\mu}+3g^2/4)} \ , \end{aligned} \tag{3.16}$$

for all α and β satisfying $0 \neq \beta \neq \alpha \neq 0$. Eqs. (A1), (A13), and (A29) give

$$\begin{aligned} \tilde{\mathcal{A}}_{0m,\alpha\pm}(\lambda,\mu) &= -\frac{3g^{5/2}b_{m\alpha}}{2\pi^2}\int_0^\pi d\theta \frac{\cos m\theta}{(2\sqrt{\lambda}\cos\theta \pm \sqrt{\mu})^2 + 3g^2/4} \\ &\quad + \left\{ \begin{array}{l} \dfrac{-\sqrt{3}g^{3/2}\xi_{m\alpha}\cos(m\cos^{-1}\pm\sqrt{\mu/\lambda})(e_\alpha-\mu)}{2\pi\sqrt{\lambda-\mu}(\lambda-\mu+g^2/4)}, \quad \text{for } \lambda > \mu \\ 0, \quad \text{for } \lambda < \mu \end{array} \right\} \\ &\equiv \tilde{\mathcal{A}}'_{0m,\alpha\pm}(\lambda,\mu) + \tilde{\mathcal{A}}''_{0m,\alpha\pm}(\lambda,\mu) \ , \end{aligned} \tag{3.17}$$

for $\alpha = 1,2,3$, and $m = 0, \pm 1, \pm 2, \ldots$, where $\tilde{\mathcal{A}}'_{0m,\alpha\pm}(\lambda,\mu)$ is the integral term and $\tilde{\mathcal{A}}''_{0m,\alpha\pm}(\lambda,\mu)$ is the term in braces in Eq. (3.17). Since $\tilde{\mathcal{A}}(\lambda,\mu)$ is a real-symmetric matrix, we may set

$$\tilde{\mathcal{A}}_{\beta\pm,0m}(\lambda,\mu) = \tilde{\mathcal{A}}_{0m,\beta\pm}(\mu,\lambda) \ , \tag{3.18}$$

and use Eq. (3.17) to evaluate the right-hand side of Eq. (3.18), for $\beta = 1,2,3$, and $m = 0, \pm 1, \pm 2, \ldots$. Finally, Eqs. (A37)–(A39) yield

$$\tilde{\mathcal{A}}_{0n,0m}(\lambda,\mu) = \begin{cases} c_{mn}\displaystyle\int_0^\pi d\theta \frac{\cos\left(n\cos^{-1}[\sqrt{(\mu/\lambda)}\cos\theta]\right)\cos m\theta}{\sqrt{\lambda-\mu\cos^2\theta}} \ , & \text{for } \lambda > \mu \\ c_{mn}\displaystyle\int_0^\pi d\theta \frac{\cos\left(m\cos^{-1}[\sqrt{(\lambda/\mu)}\cos\theta]\right)\cos n\theta}{\sqrt{\mu-\lambda\cos^2\theta}} \ , & \text{for } \lambda < \mu \end{cases} \ , \tag{3.19}$$

where

$$c_{mn} \equiv -\frac{\sqrt{3}g}{\pi^2}\sum_{\alpha=1}^{3}\xi_{m\alpha}\xi_{n\alpha} , \tag{3.20}$$

and $m,n = 0,\pm1,\pm2,\ldots$.

D. Symmetrization simplifications

A consequence of setting the masses and potential strengths of all three particles equal to the common values 1 and g, respectively, is that the particles become indistinguishable. In this case the approximate system of equations in Eqs. (1.1), (1.2), (3.2), and (3.3) may have some symmetries which allow certain simplifications. In particular, if an approximation does not have any breakup term, or has only breakup basis functions with $m \in \mathbf{I}_3$, then a simplification is possible. In fact, our numerical results show that only $m \in \mathbf{I}_3$ give nonzero contributions, but we do not yet have an analytical proof. We present the symmetrization simplifications only for Eq. (3.2), however, the analogous steps may also be applied to Eqs. (1.1), (1.2), and (3.3).

Suppose an approximation is made using only breakup basis functions $\chi_{0m}(\theta)$ with $m \in \mathbf{I}_3$. The symmetrization procedure of Refs. [12] and [13] may then be applied to combine the β=1, 2, and 3 channels. In particular, let a or $b = 0$ denote channel 0. Let $b = 1$ denote the equivalence class $\{1,2,3\}$, and let $a = 1$ denote the particular choice $\alpha = 1$ from the equivalence class $\{1,2,3\}$. Define

$$\widehat{\mathcal{K}}_{bj,ai}(\lambda,e_a) \equiv \begin{cases} \widetilde{\mathcal{K}}_{bj,ai}(\lambda,e_a), & \text{for } b=0 \\ \sum_{\beta=1}^{3}\widetilde{\mathcal{K}}_{\beta j,ai}(\lambda,e_a), & \text{for } b=1 \end{cases} \tag{3.21}$$

and

$$\widehat{\mathcal{A}}_{bj,ai}(\lambda,\mu) \equiv \begin{cases} \widetilde{\mathcal{A}}_{bj,ai}(\lambda,\mu), & \text{for } b=0 \\ \sum_{\beta=1}^{3}\widetilde{\mathcal{A}}_{\beta j,ai}(\lambda,\mu), & \text{for } b=1 \end{cases} \tag{3.22}$$

for $a,b = 0$ and 1. We note that Eqs. (3.13), and (3.17) imply that $\widetilde{\mathcal{A}}_{0m,\gamma\pm}(\lambda,\eta)$ does not depend on γ for $\gamma = 1,2,3$, and, therefore, the sum over $\gamma = 1,2,3$ in Eq. (3.2) may be moved to the right of these terms when $\beta = 0$. It follows that the summation of Eq. (3.2) over $\beta = 1,2,3$ gives

$$\widehat{\mathcal{K}}_{bj,ai}(\lambda,e_a) = \widehat{\mathcal{A}}_{bj,ai}(\lambda,e_a) + \sum_{ck}\int_0^\infty d\eta \frac{\widehat{\mathcal{A}}_{bj,ck}(\lambda,\eta)}{e_c-\eta} \times \nu_c^2(\eta)\widehat{\mathcal{K}}_{ck,ai}(\eta,e_a) , \tag{3.23}$$

where the channel indices a,b, and c now range over only the values 0 and 1. We remark that Eq. (3.23) is also valid if an approximation has no breakup term so that $a = b = c = 1$ is the only channel.

An additional simplification of Eq. (3.23) is possible if an approximation either has only the $m = 0$ breakup term or no breakup term. In these cases, the + and − basis functions may be decoupled in a manner that is similar to the decoupling used by Dodd in the 1984 Ref. [7].

E. *B*-spline solution method

In our numerical solution of Eq. (3.2), Eq. (3.3), or one of the symmetrized equations in Sec. III D, we have used the cubic B-spline collocation method described in Ref. [3]. The B-spline knots and collocation points were chosen on the interval $[-1,1]$ and then mapped to $[0,\infty)$ by the mapping

$$\lambda = \lambda(x) \equiv e_\alpha\left(\frac{1+x}{1-x}\right)^2 . \tag{3.24}$$

In particular, $\hat{n}$ knots $x_{\hat{j}}$, $\hat{j} = 1,2,\ldots,\hat{n}$, together with the extended knots x_{-2},x_{-1},x_0, and $x_{\hat{n}+1},x_{\hat{n}+2},x_{\hat{n}+3}$, were chosen in $[-1,1]$ in the following manner. $\hat{n}-4$ interior knots were chosen to be the Chebyshev points

$$x_{\hat{j}+3} \equiv -\cos\left[\frac{(2\hat{j}-1)\pi}{2(\hat{n}-4)}\right] , \tag{3.25}$$

for $\hat{j} = 1,2,\ldots,\hat{n}-4$. The four knots x_{-2},x_{-1},x_0,x_1 were all chosen at -1, and two extra knots, x_2 and x_3, were chosen to be evenly spaced between x_1 and x_4. The remaining knots were chosen to be $x_{\hat{n}+\hat{k}-1} \equiv x_{\hat{n}+\hat{k}-2} + (1-x_{\hat{n}+\hat{k}-2})/2^{\hat{k}}$, for $\hat{k} = 1,2,3$, and $x_{\hat{n}+3} \equiv 1$. The $\hat{n}+2$ collocation points $\bar{x}_{\hat{j}}$ were taken to be $\bar{x}_{\hat{j}} \equiv x_{\hat{j}}$, $\hat{j} = 2,3,\ldots,\hat{n}+1$, $\bar{x}_1 \equiv -1+(x_2+1)/2$, and $\bar{x}_0 = -1+(\bar{x}_1+1)/2$. Using the mapping of Eq. (3.24), we then defined $\lambda_{\hat{j}} \equiv \lambda(x_{\hat{j}})$, for $\hat{j} = -2,-1,0,\ldots,\hat{n}+3$, and $\bar{\lambda}_{\hat{j}} \equiv \lambda(\bar{x}_{\hat{j}})$, for $\hat{j} = 0,1,\ldots,\hat{n}+1$. By choosing an even number $\hat{n}$ of knots we enforced that $\bar{\lambda}_{\hat{j}} \neq e_\alpha$. In order to also assure that $\bar{\lambda}_{\hat{j}} \neq e_\gamma$ for $\gamma \neq \alpha$, we slightly moved any $\bar{\lambda}_{\hat{j}}$ that equals e_γ for some $\gamma \neq \alpha$.

Letting $b_{\hat{j}}(\lambda)$, $\hat{j} = 0,1,\ldots,\hat{n}+1$, denote the resulting $\hat{n}+2$ cubic B splines on $[0,\infty)$, we expanded the unknown $\widetilde{\mathcal{K}}$- or $\widetilde{\mathcal{M}}$-matrix elements by a sum of the form $\sum_{\hat{j}=0}^{\hat{n}+1} c_{\beta\hat{j}\hat{j}}b_{\hat{j}}(\lambda)$. The collocation method then yielded a system of algebraic equations which were solved for the coefficients $c_{\beta\hat{j}\hat{j}}$.

F. Regularization of singularities

The B-spline collocation method [3] requires the numerical evaluation of the integrals in Eq. (3.2) or (3.3). We write these integrals as a sum from $\hat{\ell} = -2$ to $\hat{\ell} = \hat{n}+2$ of the integrals

$$I^{\hat{n}\hat{k}\hat{\ell}}_{\beta\hat{j},\gamma k}(\bar{\lambda}_{\hat{j}}) \equiv \int_{\lambda_{\hat{\ell}}}^{\lambda_{\hat{\ell}+1}} d\eta \frac{\widetilde{\mathcal{A}}_{\beta j,\gamma k}(\bar{\lambda}_{\hat{j}},\eta)}{e_\gamma-\eta}\nu_\gamma^2(\eta)b_{\hat{k}}(\eta) . \tag{3.26}$$

In addition, if both $\bar{\lambda}_{\hat{j}}$ and e_γ belong to $[\bar{\lambda}_{\hat{\ell}},\bar{\lambda}_{\hat{\ell}+1}]$, then we further subdivide $[\bar{\lambda}_{\hat{\ell}},\bar{\lambda}_{\hat{\ell}+1}]$ into two subintervals by choosing a point $\bar{\lambda}'_{\hat{\ell}}$ halfway between $\bar{\lambda}_{\hat{j}}$ and e_γ. Each subinterval then contains at most one singular point. The

integrals that do not contain a singular point in the interval of integration were evaluated by Gauss-Legendre quadrature using 32 quadrature points.

The integrals in Eq. (3.26) containing singular integrands were evaluated using singularity subtraction [14]. In particular, when $\lambda_{\hat{\ell}} < e_\gamma < \lambda_{\hat{\ell}+1}$, there is a Cauchy singularity at $\eta = e_\gamma$, and the integral $I^{\hat{n}\hat{k}\hat{\ell}}_{\beta\hat{j},\gamma k}(\bar{\lambda}_j)$ was evaluated using the singularity subtraction Eq. (4.19) of Ref. [3]. The singularity in Eq. (3.26) at $\eta = 0$ arising from the Jacobian $\nu_\alpha(\mu)$ in Eq. (3.8), and the singularity at $\eta = \bar{\lambda}_j$ arising from the input terms in Eqs. (3.17)–(3.19) were also regularized by singularity subtraction. The regularized integrals were then approximated by a Gauss-Legendre quadrature rule using 32 quadrature points.

As one example of the singularity subtraction method, consider the integral $I^{\hat{n}\hat{k}\hat{\ell}}_{\alpha\pm,0m}(\bar{\lambda}_j)$. When $\bar{\lambda}_j \in [\lambda_{\hat{\ell}}, \lambda_{\hat{\ell}+1}]$ (but $e_0 = E$ does not lie in $[\lambda_{\hat{\ell}}, \lambda_{\hat{\ell}+1}]$), the term $\tilde{\mathcal{A}}'_{\alpha\pm,0m}(\bar{\lambda}_j, \eta)$ defined in Eqs. (3.17) and (3.18) is regular at $\eta = \bar{\lambda}_j$, but the term $\tilde{\mathcal{A}}''_{\alpha\pm,0m}(\bar{\lambda}_j, \eta)$ is singular at $\eta = \bar{\lambda}_j$ due to the factor $(\eta - \bar{\lambda}_j)^{-1/2}$. Therefore, we have evaluated the integral using the singularity subtraction formula

$$\sqrt{3} I^{\hat{n}\hat{k}\hat{\ell}}_{\alpha\pm,0m}(\bar{\lambda}_j) = \int_{\lambda_{\hat{\ell}}}^{\lambda_{\hat{\ell}+1}} d\eta \frac{\tilde{\mathcal{A}}'_{\alpha\pm,0m}(\bar{\lambda}_j, \eta) b_{\hat{k}}(\eta)}{e_0 - \eta} + \int_{\bar{\lambda}_j}^{\lambda_{\hat{\ell}+1}} d\eta \frac{\tilde{\mathcal{A}}'''_{\alpha\pm,0m}(\bar{\lambda}_j, \eta)(e_0 - \eta)^{-1} b_{\hat{k}}(\eta) - \tilde{\mathcal{A}}'''_{\alpha\pm,0m}(\bar{\lambda}_j, \bar{\lambda}_j)(e_0 - \bar{\lambda}_j)^{-1} b_{\hat{k}}(\bar{\lambda}_j)}{\sqrt{\eta - \bar{\lambda}_j}} + 2\sqrt{\lambda_{\hat{\ell}+1} - \bar{\lambda}_j}\, \tilde{\mathcal{A}}'''_{\alpha\pm,0m}(\bar{\lambda}_j, \bar{\lambda}_j)(e_0 - \bar{\lambda}_j)^{-1} b_{\hat{k}}(\bar{\lambda}_j) , \tag{3.27}$$

where

$$\tilde{\mathcal{A}}'''_{\alpha\pm,0m}(\bar{\lambda}_j, \eta) \equiv \sqrt{\eta - \bar{\lambda}_j}\, \tilde{\mathcal{A}}''_{\alpha\pm,0m}(\bar{\lambda}_j, \eta) . \tag{3.28}$$

As a second example, consider the integral $I^{\hat{n}\hat{k}\hat{\ell}}_{0n,0m}(\bar{\lambda}_j)$, which requires some special consideration. This integral has a logarithmic singularity at $\eta = \bar{\lambda}_j$. Division by $\ln|\bar{\lambda}_j - \eta|$ would remove this singularity, but may introduce new singularities when $|\bar{\lambda}_j - \eta| = 1$. Therefore, we chose a fixed constant $\delta \in (0,1)$ (we mainly used $\delta = 0.75$, but our results were insensitive to the particular choice of δ), and let $h(\eta) \equiv (1 - \eta/\delta)^2(1 + 2\eta/\delta)$, the unique cubic polynomial satisfying $h(0) = 1, h'(0) = 0, h(\delta) = 0$, and $h'(\delta) = 0$. We then defined

$$L(\eta) \equiv \begin{cases} 1 - h(\eta)\ln\eta, & 0 < \eta \le \delta \\ 1, & \delta < \eta \end{cases} \tag{3.29}$$

and

$$\tilde{\mathcal{A}}'_{0n,0m}(\lambda, \mu) \equiv \frac{\tilde{\mathcal{A}}_{0n,0m}(\lambda, \mu)}{L(|\lambda - \mu|)} , \tag{3.30}$$

where $\tilde{\mathcal{A}}_{0n,0m}(\lambda, \mu)$ is defined by Eq. (3.19) with c_{mn} defined in Eq. (3.20). We then analytically computed the limit

$$\tilde{\mathcal{A}}'_{0n,0m}(\mu, \mu) \equiv \lim_{\varepsilon \to 0} \tilde{\mathcal{A}}'_{0n,0m}(\mu + \varepsilon, \mu) = c_{mn} \frac{1 + (-1)^{n+m}}{2\sqrt{\mu}} . \tag{3.31}$$

Using singularity subtraction, we wrote

$$\sqrt{3} I^{\hat{n}\hat{k}\hat{\ell}}_{0n,0m}(\bar{\lambda}_j) = \int_{\lambda_{\hat{\ell}}}^{\lambda_{\hat{\ell}+1}} d\eta L(|\bar{\lambda}_j - \eta|) \left[\frac{\tilde{\mathcal{A}}'_{0n,0m}(\bar{\lambda}_j, \eta) b_{\hat{k}}(\eta)}{e_0 - \eta} - \frac{\tilde{\mathcal{A}}'_{0n,0m}(\bar{\lambda}_j, \bar{\lambda}_j) b_{\hat{k}}(\bar{\lambda}_j)}{e_0 - \bar{\lambda}_j} \right] + \frac{\tilde{\mathcal{A}}'_{0n,0m}(\bar{\lambda}_j, \bar{\lambda}_j) b_{\hat{k}}(\bar{\lambda}_j)}{e_0 - \bar{\lambda}_j} \int_{\lambda_{\hat{\ell}}}^{\lambda_{\hat{\ell}+1}} d\eta L(|\bar{\lambda}_j - \eta|) . \tag{3.32}$$

The first integral in Eq. (3.32) was numerically evaluated using a 32-point Gauss-Legendre quadrature, and the second integral was evaluated analytically.

For $\alpha \neq 0$, the nonhomogeneous terms $\tilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda, e_\alpha)$ in Eq. (3.2) are nonsingular for all $\lambda \in \mathbf{R}^+$, and for all β including $\beta = 0$ [since the second term in Eq. (3.17) vanishes at $\mu = e_\alpha$]. However, the $\alpha = 0$ terms given in Eqs. (3.18) and (3.19) have integrable singularities at $\lambda = e_0$. Consequently, it would not be practical to use the collocation method to solve Eq. (3.2) with $\alpha = 0$. Instead, the Galerkin method [3] should be used in this case. Since the published analytical solutions in Ref. [7] do not include any formulas with the input channel α set equal to the breakup channel, we have nothing to

compare with in this case anyway, and we have not attempted to compute solutions with $\alpha = 0$. We do include the $\gamma = 0$ terms in the kernels of Eqs. (3.2) and (3.3). We note that since $\mathcal{S}(E)$ and $\mathcal{K}(E)$ are block diagonal, the matrix elements $\mathcal{K}_{0n,0m}(\lambda, e_0)$, which we did not compute, do not contribute to $\mathcal{S}_{\beta j,1+}(E)$. Since it is known analytically that our on-shell $\mathcal{K}$ matrix $\mathcal{K}(E)$ is symmetric, we have used this symmetry to obtain the full computed on-shell $\mathcal{K}$ matrix $\mathcal{K}(E)$.

We remark that the $(\lambda - \mu)^{-1/2}$ singularities in Eqs. (3.18) and (3.19) arise from the Jacobians $\nu_\alpha^2(\mu)$ in Eq. (3.8) for this problem in a space dimension of $n = 1$. If $n = 3$, the analogous terms will be $(\lambda - \mu)^{1/2}$. Consequently, the $\alpha = 0$ terms should not be a problem for the collocation method when the space dimension is $n = 3$.

G. Computation of the scattering operator

Since our off-shell $\mathcal{K}$ and $\mathcal{M}$ operators are different from previous operators, it is possible to compare only our on-shell values. At total energy E the kernel of the on-shell approximate scattering matrix $S(E)$ has matrix elements given by the equation [2, 3]

$$\text{kernel of } S_{\beta\alpha}(E) = \nu_\beta^{-1}(e_\beta)\nu_\alpha^{-1}(e_\alpha)\phi_\beta(p_\beta)\phi_\alpha^*(p_\alpha) \times \sum_{\substack{i\in\alpha \\ j\in\beta}} \chi_{\beta j}(\hat{k}_\beta)\mathcal{S}_{\beta j,\alpha i}(E)\chi_{\alpha i}^*(\hat{k}_\alpha) \ . \tag{3.33}$$

The matrix $\mathcal{S}(E)$ with matrix elements $\mathcal{S}_{\beta j,\alpha i}(E)$ is related to our $\mathcal{K}$ matrix $\mathcal{K}(E)$ by the Cayley-type transform [3]

$$\mathcal{S}(E) = [\mathcal{I}(E) - i\pi\mathcal{K}(E)][\mathcal{I}(E) + i\pi\mathcal{K}(E)]^{-1} \ , \tag{3.34}$$

and our approximate on-shell transition matrix $\mathcal{M}(E)$ is related to $\mathcal{S}(E)$ by the formula

$$\mathcal{S}(E) = \mathcal{I}(E) - 2\pi i\mathcal{M}(E) \ . \tag{3.35}$$

The exact values of the matrix $\mathcal{S}(E)$ follow from the work of Dodd [7]. In particular, the limit $p_1' \to p_1$ in Eq. (14) of the 1971 Ref. [7] yields

$$X(p_1, p_1) = \frac{12p_1^2}{g^2(p_1 - ig)(3p_1 - ig)} \ , \tag{3.36}$$

and Dodd shows that

$$\mathcal{S}_{1+,1+}(E(p_1)) = \mathcal{S}_{1-,1-}(E(p_1)) = 1 + \frac{2ig^3}{3p_1}X(p_1, p_1) \ , \tag{3.37}$$

and all other matrix elements are zero. Removing the complex quantities from the denominator in Eq. (3.36), and expressing Eq. (3.37) as a function of the total energy

$$E = E(p_1) \equiv \frac{3p_1^2}{4} - \frac{g^2}{4} \ , \tag{3.38}$$

gives

$$\mathcal{S}_{1+,1+}(E) = \mathcal{S}_{1-,1-}(E) = \frac{E^2 - \sigma^2(E)}{E^2 + \sigma^2(E)} + i\frac{2E\sigma(E)}{E^2 + \sigma^2(E)} \ , \tag{3.39}$$

where

$$\sigma(E) \equiv 2g\sqrt{\tfrac{1}{3}(E + g^2/4)} \ , \tag{3.40}$$

and all other matrix elements of $\mathcal{S}(E)$ are zero. Using the inverse transform to Eq. (3.34), we also learn that the exact on-shell $\mathcal{K}$-matrix $\mathcal{K}(E)$ has matrix elements

$$\mathcal{K}_{1+,1+}(E) = \mathcal{K}_{1-,1-}(E) = -\frac{\sigma(E)}{\pi E} \ , \tag{3.41}$$

with all other matrix elements equal to zero. In our work we have used Eqs. (3.39)–(3.41) to compare our numerically computed values with the exact quantities.

IV. NUMERICAL RESULTS

We have solved Eqs. (3.2) and (3.3) using the breakup basis functions in Eq. (2.30) for several integer values of m. Although we do not have a complete analytical proof, our numerical results show that only the values of m which are nonnegative multiples of 3 have nonzero contributions. In this case, the system in Eq. (3.2) may be symmetrized as shown in Eq. (3.23). Since computations using the symmetrized equations are considerably faster, all of our subsequent $\mathcal{K}$-equation calculations were performed using Eq. (3.23), and our transition operator calculations were performed using the $\widehat{\mathcal{M}}$ equations which are analogous to Eq. (3.23).

The breakup threshold total energy is $E = 0.0$, but as is well known [7], there is no actual physical breakup for this identical particle problem. Figure 1 is a graph of our computed half-on-shell $\widehat{\mathcal{K}}$-matrix elements $\widehat{\mathcal{K}}_{0m,1+}(\lambda, e_1)$, using 28 B-spline basis functions and the four breakup Fourier cosine terms in Eq. (2.30) with m=0, 3, 6, and 9. The above-breakup total energy is $E = 0.75$, which corresponds to the input kinetic energy $e_1 = 3.0$. The on-shell value of λ is $\lambda = e_0 = 0.75$, and we note that all

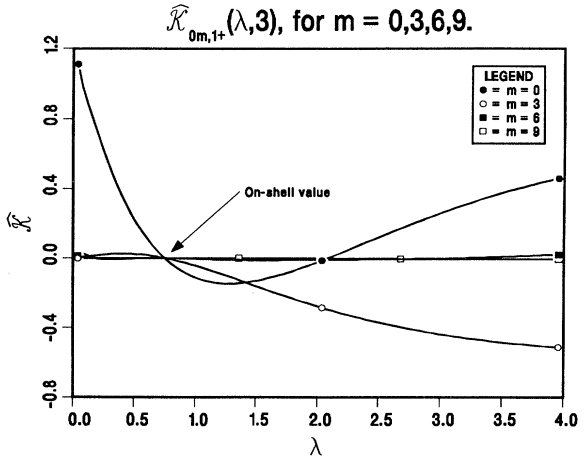

FIG. 1. Plot of $\widehat{\mathcal{K}}_{0m,1+}(\lambda, 3)$ vs λ, for $m = 0, 3, 6, 9$, computed using 28 B-spline basis functions. The on-shell value of λ is $\lambda = 0.75$.

four of the curves vanish there, explaining why there is no physical breakup in this problem.

The Faddeev equations [5] have been solved analytically for this problem by Dodd [7]. Since our half-on-shell operators are different from those arising in the Faddeev equations, it is only possible to compare our on-shell solutions with those of Dodd. Fig. 2 contains a graph of the real and imaginary parts of the exact on-shell matrix element $\mathcal{S}_{1+,1+}(E)$. The exact matrix element $\mathcal{S}_{1-,1-}(E)$ is identical. All other matrix elements of the exact on-shell scattering matrix $\mathcal{S}(E)$ are equal to zero.

In Fig. 3 we show a logarithmic scale graph of the absolute value of the difference between our computed $\mathcal{S}_{1+,1+}(E)$ matrix element and the exact $\mathcal{S}_{1+,1+}(E)$ matrix element for all energies from the 2-cluster threshold $E = -2.25$ to $E = 1.75$, using Eq. (3.23) and 28 B-spline basis functions. The top curve is the solution using no Eq. (2.30) breakup terms, the middle curve is the solution using only the $m = 0$ breakup term, and the bottom curve is the solution using the three breakup terms with $m = 0, 3, 6$. We note that the solutions are converging for all energies E, both below and above breakup, as the number of breakup basis functions increases.

Tables I–III show the results of our calculations using Eq. (3.23). In particular, our computed values of the real and imaginary parts of $\mathcal{S}_{1+,1+}(E)$ for the below-breakup energy $E = -1.25$ are shown in Table I and compared with the known exact values. Table II shows a corresponding comparison for the above breakup energy $E = 0.75$. The columns labeled m in 0 give the index values m of the included Eq. (2.30) breakup basis functions. $\text{Prob}_{1+,1+}$ is the probability of elastic scattering in the forward direction. Table III shows our computed values of the additional scattering operator matrix elements $\mathcal{S}_{\beta j,1+}(E)$, and the corresponding probabilities $\text{Prob}_{\beta j,1+}(E)$, at the above breakup energy $E = 0.75$ using $m = 0, 3, 6$, and 9. Tables IV and V show the corresponding results of our $E = 0.75$ above-breakup calculations using the transition operator Eq. (3.3) symmetrized as in Eq. (3.23).

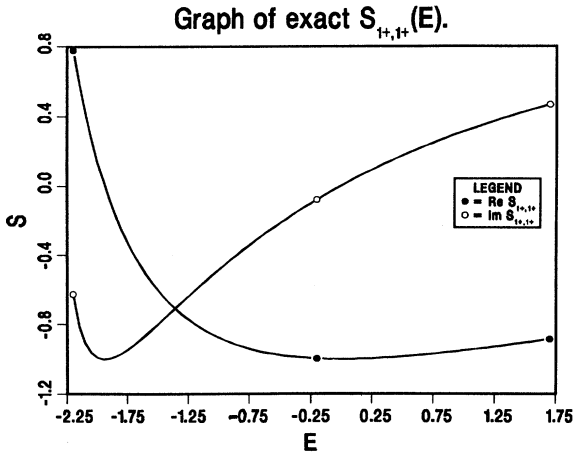

FIG. 2. Graph of the real and imaginary parts of the exact elastic $\mathcal{S}$-matrix element $\mathcal{S}_{1+,1+}(E)$.

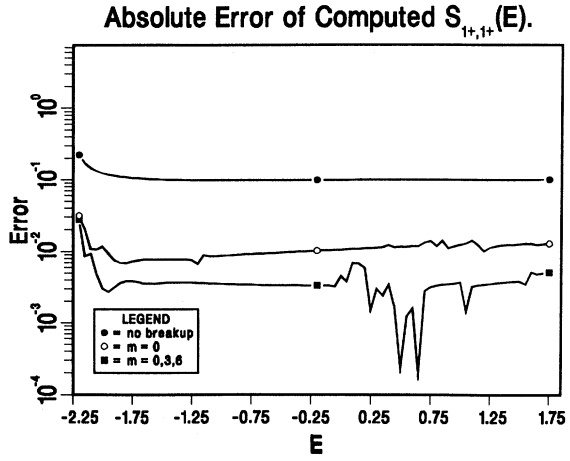

FIG. 3. Absolute error of computed $\mathcal{S}_{1+,1+}(E)$ using no breakup term, only the $m = 0$ breakup term, and the three breakup terms with $m = 0, 3$, and 6.

Tables I, II, and IV show the effect on the elastic (1+) channel of increasing the number of Fourier cosine series breakup basis functions in Eq. (2.30) from zero to the four values m=0, 3, 6, and 9. Our computer program also has good numerical stability with respect to increasing the number of B-spline basis functions $b_j(\lambda)$.

We note that the computed probabilities in Table III sum to 1.000 000 000, reflecting the fact that our use of a symmetrized $\mathcal{K}(E)$ matrix automatically yields a unitary approximate scattering matrix $\mathcal{S}(E)$. On the other hand, the computed probabilities in Table V sum to near 1, but not exactly 1, showing that the scattering matrix $\mathcal{S}(E)$ computed using the CG transition operator equations is approximately, but not exactly, unitary.

The calculations shown in the tables were done on a SUN 3 workstation. The more time-consuming calculations required to make Fig. 3 were done on an IBM 6000-320 workstation.

V. CONCLUSIONS

In order to test the Chandler-Gibson N-body quantum scattering theory [1, 2], and to test our computer programs under development, we have solved the 3-body problem consisting of three particles moving on a line and interacting through attractive delta-function potentials. This problem has been used previously as a test problem [7–9], and the analytically known on-shell solution [7] is available for comparison.

The CG equations differ from previous N-particle equations in that the projections onto the channel subspaces are included in the unknowns of the equations, and the equations contain an overlap term which correctly couples these channel subspaces. These N-body equations may be written in either a $\mathcal{K}$-matrix [Eq. (1.1) or (3.2)] or a transition matrix [Eq. (1.2) or (3.3)] form.

Our computed scattering matrix elements using the CG $\widehat{\mathcal{K}}$ equations (see Fig. 3 and Tables I–III) and the CG $\widehat{\mathcal{M}}$ equations (see Tables IV and V) are generally

TABLE I. Elastic channel solution of the 3-body test problem at the below-breakup total energy $E = -1.25$, computed using the $\widehat{K}$-equations with 20 B-spline basis functions.

m in 0	Re $\mathcal{S}_{1+,1+}$	Im $\mathcal{S}_{1+,1+}$	$\text{Prob}_{1+,1+}$
None	−0.82531284	−0.55679530	0.99116229
0	−0.78083425	−0.62456428	0.99978267
0,3	−0.77962675	−0.62602347	0.99972324
0,3,6	−0.76774937	−0.64074621	0.99999480
0,3,6,9	−0.76757214	−0.64095944	0.99999599
Exact	−0.76958525	−0.63854408	1.00000000

TABLE II. Elastic channel solution of the 3-body test problem at the above-breakup total energy $E = 0.75$, computed using the $\widehat{K}$-equations with 28 B-spline basis functions.

m in 0	Re $\mathcal{S}_{1+,1+}$	Im $\mathcal{S}_{1+,1+}$	$\text{Prob}_{1+,1+}$
None	−0.93636329	0.34060714	0.99278944
0	−0.96568304	0.25959080	0.99993112
0,3	−0.96762656	0.25216256	0.99988712
0,3,6	−0.96999486	0.24311060	0.99999280
0,3,6,9	−0.96999538	0.24310856	0.99999280
Exact	−0.96923077	0.24615385	1.00000000

TABLE III. Above breakup solution of the 3-body test problem at the total energy $E = 0.75$, computed using the $\widehat{K}$-equations with 28 B-spline basis functions, and using the m=0, 3, 6, and 9 breakup basis functions.

$\beta j, \alpha i$	Re $\mathcal{S}_{\beta j,\alpha i}$	Im $\mathcal{S}_{\beta j,\alpha i}$	$\text{Prob}_{\beta j,\alpha i}$	Exact $\text{Prob}_{\beta j,\alpha i}$
1+,1+	−0.96999538	0.24310856	0.9999928026	1.0000000000
1−,1+	−0.00064432	−0.00257113	0.0000070258	0.0000000000
00,1+	0.00005706	−0.00000697	0.0000000033	0.0000000000
03,1+	0.00008786	−0.00001096	0.0000000078	0.0000000000
06,1+	0.00039685	−0.00004844	0.0000001598	0.0000000000
09,1+	−0.00002458	0.00000307	0.0000000006	0.0000000000

TABLE IV. Elastic channel solution of the 3-body test problem at the above breakup total energy $E = 0.75$, computed using the $\widehat{\mathcal{M}}$-equations with 28 B-spline basis functions.

m in 0	Re $\mathcal{S}_{1+,1+}$	Im $\mathcal{S}_{1+,1+}$	$\text{Prob}_{1+,1+}$
None	−0.93632327	0.34063767	0.99273528
0	−0.96611137	0.25780599	0.99983511
0,3	−0.96800600	0.25043252	0.99975206
0,3,6	−0.97003585	0.24314682	1.00008994
0,3,6,9	−0.96996391	0.24303049	0.99989381
Exact	−0.96923077	0.24615385	1.00000000

TABLE V. Above breakup solution of the 3-body test problem at the total energy $E = 0.75$, computed using the $\widehat{\mathcal{M}}$ equations with 28 B-spline basis functions, and using the m=0, 3, 6, and 9 breakup basis functions.

$\beta j, \alpha i$	Re $\mathcal{S}_{\beta j,\alpha i}$	Im $\mathcal{S}_{\beta j,\alpha i}$	$\text{Prob}_{\beta j,\alpha i}$	Exact $\text{Prob}_{\beta j,\alpha i}$
1+,1+	−0.96996391	0.24303049	0.9998938074	1.0000000000
1−,1+	−0.00085556	−0.00253016	0.0000071337	0.0000000000
00,1+	0.00003203	0.00002322	0.0000000016	0.0000000000
03,1+	−0.00002711	−0.00011306	0.0000000135	0.0000000000
06,1+	0.00035433	0.00009323	0.0000001342	0.0000000000
09,1+	0.00007226	−0.00003158	0.0000000062	0.0000000000

within 0.5% of the exact $\mathcal{S}$-matrix solutions, and the corresponding probabilities are within 0.001% of the exact probabilities, at all tested energies both below and above the 3-body breakup threshold. These results are particularly impressive in light of the singular delta distribution potentials and the singular Jacobians which arise from a space dimension of $n = 1$.

We conclude that the CG theory works very well for the 3-body test problem. Either the $\mathcal{K}$-matrix approach or transition operator approach may be used, the results being comparable. The $\mathcal{K}$-matrix method has the advantage that the unknowns are real valued for real-valued potentials. The transition operator method has the advantage that the calculations need to be performed only for the input channels of interest.

We believe that our test problem results verify that the CG equations are attractive from a practical, as well as theoretical, point of view. The CG equations appear to provide an attractive alternative to other N-body equations, especially for scattering problems with (a) nonseparable potentials, (b) energies above the breakup threshold, and/or (c) more than three particles. The major remaining obstacle for more complicated problems is the analytical/numerical evaluation of the input Born and overlap functions. A further study of these integrals is in progress.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge fruitful discussions about this work with E. O. Alt, Gy. Bencze, F. Coester, B. J. Fisk, Z. C. Kuruoglu, F. S. Levin, G. W. Pletsch, E. F. Redish, W. Sandhas, I. H. Sloan, and H. J. Taijeron. We thank Arthur G. Cannon of the Albuquerque office of IBM Corporation for arranging our use of an IBM 6000-320. We also gratefully acknowledge the financial support of Grants No. PHY-8802774 and No. INT-8800898 from the National Science Foundation.

APPENDIX: EVALUATION OF $\mathcal{A}(\lambda,\mu)$

The input terms in Eqs. (1.1) and (1.2) are of the form of Eq. (1.3). Multiplying Eq. (1.3) on the left by $\nu_\beta^{-1}(\lambda)$ and on the right by $\nu_\alpha^{-1}(\mu)$ yields

$$\tilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda,\mu) = \tilde{\mathcal{B}}_{\beta j,\alpha i}(\lambda,\mu) - \tilde{\mathcal{C}}_{\beta j,\alpha i}(\lambda,\mu)(e_\alpha - \mu) , \tag{A1}$$

where $\tilde{\mathcal{A}}_{\beta j,\alpha i}(\lambda,\mu)$ is defined in Eq. (3.1), and $\tilde{\mathcal{B}}_{\beta j,\alpha i}(\lambda,\mu)$ and $\tilde{\mathcal{C}}_{\beta j,\alpha i}(\lambda,\mu)$ are similarly defined with $\mathcal{A}$ replaced by $\mathcal{B}$ and $\mathcal{C}$, respectively. General formulas for evaluating $\tilde{\mathcal{C}}_{\beta j,\alpha i}(\lambda,\mu)$ and $\tilde{\mathcal{B}}_{\beta j,\alpha i}(\lambda,\mu)$ are given in Ref. [2]. In this appendix we use these general formulas to obtain specific formulas for our three-body test problem. The formulas derived in this appendix are general enough to permit the masses m_α and the potential strength constants g_α to be different for different values of α, $\alpha = 1,2,3$.

1. Evaluation of $\tilde{\mathcal{C}}(\lambda,\mu)$

In this subsection we evaluate the entries in the overlap matrix $\tilde{\mathcal{C}}(\lambda,\mu)$.

Let P_α denote the orthogonal projection operator of $\mathcal{H}_N$ onto $\mathcal{H}_\alpha$, where $\mathcal{H}_\alpha$ is the closed subspace of $\mathcal{H}_N$ spanned by vectors of the form $\hat{\phi}_\alpha(p_\alpha)\psi(q_\alpha)$ with $\psi \in \mathcal{L}^2(\mathbf{R})$, and $\alpha = 1,2,3$. For $\psi \in \mathcal{H}_N$, the vector $P_\alpha\psi \in \mathcal{H}_\alpha$ is thus given by

$$(P_\alpha\psi)(p'_\alpha,q'_\alpha) = \int dp_\alpha dq_\alpha \hat{\phi}_\alpha(p'_\alpha)\hat{\phi}^*_\alpha(p_\alpha) \times \delta(q'_\alpha - q_\alpha)\psi(p_\alpha,q_\alpha) . \tag{A2}$$

Hence, P_α is an integral operator on $\mathcal{H}_N$ with kernel given by the distribution

$$\langle p'_\alpha q'_\alpha | P_\alpha | p_\alpha q_\alpha\rangle \equiv \hat{\phi}_\alpha(p'_\alpha)\delta(q'_\alpha - q_\alpha)\hat{\phi}^*_\alpha(p_\alpha) . \tag{A3}$$

In Eqs. (A2) and (A3) $\hat{\phi}^*_\alpha(p_\alpha)$ denotes the complex conjugate of $\hat{\phi}_\alpha(p_\alpha)$. Since the $\hat{\phi}_\alpha(p_\alpha)$ in Eq. (2.12) is a real-valued function these quantities are equal, however, we will include the asterisk in order to illustrate the more general case [2]. Using Eq. (2.13), the momenta (p'_α,q'_α) in Eq. (A3) may be transformed to those for (p'_β,q'_β) to obtain

$$\langle p'_\beta q'_\beta | P_\alpha | p_\alpha q_\alpha\rangle = \hat{\phi}_\alpha\left(-\frac{\mu_\alpha}{m_\gamma}p'_\beta - \epsilon_{\alpha\beta}\frac{\mu_\beta}{\bar{\mu}_\alpha}q'_\beta\right)\delta\left(\epsilon_{\alpha\beta}p'_\beta - \frac{\mu_\beta}{m_\gamma}q'_\beta - q_\alpha\right)\hat{\phi}^*_\alpha(p_\alpha) . \tag{A4}$$

Combining Eqs. (A3) and (A4) gives the kernel for $P_\beta P_\alpha$,

$$\begin{aligned}\langle p'_\beta q'_\beta | P_\beta P_\alpha | p_\alpha q_\alpha\rangle &= \int dpdq \langle p'_\beta q'_\beta | P_\beta | pq\rangle\langle pq | P_\alpha | p_\alpha q_\alpha\rangle \\ &= \hat{\phi}_\beta(p'_\beta)\hat{\phi}^*_\beta\left(\epsilon_{\alpha\beta}\left[\frac{\mu_\beta}{m_\gamma}q'_\beta + q_\alpha\right]\right)\hat{\phi}_\alpha\left(-\epsilon_{\alpha\beta}\left[q'_\beta + \frac{\mu_\alpha}{m_\gamma}q_\alpha\right]\right)\hat{\phi}^*_\alpha(p_\alpha) ,\end{aligned} \tag{A5}$$

valid for all α and β satisfying $0 \neq \beta \neq \alpha \neq 0$. In obtaining Eq. (A5) we have made use of the identity $\mu_\alpha\mu_\beta m_\gamma^{-2} + \mu_\beta\bar{\mu}_\alpha^{-1} = 1$.

The next step is to express the kernel in Eq. (A5) in KEHS coordinates. Let $\mu \equiv |k_\alpha|^2$ denote the input kinetic energy, and let $\lambda \equiv |k'_\beta|^2$ denote the output kinetic energy. Substituting q_α from Eq. (2.15) and $q'_\beta = \hat{k}'_\beta\sqrt{2\bar{\mu}_\beta\lambda}$ into Eq. (A5) yields a formula for the kernel

$$C_{\beta\alpha}(p'_\beta,\hat{k}'_\beta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)\equiv\langle p'_\beta\hat{k}'_\beta\lambda|\bar{\delta}_{\beta\alpha}P_\beta P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle\ , \tag{A6}$$

valid for each $0\neq\beta\neq\alpha\neq 0$. In Eq. (A6) $\bar{\delta}_{\beta\alpha}\equiv 1-\delta_{\beta\alpha}$ with $\delta_{\beta\alpha}$ the Kronecker delta, which implies that $C_{\alpha\alpha}=0$ for all $\alpha=1,2,3$.

Using the basis functions in Eq. (2.17), the expansion given in Eq. (7.10) of Ref. [2] becomes

$$C_{\beta\alpha}(p'_\beta,\hat{k}'_\beta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)=\hat{\phi}_\beta(p'_\beta)\left(\sum_{\substack{m=+,-\\ n=+,-}}\chi_{\beta n}(\hat{k}'_\beta)\widetilde{C}_{\beta n,\alpha m}(\lambda,\mu)\chi^*_{\alpha m}(\hat{k}_\alpha)\right)\hat{\phi}^*_\alpha(p_\alpha)\ , \tag{A7}$$

where

$$\widetilde{C}_{\beta+,\alpha\pm}(\lambda,\mu)=\widetilde{C}_{\beta-,\alpha\mp}(\lambda,\mu)\equiv\frac{(2/\pi)(a_\alpha a_\beta)^{3/2}}{[(\mu_\beta m_\gamma^{-1}\sqrt{2\bar{\mu}_\beta\lambda}\pm\sqrt{2\bar{\mu}_\alpha\mu})^2+a_\beta^2][(\sqrt{2\bar{\mu}_\beta\lambda}\pm\mu_\alpha m_\gamma^{-1}\sqrt{2\bar{\mu}_\alpha\mu})^2+a_\alpha^2]}\ , \tag{A8}$$

for all $0\neq\beta\neq\alpha\neq 0$.

Consider now the breakup partition 0. Since $P_0=I_N$, the identity operator on $\mathcal{H}_N$, the kernel of P_0P_α is obtained from Eq. (A3). In order to express this kernel in KEHS coordinates, we replace q_α by the right-hand side of Eq. (2.15), and, by Lemma 2, let

$$p'_\alpha=\sqrt{2\mu_\alpha\lambda}\sin(\theta+\tau_{\alpha1})\ ,\quad q'_\alpha=\sqrt{2\bar{\mu}_\alpha\lambda}\cos(\theta+\tau_{\alpha1})\ . \tag{A9}$$

It follows that

$$C_{0\alpha}(\theta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)\equiv\langle\theta\lambda|\bar{\delta}_{0\alpha}P_0P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle=\frac{\bar{\delta}_{0\alpha}(2/\pi)^{1/2}a_\alpha^{3/2}\delta(\sqrt{2\bar{\mu}_\alpha\lambda}\cos(\theta+\tau_{\alpha1})-\sqrt{2\bar{\mu}_\alpha\mu}\hat{k}_\alpha)\hat{\phi}^*_\alpha(p_\alpha)}{[2\mu_\alpha\lambda\sin^2(\theta+\tau_{\alpha1})+a_\alpha^2]}\ . \tag{A10}$$

Thus [2]

$$\begin{aligned}\widetilde{C}_{0m,\alpha\pm}(\lambda,\mu)&\equiv\int d\theta dp_\alpha d\hat{k}_\alpha\chi^*_{0m}(\theta)C_{0\alpha}(\theta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)\hat{\phi}_\alpha(p_\alpha)\chi_{\alpha\pm}(\hat{k}_\alpha)\\&=\bar{\delta}_{0\alpha}(2/\pi)^{1/2}a_\alpha^{3/2}\int_{-\pi}^{\pi}d\theta\chi^*_{0m}(\theta)\frac{\delta(\sqrt{2\bar{\mu}_\alpha\lambda}\cos(\theta+\tau_{\alpha1})\mp\sqrt{2\bar{\mu}_\alpha\mu})}{[2\mu_\alpha\lambda\sin^2(\theta+\tau_{\alpha1})+a_\alpha^2]}\\&=\bar{\delta}_{0\alpha}(2/\pi)^{1/2}a_\alpha^{3/2}\int_{-\pi}^{\pi}d\theta\chi^*_{0m}(\theta-\tau_{\alpha1})\frac{\delta(\sqrt{2\bar{\mu}_\alpha\lambda}\cos\theta\mp\sqrt{2\bar{\mu}_\alpha\mu})}{(2\mu_\alpha\lambda\sin^2\theta+a_\alpha^2)}\ ,\end{aligned} \tag{A11}$$

for $m=0,\pm1,\pm2,\ldots$. In the second of Eqs. (A11) the integration with respect to $d\hat{k}_\alpha$ has been evaluated using Eqs. (2.17), and the integration with respect to dp_α is equal to 1. In the third of Eqs. (A11) we have used the periodicity of the integrand to translate the interval of integration. If $m=0$, then the integrand of the last integral in Eq. (A11) is an even function of θ. If $m\neq0$, then trigonometric identities for the cosine and sine of the difference of two angles may be used to express $\chi^*_{0m}(\theta-\tau_{\alpha1})$ as a sum of even ($\cos m\theta$) and odd ($\sin m\theta$) terms. It follows that

$$\widetilde{C}_{0m,\alpha\pm}(\lambda,\mu)=2^{3/2}\pi^{-1}a_\alpha^{3/2}\xi_{m\alpha}\int_0^\pi d\theta\cos m\theta\frac{\delta(\sqrt{2\bar{\mu}_\alpha\lambda}\cos\theta\mp\sqrt{2\bar{\mu}_\alpha\mu})}{(2\mu_\alpha\lambda\sin^2\theta+a_\alpha^2)}\ , \tag{A12}$$

for $\alpha=1,2,3$, where $\xi_{m\alpha}$ are the constants defined in Eq. (3.11). If the substitution $q=\sqrt{2\bar{\mu}_\alpha\lambda}\cos\theta$, $d\theta=-(2\bar{\mu}_\alpha\lambda-q^2)^{-1/2}dq$, is made in the integrand of Eq. (A12), then the resulting integral containing a delta function can be evaluated to yield

$$\widetilde{C}_{0m,\alpha\pm}(\lambda,\mu)=\begin{cases}\dfrac{(\pi\mu_\alpha)^{-1}\bar{\mu}_\alpha^{-1/2}a_\alpha^{3/2}\xi_{m\alpha}\cos\left(m\cos^{-1}\pm\sqrt{\mu/\lambda}\right)}{\sqrt{\lambda-\mu}(\lambda-\mu-\varepsilon_\alpha)}, & \text{for } \lambda>\mu\\ 0, & \text{for } \lambda<\mu\end{cases} \tag{A13}$$

for $\alpha=1,2,3$, and $m=0,\pm1,\pm2,\ldots$, where ε_α is defined in Eq. (2.10). Since the operator $\bar{\delta}_{\alpha0}P_\alpha P_0$ is the adjoint of the operator $\bar{\delta}_{0\alpha}P_0P_\alpha$, it follows that

$$\widetilde{C}_{\alpha\pm,0m}(\lambda,\mu)=\widetilde{C}^*_{0m,\alpha\pm}(\mu,\lambda)=\widetilde{C}_{0m,\alpha\pm}(\mu,\lambda) \tag{A14}$$

for $\alpha=1,2,3$, and $m=0,\pm1,\pm2,\ldots$, with the right-hand side function given by Eq. (A13). Finally,

$$\widetilde{C}_{\alpha j,\alpha i}(\lambda,\mu)=0\ , \tag{A15}$$

for $\alpha=0,1,2,3$, and all combinations of i and j. This completes the evaluation of all of the matrix elements of $\widetilde{C}(\lambda,\mu)$.

2. Evaluation of $\tilde{\mathcal{B}}(\lambda,\mu)$

In this subsection we evaluate the entries in the matrix $\tilde{\mathcal{B}}(\lambda,\mu)$.

Since the potential V_α is given in (x_α, y_α) coordinates as multiplication by the distribution $-g_\alpha\delta(x_\alpha)$, its value in (p_α, q_α) momentum space is obtained by Fourier transformation $\mathcal{F}$ to be

$$\begin{aligned}(V_\alpha\psi)(p'_\alpha,q'_\alpha)&=\mathcal{F}\{-g_\alpha\delta(x_\alpha)\psi(x_\alpha,y_\alpha)\}\\&=\mathcal{F}\{-g_\alpha\delta(x_\alpha)\mathcal{F}^{-1}\{\psi(p_\alpha,q_\alpha)\}\}\\&=\int dp_\alpha dq_\alpha\left[-\frac{g_\alpha}{2\pi}\delta(q'_\alpha-q_\alpha)\right]\psi(p_\alpha,q_\alpha)\end{aligned}\tag{A16}$$

It follows that V_α is an integral operator on $\mathcal{H}_N$ with kernel given by the distribution

$$\langle p'_\alpha q'_\alpha|V_\alpha|p_\alpha q_\alpha\rangle\equiv-\frac{g_\alpha}{2\pi}\delta(q'_\alpha-q_\alpha)\,.\tag{A17}$$

Combining Eq. (A17) (with α replaced by β) and Eq. (A4) yields

$$\begin{aligned}\langle p'_\beta q'_\beta|V_\beta P_\alpha|p_\alpha q_\alpha\rangle&=\int dpdq\langle p'_\beta q'_\beta|V_\beta|pq\rangle\langle pq|P_\alpha|p_\alpha q_\alpha\rangle\\&=-\frac{g_\beta}{2\pi}\hat\phi_\alpha\left(-\epsilon_{\alpha\beta}\left[q'_\beta+\frac{\mu_\alpha}{m_\gamma}q_\alpha\right]\right)\\&\quad\times\hat\phi^*_\alpha(p_\alpha)\,,\end{aligned}\tag{A18}$$

for all α and β satisfying $0\neq\beta\neq\alpha\neq0$. Eqs. (2.12), (A3), and (A18) then give

$$\langle p'_\beta q'_\beta|P_\beta V_\beta P_\alpha|p_\alpha q_\alpha\rangle=\frac{-\pi^{-1}g_\beta(a_\alpha a_\beta)^{1/2}a_\alpha\hat\phi_\beta(p'_\beta)\hat\phi^*_\alpha(p_\alpha)}{(q'_\beta+\mu_\alpha m_\gamma^{-1}q_\alpha)^2+a_\alpha^2}\,.\tag{A19}$$

Using Eq. (A18) with β and γ interchanged, and then using Eqs. (2.13) to convert to (p'_β, q'_β) momenta results in

$$\langle p'_\beta q'_\beta|V_\gamma P_\alpha|p_\alpha q_\alpha\rangle=-\frac{g_\gamma}{2\pi}\hat\phi_\alpha\left(-p'_\beta+\epsilon_{\alpha\gamma}\left[\frac{\mu_\beta}{m_\alpha}q'_\beta-\frac{\mu_\alpha}{m_\beta}q_\alpha\right]\right)\hat\phi^*_\alpha(p_\alpha)\,.\tag{A20}$$

Eqs. (2.12), (A3), and (A20) imply that

$$\begin{aligned}\langle p'_\beta q'_\beta|P_\beta V_\gamma P_\alpha|p_\alpha q_\alpha\rangle&=\int dpdq\langle p'_\beta q'_\beta|P_\beta|pq\rangle\langle pq|V_\gamma P_\alpha|p_\alpha q_\alpha\rangle\\&=\int_{-\infty}^{\infty}dp\frac{-\pi^{-2}g_\gamma(a_\alpha a_\beta)^{3/2}\hat\phi_\beta(p'_\beta)\hat\phi^*_\alpha(p_\alpha)}{(p^2+a_\beta^2)\{[p-\epsilon_{\alpha\gamma}(\mu_\beta m_\alpha^{-1}q'_\beta-\mu_\alpha m_\beta^{-1}q_\alpha)]^2+a_\alpha^2\}}\\&=\frac{-\pi^{-1}g_\gamma(a_\alpha a_\beta)^{1/2}(a_\alpha+a_\beta)\hat\phi_\beta(p'_\beta)\hat\phi^*_\alpha(p_\alpha)}{(\mu_\beta m_\alpha^{-1}q'_\beta-\mu_\alpha m_\beta^{-1}q_\alpha)^2+(a_\alpha+a_\beta)^2}\,,\end{aligned}\tag{A21}$$

for all nonzero and nonequal α, β, and γ. The last equation in Eqs. (A21) has been obtained by using contour integration and the residue theorem to evaluate the integral with respect to p and then algebraically simplifying the result. Adding Eqs. (A19) and (A21) gives a formula for $\langle p'_\beta q'_\beta|P_\beta\bar V_\alpha P_\alpha|p_\alpha q_\alpha\rangle$ valid for all $0\neq\beta\neq\alpha\neq0$, where $\bar V_\alpha$ is defined in Eq. (2.8). Finally, replacing q_α by Eq. (2.15) and q'_β by $q'_\beta=\hat k'_\beta\sqrt{2\bar\mu_\beta\lambda}$, gives a formula for the kernel function

$$B_{\beta\alpha}(p'_\beta,\hat k'_\beta,\lambda;p_\alpha,\hat k_\alpha,\mu)\equiv\langle p'_\beta\hat k'_\beta\lambda|P_\beta\bar V_\alpha P_\alpha|p_\alpha\hat k_\alpha\mu\rangle\,,\tag{A22}$$

valid for all $0\neq\beta\neq\alpha\neq0$.

The expansion analogous to Eq. (A7) for $B_{\beta\alpha}(p'_\beta,\hat k'_\beta,\lambda;p_\alpha,\hat k_\alpha,\mu)$ then gives

$$\begin{aligned}\tilde{\mathcal{B}}_{\beta+,\alpha\pm}(\lambda,\mu)&=\tilde{\mathcal{B}}_{\beta-,\alpha\mp}(\lambda,\mu)\\&\equiv-\frac{\sqrt{a_\alpha a_\beta}}{\pi}\left[\frac{g_\beta a_\alpha}{(\sqrt{2\bar\mu_\beta\lambda}\pm\mu_\alpha m_\gamma^{-1}\sqrt{2\bar\mu_\alpha\mu})^2+a_\alpha^2}+\frac{g_\gamma(a_\alpha+a_\beta)}{(\mu_\beta m_\alpha^{-1}\sqrt{2\bar\mu_\beta\lambda}\mp\mu_\alpha m_\beta^{-1}\sqrt{2\bar\mu_\alpha\mu})^2+(a_\alpha+a_\beta)^2}\right],\end{aligned}\tag{A23}$$

for all α and β satisfying $0\neq\beta\neq\alpha\neq0$.

Equation (A23) does not hold when $\beta=\alpha$. In this case both of the kernel terms will be similar to Eq. (A20). In particular, Eqs. (A18) and (2.13) yield

$$\langle p'_\alpha q'_\alpha|V_\beta P_\alpha|p_\alpha q_\alpha\rangle=-\frac{g_\beta}{2\pi}\hat\phi_\alpha\left(p'_\alpha+\epsilon_{\alpha\beta}\frac{\mu_\alpha}{m_\gamma}(q'_\alpha-q_\alpha)\right)\hat\phi^*_\alpha(p_\alpha)\,,\tag{A24}$$

and the corresponding equation with β and γ interchanged. A derivation similar to Eqs. (A21)–(A23) then gives the identities

$$\widetilde{\mathcal{B}}_{\alpha+,\alpha\pm}(\lambda,\mu)=\widetilde{\mathcal{B}}_{\alpha-,\alpha\mp}(\lambda,\mu)\equiv-\frac{a_\alpha^2}{\pi}\left[\frac{g_\beta}{\mu_\alpha^2 m_\gamma^{-2}\bar{\mu}_\alpha(\sqrt{\lambda}\mp\sqrt{\mu})^2+2a_\alpha^2}+\frac{g_\gamma}{\mu_\alpha^2 m_\beta^{-2}\bar{\mu}_\alpha(\sqrt{\lambda}\mp\sqrt{\mu})^2+2a_\alpha^2}\right], \tag{A25}$$

valid for all $\alpha\neq 0$.

We now consider the breakup cases. First, consider the operator $P_0\bar{V}_\alpha P_\alpha=(V_\beta+V_\gamma)P_\alpha$. The kernel in Eq. (A18) may be transformed to KEHS coordinates by replacing q_α by the right-hand side of Eq. (2.15) and q'_β by the right-hand side of the second equation in Eq. (A9) (with α replaced by β). The result is

$$\langle\theta\lambda|V_\beta P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle=\frac{-(a_\alpha/2\pi)^{3/2}g_\beta\bar{\mu}_\beta^{-1}\hat{\phi}_\alpha^*(p_\alpha)}{[\sqrt{\lambda}\cos(\theta+\tau_{\beta 1})-\hat{k}_\alpha\sqrt{\mu}\cos\tau_{\beta\alpha}]^2+a_\alpha^2/(2\bar{\mu}_\beta)}\ . \tag{A26}$$

Here we have used the identity

$$\cos\tau_{\beta\alpha}\equiv-\frac{\mu_\alpha}{m_\gamma}\sqrt{\frac{\bar{\mu}_\alpha}{\bar{\mu}_\beta}}\ , \tag{A27}$$

valid for all $\beta\neq\alpha$. Defining the kernel

$$B_{0\alpha}(\theta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)\equiv\sum_{\beta\neq\alpha,0}\langle\theta\lambda|V_\beta P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle\ , \tag{A28}$$

and using the same procedure as in Eqs. (A11) and (A12), we obtain

$$\begin{aligned}\widetilde{\mathcal{B}}_{0m,\alpha\pm}(\lambda,\mu)&\equiv\int d\theta dp_\alpha d\hat{k}_\alpha\chi_{0m}^*(\theta)B_{0\alpha}(\theta,\lambda;p_\alpha,\hat{k}_\alpha,\mu)\hat{\phi}_\alpha(p_\alpha)\chi_{\alpha\pm}(\hat{k}_\alpha)\\&=-\frac{a_\alpha^{3/2}}{(2\pi)^{3/2}}\sum_{\beta\neq\alpha,0}\int_{-\pi}^{\pi}d\theta\frac{\chi_{0m}^*(\theta)}{[\sqrt{\lambda}\cos(\theta+\tau_{\beta 1})\mp\sqrt{\mu}\cos\tau_{\beta\alpha}]^2+a_\alpha^2/(2\bar{\mu}_\beta)}\\&=-\frac{a_\alpha^{3/2}}{2^{1/2}\pi^2}\sum_{\beta\neq\alpha,0}\frac{g_\beta\xi_{m\beta}}{\bar{\mu}_\beta}\int_0^{\pi}d\theta\frac{\cos m\theta}{(\sqrt{\lambda}\cos\theta\mp\sqrt{\mu}\cos\tau_{\beta\alpha})^2+a_\alpha^2/(2\bar{\mu}_\beta)}\ ,\end{aligned} \tag{A29}$$

for $\alpha=1,2,3$, and $m=0,\pm1,\pm2,\ldots$. These integrals are finite and may be easily evaluated numerically.

The kernel $\widetilde{\mathcal{B}}_{\alpha\pm,0m}(\lambda,\mu)$ of the operator $P_\alpha\bar{V}_0P_0$ may be obtained from the kernel of the adjoint operator $P_0\bar{V}_0P_\alpha=(V_\alpha+V_\beta+V_\gamma)P_\alpha$. The kernels of the $V_\beta P_\alpha$ terms have already been obtained in Eq. (A29). Consider the operator $V_\alpha P_\alpha$. By Eqs. (A3), (A17), and (2.12),

$$\begin{aligned}\langle p'_\alpha q'_\alpha|V_\alpha P_\alpha|p_\alpha q_\alpha\rangle&=\int dpdq\left[-\frac{g_\alpha}{2\pi}\delta(q'_\alpha-q)\right]\hat{\phi}_\alpha(p)\delta(q-q_\alpha)\hat{\phi}_\alpha^*(p_\alpha)\\&=-\frac{g_\alpha}{2\pi}\delta(q'_\alpha-q_\alpha)\hat{\phi}_\alpha^*(p_\alpha)\int dp\hat{\phi}_\alpha(p)\\&=-g_\alpha\sqrt{\frac{a_\alpha}{2\pi}}\delta(q'_\alpha-q_\alpha)\hat{\phi}_\alpha^*(p_\alpha)\ .\end{aligned} \tag{A30}$$

Using Eqs. (2.15) and (A9), this becomes

$$\langle\theta\lambda|V_\alpha P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle=-g_\alpha\sqrt{\frac{a_\alpha}{2\pi}}\delta\left(\sqrt{2\bar{\mu}_\alpha\lambda}\cos(\theta+\tau_{\alpha 1})-\hat{k}_\alpha\sqrt{2\bar{\mu}_\alpha\mu}\right)\hat{\phi}_\alpha^*(p_\alpha)\ . \tag{A31}$$

The term that must be added to Eq. (A29) is thus

$$\begin{aligned}\widetilde{\mathcal{B}}'_{0m,\alpha\pm}(\lambda,\mu)&\equiv\int d\theta dp_\alpha d\hat{k}_\alpha\chi_{0m}^*(\theta)\langle\theta\lambda|V_\alpha P_\alpha|p_\alpha\hat{k}_\alpha\mu\rangle\hat{\phi}_\alpha(p_\alpha)\chi_{\alpha\pm}(\hat{k}_\alpha)\\&=\frac{-g_\alpha(2a_\alpha)^{1/2}\xi_{m\alpha}}{\pi}\int_0^{\pi}d\theta\cos m\theta\delta\left(\sqrt{2\bar{\mu}_\alpha}(\sqrt{\lambda}\cos\theta\mp\sqrt{\mu})\right)\ .\end{aligned} \tag{A32}$$

Letting $q\equiv\sqrt{2\bar{\mu}_\alpha\lambda}\cos\theta$, and $d\theta=-(2\bar{\mu}_\alpha\lambda-q^2)^{-1/2}dq$, the last integral in Eq. (A32) may be evaluated to obtain

$$\widetilde{\mathcal{B}}'_{0m,\alpha\pm}(\lambda,\mu)=\begin{cases}\dfrac{-g_\alpha a_\alpha^{1/2}\xi_{m\alpha}\cos(m\cos^{-1}\pm\sqrt{\mu/\lambda})}{\pi\bar{\mu}_\alpha^{1/2}\sqrt{\lambda-\mu}}, & \text{for } \lambda>\mu\\ 0, & \text{for } \lambda<\mu.\end{cases} \tag{A33}$$

Then

$$\widetilde{\mathcal{B}}_{\alpha\pm,0m}(\lambda,\mu)=\widetilde{\mathcal{B}}_{0m,\alpha\pm}(\mu,\lambda)+\widetilde{\mathcal{B}}'_{0m,\alpha\pm}(\mu,\lambda)\,, \tag{A34}$$

with the right-hand side functions given by Eqs. (A29) and (A33), respectively.

The kernel of $P_0\bar{V}_0P_0=V_1+V_2+V_3$ is the sum of three terms of the form of Eq. (A17). Substituting Eqs. (2.27), (2.28), and (A9) into Eq. (A17) gives the kernel

$$\langle\theta'\lambda|V_\alpha|\theta\mu\rangle\equiv-\frac{g_\alpha}{2\pi}\delta\left(\sqrt{2\bar{\mu}_\alpha}[\sqrt{\lambda}\cos(\theta'+\tau_{\alpha1})-\sqrt{\mu}\cos(\theta+\tau_{\alpha1})]\right)\,, \tag{A35}$$

in KEHS coordinates for $\alpha=1,2,3$. Thus

$$\begin{aligned}\widetilde{\mathcal{B}}^{(\alpha)}_{0n,0m}(\lambda,\mu)&\equiv\int_{-\pi}^{\pi}d\theta'\int_{-\pi}^{\pi}d\theta\chi^*_{0n}(\theta')\langle\theta'\lambda|V_\alpha|\theta\mu\rangle\chi_{0m}(\theta)\\&=-\frac{g_\alpha}{2\pi}\int_{-\pi}^{\pi}d\theta'\int_{-\pi}^{\pi}d\theta\chi^*_{0n}(\theta'-\tau_{\alpha1})\delta\left(\sqrt{2\bar{\mu}_\alpha}(\sqrt{\lambda}\cos\theta'-\sqrt{\mu}\cos\theta)\right)\chi_{0m}(\theta-\tau_{\alpha1})\\&=-\frac{2g_\alpha\xi_{m\alpha}\xi_{n\alpha}}{\pi^2}\int_0^{\pi}d\theta'\int_0^{\pi}d\theta\cos n\theta'\cos m\theta\;\delta\left(\sqrt{2\bar{\mu}_\alpha}(\sqrt{\lambda}\cos\theta'-\sqrt{\mu}\cos\theta)\right)\,,\end{aligned} \tag{A36}$$

for $m,n=0,\pm1,\pm2,\ldots$, and $\alpha=1,2,3$. The integrand of the last integral is symmetric in λ and μ. Suppose that $\lambda>\mu$, and let $q=\sqrt{2\bar{\mu}_\alpha\lambda}\cos\theta'$. Then $d\theta'=-(2\bar{\mu}_\alpha\lambda-q^2)^{-1/2}dq$, and the resulting integral with respect to q may be evaluated to yield

$$\widetilde{\mathcal{B}}^{(\alpha)}_{0n,0m}(\lambda,\mu)=-\frac{2^{1/2}g_\alpha\xi_{m\alpha}\xi_{n\alpha}}{\pi^2\bar{\mu}_\alpha^{1/2}}\int_0^{\pi}d\theta\frac{\cos\left(n\cos^{-1}[\sqrt{\mu/\lambda}\cos\theta]\right)\cos m\theta}{\sqrt{\lambda-\mu\cos^2\theta}}\,, \tag{A37}$$

for $\lambda>\mu$, $m,n=0,\pm1,\pm2\ldots$, and $\alpha=1,2,3$. Then, for $m,n=0,\pm1,\pm2,\ldots$,

$$\widetilde{\mathcal{B}}_{0n,0m}(\lambda,\mu)=\sum_{\alpha=1}^{3}\widetilde{\mathcal{B}}^{(\alpha)}_{0n,0m}(\lambda,\mu)\,,\quad\text{for }\lambda>\mu\,, \tag{A38}$$

and

$$\widetilde{\mathcal{B}}_{0n,0m}(\lambda,\mu)=\widetilde{\mathcal{B}}_{0m,0n}(\mu,\lambda)\,,\quad\text{for }\lambda<\mu\,, \tag{A39}$$

with the right-hand side of Eq. (A39) defined by Eqs. (A37) and (A38).

In summary, we have evaluated, or obtained integral formulas for, all of the matrix elements of $\widetilde{\mathcal{C}}(\lambda,\mu)$ and $\widetilde{\mathcal{B}}(\lambda,\mu)$. In particular, the matrix elements of $\widetilde{\mathcal{C}}(\lambda,\mu)$ are given in Eqs. (A8), (A13), and (A14). The matrix elements of $\widetilde{\mathcal{B}}(\lambda,\mu)$ are given in Eqs. (A23), (A25), (A29), (A33), (A34), and (A37)–(A39). Substituting these formulas for the matrix elements of $\widetilde{\mathcal{C}}(\lambda,\mu)$ and $\widetilde{\mathcal{B}}(\lambda,\mu)$ into Eq. (A1) yields formulas for all of the matrix elements of $\widetilde{\mathcal{A}}(\lambda,\mu)$. We note that $\widetilde{\mathcal{A}}(\lambda,\mu)$ is a real-valued symmetric matrix, as expected, since $\widetilde{\mathcal{A}}(\lambda,\mu)$ is the kernel of a symmetric operator.

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