

SINGULAR CORES IN THE THREE-BODY PROBLEM I: THEORY*

D. D. Brayshaw

Stanford Linear Accelerator Center
Stanford University, Stanford, California 94305

ABSTRACT

The three-body formalism for singular cores previously introduced by the author is considered in some detail. A new derivation is presented which clearly demonstrates the uniqueness of this formalism, and a detailed proof of three-particle unitarity is given for the amplitudes so defined. The kernel for the special case of BCM alone is explicitly evaluated, and the result is used to analyze some problems of solution common to these models. Applications of the formalism and its relation to other approaches are discussed, and a generalization of the BCM is introduced which leads to a potentially interesting and readily calculable three-body model.

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I. INTRODUCTION

In a recent Letter¹, the present author introduced a generalization of the Faddeev formalism to include two-body interactions whose extremely short-range behavior is characterized by a hard core, or by a boundary-condition on the wave-function (BCM). Using the special properties of the BCM t-matrix developed earlier,² it was shown that the usual Faddeev equations do not yield a unique solution for such interactions, but that a particular solution can be defined which yields the desired physical properties. In particular, the resultant three-body wave-function vanishes whenever any pair of particles are within their respective core radius, while its asymptotic behavior corresponds to a unitary three-particle t-matrix. In this paper we give detailed proofs of these assertions, present a new derivation of our equation which clearly demonstrates its uniqueness, and explicitly evaluate the kernel for the special case of BCM alone (no external potential). This provides the theoretical groundwork for subsequent articles in this series dealing with the actual solution of our equations for specific models.

The principal motivation for this development is the versatility afforded by being able to utilize this additional class of interactions in the three-body problem. For example, calculations to-date in the three-nucleon system with realistic interactions have been restricted to soft core models and have generated some doubt as to the ability of such models to fit the experimental data.³ It is not unreasonable to expect the singular core models to produce qualitatively different behavior; functionally, the corresponding off-shell t-matrices are quite different from those of soft cores, exhibiting the typical oscillatory properties of entire functions. Whether or not singular cores can reduce the discrepancy with experiment is of course speculation, but it seems important to explore this possibility.

Nuclear physics aside, the formalism also leads to a number of applications of interest to statistical and chemical physics. An example is the third virial coefficient for a (quantum-mechanical) system of hard spheres. This can be obtained knowing the wave-function for three particles interacting via hard cores,⁴ a special case of our formalism. In fact, with no increase in difficulty, one could also perform such a calculation with hard cores plus weak attractive forces characterized by the BCM. Such computations would be facilitated by a fact pointed out in B1; namely, that for the BCM (or hard core) alone, our equation can be reduced to integral equations in only one variable. Finally, one can take advantage of this property in introducing a generalization of the BCM which is readily amenable to three-body calculations; we shall return to this point in the final section.

We begin in section II with a brief review of the development given in B1. By observing a special property of the BCM t-matrix unnoticed in our earlier work, we are able to present a new derivation for our equation which emphasizes the fact that it is unique. Section III is devoted to explicit proofs of the three-particle unitarity relations for our amplitudes. At the same time, the algebraic notation introduced in B1 (and recapitulated in section II) is employed to construct particularly transparent derivations of unitarity for the usual Faddeev amplitudes.

In section IV we introduce a "super-vector" notation in order to simplify evaluation of the operator product IQ appearing in our kernel; this result is then employed in section V, where we explicitly evaluate the kernel for the special case of BCM alone. Here the separability of the kernel in one of its (vector) variables leads to a coupled set of integral equations in one vector variable; projection onto states of definite total angular momentum results in coupled one-dimensional equations. At the end of this section we take advantage of the relative

simplicity of this case to consider in some detail the relationship between our amplitudes and the three-body wave-function.

Finally, section VI is devoted to a discussion of various aspects of the formalism, its relation to the work of other authors, and to problems involved in obtaining actual solutions. Here we also consider a potentially interesting generalization of the BCM and outline the calculational program now underway. In the Appendix we give a derivation of the operator Q which plays a crucial role in our development.

II. THREE-BODY FORMALISM FOR SINGULAR CORES

In this section we briefly review the theoretical development given in B1, recapitulating some useful notational conventions. We also present a new derivation of the integral equation introduced in B1. This derivation supplements the previous (more physical) argument by clearly demonstrating the fact that our new equation is unique. As in B1, we make the nonessential but simplifying assumption that our three particles are spinless.

We denote the mass of particle α by m_α and the total three-body c.m. energy by W . Three-particle states are described by the usual Jacobi variables $\vec{p}_\alpha, \vec{q}_\alpha$, with the corresponding reduced masses μ_α, M_α ;

$$\mu_\alpha^{-1} = m_\beta^{-1} + m_\gamma^{-1}, \quad (1)$$

$$M_\alpha^{-1} = m_\alpha^{-1} + (m_\beta + m_\gamma)^{-1},$$

and $(\alpha\beta\gamma)$ are cyclic permutations of (123). In the usual channel decomposition, the three-body state vector is $|\Psi\rangle = \sum_\alpha |\psi_\alpha\rangle$, where the $|\psi_\alpha\rangle$ satisfy

$$|\psi_\alpha\rangle = (1 - G_0 t_\alpha) |\phi\rangle - G_0 t_\alpha \sum_{\beta \neq \alpha} |\psi_\beta\rangle. \quad (2)$$

Here t_α represents the two-body t -matrix as an operator in the three-body Hilbert space, $|\phi\rangle$ is a plane-wave state, and $G_0 = G_0(W)$ is the free Green function. Equation (2) is one expression of the Faddeev equations.⁵

It is convenient to introduce the states $|\alpha \vec{p} \vec{q}\rangle$, where

$$\langle \alpha \vec{p}' \vec{q}' | \beta \vec{p} \vec{q} \rangle = \delta_{\alpha\beta} \delta(\vec{p}' - \vec{p}) \delta(\vec{q}' - \vec{q}), \quad (3)$$

$$\sum_\alpha \int d\vec{p} d\vec{q} |\alpha \vec{p} \vec{q}\rangle \langle \alpha \vec{p} \vec{q}| = 1.$$

We can then define the operators t , I such that

$$\begin{aligned}
\langle \alpha \vec{p}' \vec{q}' | t | \beta \vec{p} \vec{q} \rangle &= \delta_{\alpha\beta} \delta(\vec{q}' - \vec{q}) t_{\alpha}(\vec{p}', \vec{p}; W - q^2/2M_{\alpha}), \\
\langle \alpha \vec{p}' \vec{q}' | I | \beta \vec{p} \vec{q} \rangle &= - \delta\left(\vec{p} + \frac{\mu\beta}{m_{\gamma}} \vec{p}' - \frac{\mu\beta}{M_{\alpha}} \vec{q}'\right) \delta\left(\vec{q} + \vec{p}' + \frac{\mu_{\alpha}}{m_{\gamma}} \vec{q}'\right) \\
&\quad \text{if } \alpha\beta\gamma \text{ are cyclic,} \\
&\quad (4) \\
&= - \delta\left(\vec{p} + \frac{\mu\beta}{m_{\gamma}} \vec{p}' + \frac{\mu\beta}{M_{\alpha}} \vec{q}'\right) \delta\left(\vec{q} - \vec{p}' + \frac{\mu_{\alpha}}{m_{\gamma}} \vec{q}'\right) \\
&\quad \text{if } \beta\alpha\gamma \text{ are cyclic.}
\end{aligned}$$

Here $t_{\alpha}(\vec{p}', \vec{p}; s)$ is the off-shell two-body t -matrix for particles β and γ , energy s ; the diagonal elements of I vanish. With the identification

$$\psi_{\alpha}(\vec{p}_{\alpha}, \vec{q}_{\alpha}) = \langle \vec{p}_{\alpha} \vec{q}_{\alpha} | \psi_{\alpha} \rangle \equiv \langle \alpha \vec{p}_{\alpha} \vec{q}_{\alpha}' | \psi \rangle, \quad (5)$$

and letting $|\psi\rangle = M |\phi\rangle$, we can rewrite Eq. (2) in the form

$$M = 1 - G_0 t + G_0 t I M. \quad (6)$$

It is important to keep in mind that the operators in Eq. (6) act on the states of Eq. (3); in particular

$$\langle \alpha \vec{p}' \vec{q}' | G_0 | \beta \vec{p} \vec{q} \rangle = \frac{\delta_{\alpha\beta} \delta(\vec{p}' - \vec{p}) \delta(\vec{q}' - \vec{q})}{p^2/2\mu_{\alpha} + q^2/2M_{\alpha} - W - i\epsilon}. \quad (7)$$

One can easily verify that I and G_0 commute.

The development up to this point is completely general, with the object of obtaining the operator equation for M , Eq. (6). Since Eq. (6) is exactly equivalent to the equations of Faddeev, one can immediately infer that it serves

to uniquely define M for a large class of two-body potentials. However, it was shown in B1 that this is not the case in the presence of singular cores. The proof is based on the fact that for such interactions, the two-body t-matrix has the special property that

$$\tilde{V} G_0 t = t G_0 \tilde{V} = \tilde{V} \quad , \quad (8)$$

where $\tilde{V} = \tilde{V} \tilde{V}$ corresponds to a square-well potential of unit strength and a range a_α for the matrix element

$$\langle \alpha \vec{p}' \vec{q}' | \tilde{V} | \beta \vec{p} \vec{q} \rangle = \delta_{\alpha\beta} \delta(\vec{q}' - \vec{q}) \tilde{V}_\alpha(\vec{p}' - \vec{p}) . \quad (9)$$

That is, $\tilde{V}_\alpha(\vec{p})$ is the Fourier transform of the unit step-function $\theta(a_\alpha - r)$.

Moreover, one can construct an operator Q of the form $Q = 1 + \tilde{V} B (I - 1)$ with the following properties:

$$\begin{aligned} Q Q &= Q , \\ V (1 - I) Q &= (1 - I) Q \tilde{V} = 0 , \\ (1 - \tilde{V} I) Q &= 1 - \tilde{V} , \\ Q \tilde{V} &= \tilde{V} Q \tilde{V} . \end{aligned} \quad (10)$$

(An explicit derivation of Q is given in the Appendix.) Using Eqs. (8) and (10), one observes that

$$(1 - G_0 t I) G_0 Q \tilde{V} = 0 , \quad (11)$$

and hence that $(1 - G_0 t I)^{-1}$ does not exist. Therefore, one cannot use the ordinary Faddeev equations (Eq. (6)) to uniquely determine M in the presence of singular cores.

To overcome this difficulty, a generalization of the Faddeev formalism was presented in B1. We consider a new operator \tilde{t} chosen such that

$$1 - G_0 t = (1 - \tilde{V}) (1 - G_0 \tilde{t}) . \quad (12)$$

A particular solution M to Eq. (6) can then be defined as $M = Q M_e$, where M_e satisfies the new equation

$$M_e = 1 - G_0 \tilde{t} + G_0 \tilde{t} I Q M_e . \quad (13)$$

This new equation was motivated in B1 by imposing reasonable physical requirements on the resultant three-body wave-function; namely, that it should vanish whenever any two particles are within their respective core radius, and must correspond to a unitary three-body t -matrix.

We now consider a somewhat different derivation which employs another special relation concerning the two-body t -matrix: the fact that \tilde{t} can be chosen such that

$$\tilde{t} \tilde{V} = 0 . \quad (14)$$

Postponing a proof of this assertion until the end of this section, we proceed by assuming that M is any solution of Eq. (6). Employing Eq. (8), it follows that

$$\begin{aligned} \tilde{V} M &= \tilde{V} (1 - G_0 t + G_0 t I M) , \\ &= \tilde{V} I M . \end{aligned} \quad (15)$$

The form of Q then implies that $Q M = M$. Noting that with our choice of states (Eq. (3)) the relationship between M and the three-body state vector is given by $|\Psi\rangle = (1 - I) M |\phi\rangle$, we have that

$$|\Psi\rangle = (1 - I) Q M |\phi\rangle . \quad (16)$$

We next observe that, as a consequence of Eq. (14) and the properties of Q ,

$$\begin{aligned} \tilde{t} I Q \tilde{V} &= \tilde{t} Q \tilde{V} \\ &= \tilde{t} \tilde{V} Q \tilde{V} \\ &= 0 . \end{aligned} \quad (17)$$

Hence, substituting Eq. (12) into Eq. (6), we deduce that

$$\tilde{t} I Q M = \tilde{t} I Q (1 - G_0 \tilde{t} + G_0 \tilde{t} I M) . \quad (18)$$

Defining

$$X = \tilde{t} I Q M = \tilde{t} I M , \quad (19)$$

we obtain an integral equation for X ;

$$X = \tilde{t} I Q (1 - G_0 \tilde{t}) + \tilde{t} I Q G_0 X . \quad (20)$$

Comparing this equation to Eq. (13), we infer that $X = \tilde{t} I Q M_e$, i. e. , the two equations are totally equivalent.

Moreover, we observe that X is all that is required to form $|\psi\rangle$, since Eqs. (6) and (12) imply that

$$M = \tilde{V} (1 - G_0 \tilde{t}) \cdot (-1 + I M) + 1 - G_0 \tilde{t} + G_0 X . \quad (21)$$

Hence, due to Eq. (16), we have

$$\begin{aligned} |\psi\rangle &= (1 - I) Q (1 - G_0 \tilde{t} + G_0 X) |\phi\rangle \\ &= (1 - I) Q M_e |\phi\rangle . \end{aligned} \quad (22)$$

Finally, we note that although \tilde{t} is not uniquely defined by Eqs. (12) and (14), any change in \tilde{t} must be of the form $\Delta\tilde{t} = G_0^{-1} \tilde{V} A$. If we suppose that M_e^1 is the solution of Eq. (13) under the replacement $\tilde{t} \rightarrow \tilde{t}' = \tilde{t} + \Delta\tilde{t}$, it follows from Eq. (17) that

$$M_e^1 = M_e + \tilde{V} A (-1 + I Q M_e^1) . \quad (23)$$

However, $|\psi\rangle$ is invariant under such a change. We thus conclude that our equation is to all intents unique.

We conclude this section by considering the nature of \tilde{t} and the proof of Eq. (14). To do so it is clearly adequate to drop subscripts and work in a two-body space. Denoting the core radius by a , we shall first deal with the

case of the BCM alone ($\tilde{t} = \tilde{t}^{\text{BC}}$); the subsequent generalization to BCM plus external potential is trivial. We look for $\tilde{t}_\ell^{\text{BC}}$, the projection of \tilde{t}^{BC} on partial-wave ℓ , in the form

$$\tilde{t}_\ell^{\text{BC}}(p', p; s) = G_\ell(p', s) t_\ell^{\text{BC}}(\kappa, p; s). \quad (24)$$

Here $\kappa = (2 M_r s)^{1/2}$ is the on-shell momentum value; t_ℓ^{BC} is thus proportional to the half-on-shell BCM amplitude. We assert that G_ℓ may be constructed in the form

$$\begin{aligned} G_\ell(p, s) &= 1 + (p^2 - \kappa^2) \sum_{n=0, 2, \dots}^{\ell} \alpha_n(\kappa^2) j_{n-2}(ap), \\ &\quad (\ell \text{ even}), \quad (25) \\ &= \frac{1}{\kappa} \left\{ p + (p^2 - \kappa^2) \sum_{n=1, 3, \dots}^{\ell} \beta_n(\kappa^2) j_{n-2}(ap) \right\}, \\ &\quad (\ell \text{ odd}), \end{aligned}$$

with $\alpha_0 = \beta_1 \equiv 0$, and the remaining α_n, β_n chosen such that $G_\ell(p, s) \propto p^\ell$ as $p \rightarrow 0$. To prove the latter statement we note that the $\alpha_n (\beta_n)$ can be determined inductively, i. e., suppose that the statement is true for a given ℓ (say ℓ is even for definiteness), then

$$G_\ell(p, s) \xrightarrow{p \rightarrow 0} \frac{G_\ell^{(\ell)}(0, s)}{\ell!} p^\ell, \quad (26)$$

with $G_\ell^{(\ell)}(0, s)$ completely determined by the $\alpha_n, n \leq \ell$. Noting that

$$G_{\ell+2}(p, s) - G_\ell(p, s) = (p^2 - \kappa^2) \alpha_{\ell+2}(\kappa^2) j_\ell(ap), \quad (27)$$

we can clearly satisfy the condition for $l+2$ by taking

$$\alpha_{l+2}^{(\kappa^2)} = \frac{(2l+1)!!}{\kappa^{2l!}} \cdot \frac{G_l^{(\ell)}(0, s)}{a^l}. \quad (28)$$

Since the condition holds for $l = 0$ we are done (the proof for odd l follows similarly). Given G_l , we can now apply equation [39] of B2 to evaluate the operator product $\tilde{V} G_0 \tilde{t}^{BC}$; together with the explicit form for t^{BC} given in equation [48] of B2, this immediately verifies Eq. (12) for the BCM alone.

In order to generalize this result to the case-of BCM plus external potential, we remind the reader of equation [71] of B2, which states that

$$t = t^{BC} + (1 - t^{BC} G_0) V_e (1 - G_0 t), \quad (29)$$

in which V_e is the external potential. In view of the pure BCM result, we simply observe that the choice

$$\tilde{t} = \tilde{t}^{BC} + (1 - \tilde{t}^{BC} G_0) V_e (1 - G_0 t) \quad (30)$$

satisfies Eq. (12). Given Eqs. (24) and (30) it is straight forward to verify that \tilde{t} satisfies the unitarity relation

$$\tilde{t}_\ell(p', p; s+i\epsilon) - \tilde{t}_\ell(p', p; s-i\epsilon) = -i\pi 2M_r \kappa \tilde{t}_\ell(p', \kappa; s+i\epsilon) \tilde{t}_\ell(\kappa, p; s-i\epsilon). \quad (31)$$

In the subsequent sections we shall denote this symbolically by

$$\begin{aligned} \Delta \tilde{t} &\equiv \tilde{t}^+ - \tilde{t}^- = -\tilde{t}^+ \Delta G_0 \tilde{t}^- \\ &= -\tilde{t}^- \Delta G_0 \tilde{t}^+, \end{aligned} \quad (32)$$

ΔG_0 being the discontinuity of the free Green function.

Finally, having established the form of \tilde{t} , we turn to the consideration of Eq. (14). It is clear from Eq. (30) that \tilde{t} is of the form $\tilde{t} = A \tilde{t}^{BC} + B V_e$. However, since $V_e = (1 - \tilde{V}) V_e = V_e (1 - \tilde{V})$, we infer that $\tilde{t} \tilde{V} \propto \tilde{t}^{BC} \tilde{V}$; hence it

is only necessary to treat the case of BCM alone. From the formulas developed in B2 one can easily show that

$$t_{\ell}^{\text{BC}}(\kappa, p; s) = \frac{g_{\ell}(p)}{D_{\ell}(\kappa)} , \quad (33)$$

with

$$g_{\ell}(p) = (a\lambda_{\ell} - \ell) j_{\ell}(ap) + ap j_{\ell+1}(ap),$$

$$D_{\ell}(\kappa) = i\pi M_{\text{r}} \kappa \left[(a\lambda_{\ell} - \ell) h_{\ell}(a\kappa) + a\kappa h_{\ell+1}(a\kappa) \right] . \quad (34)$$

(With our convention $\psi'_{\ell}/\psi_{\ell} = \lambda_{\ell}$ at the core radius). Note that the verification of the above is greatly aided by the alternative formula

$$f_{\ell}(p, a, \kappa) = ia\kappa \left[a\kappa h_{\ell+1}(a\kappa) j_{\ell}(ap) - h_{\ell}(a\kappa) ap j_{\ell+1}(ap) \right] , \quad (35)$$

for the quantity f_{ℓ} defined in B2.

Consequently, the proof that $\tilde{t} \tilde{V} = 0$ rests on showing that

$$I_{\ell} \equiv \int_0^{\infty} dp p^2 g_{\ell}(p) \tilde{V}_{\ell}(p, p') = 0 . \quad (36)$$

This, however, is somewhat delicate since I_{ℓ} is ill-defined. To see this it is convenient to employ the representation

$$g_{\ell}(p) = \int_0^{\infty} dr r^2 j_{\ell}(pr) \hat{g}_{\ell}(r) , \quad (37)$$

$$\hat{g}_{\ell}(r) = \frac{(a\lambda_{\ell} + 1)}{a^2} \delta(r-a) + \frac{\delta'(r-a)}{r} .$$

Thus

$$I_{\ell} = \int_0^{\infty} dr r^2 \hat{g}_{\ell}(r) \theta(a-r) j_{\ell}(rp') , \quad (38)$$

$$= \theta(0)g_{\ell}(p') - a \delta(0)j_{\ell}(ap') ,$$

and hence is dependent on the ambiguous quantities $\theta(0)$, $\delta(0)$.

In this circumstance we argue that I_ℓ must be evaluated as a limit in which the radial parameter related to g_ℓ is taken to be $b > a$, the integral is performed, and the limit $b \rightarrow a$ is taken at the end; this prescription clearly gives zero as a result. In order to justify this with respect to the alternative choice of limit ($a > b$), we first observe that the pure BCM is a model in which the wave-function vanishes in the core region and its asymptotic behavior sets in immediately exterior to the core. However, the latter behavior is defined by the t-matrix, and it is thus reasonable to associate the parameters of the t-matrix with the external region ($b > a$). Moreover, if one re-examines relations such as Eqs. (11) and (15) in terms of such a limit, one finds that only the choice $b > a$ is compatible. Finally, a more detailed analysis shows that the choice $a > b$ leads to an exponentially divergent kernel in Eq. (13).

III. THREE-BODY UNITARITY

In this section we give an explicit proof of the three-particle unitarity relations for our new formalism, Eq. (13). In doing so, it will be convenient to adopt a notation of the type illustrated in Eq. (32) in order to express the discontinuities of an amplitude across its cut. As is well known, the discontinuities of the off-shell three-body t-matrix T as a function of the total energy W arise from two sources: (1) scattering to states consisting of three free particles, with a threshold $W=0$, (2) elastic scattering of a single particle from a bound state of two others. In the latter case thresholds are found at $W = \nu_{\alpha j}$, where $-\nu_{\alpha j}$ is the binding energy for the j-th bound state of particles β and γ . The cuts from both sources are taken to lie to the right of the corresponding threshold along the real W-axis.

As an illustration, we first consider the relation for cut (1) in the ordinary Faddeev formalism. We note that the relationship between M and T is given by

$$1 - G_0 T = (1-I) M. \quad (39)$$

By assumption, we have that in this case the operator

$$Z = (1 - G_0 t I)^{-1} \quad (40)$$

exists. The unitarity condition for t is that $\Delta t = -t^- \Delta G_0 t^+$; thus

$$\Delta Z = Z^- (1 - G_0^- t^-) \Delta G_0 t^+ I Z^+. \quad (41)$$

From Eq. (6) we have $M = Z (1 - G_0 t)$; it follows that

$$\begin{aligned} \Delta M &= \Delta Z (1 - G_0^+ t) - Z^- (1 - G_0^- t^-) \Delta G_0 t^+, \\ &= M^- \Delta G_0 t^+ (I Z^+ [1 - G_0^+ t] - 1) , \\ &= M^- \Delta G_0 t^+ (I M^+ - 1) . \end{aligned} \quad (42)$$

However, Eq. (6) implies that

$$t(IM-1) = G_0^{-1} (M-1) , \quad (43)$$

while $\Delta G_0 G_0^{-1} A = 0$ unless a corresponding factor of G_0 occurs in A (ΔG_0 puts operator to the right on-shell). Thus

$$\Delta M = M^- \Delta G_0 G_0^{-1} M^+ . \quad (44)$$

On the other hand, Eq. (39) says that

$$T = -G_0^{-1} [(1-I) M-1] , \quad (45)$$

and hence

$$\Delta T = -G_0^{-1} (1-I) \Delta M . \quad (46)$$

At this point we observe that the definition of I , Eq. (4), implies that

$$\begin{aligned} I^{-1} &= \frac{1}{2} (1+I) , \\ (1-I)^2 &= 3(1-I) , \\ (1-I)(2+I) &= 0 . \end{aligned} \quad (47)$$

Since

$$\begin{aligned} M &= Z (1-G_0 t I + I - 1) I^{-1} , \\ &= I^{-1} + Z (I-1) I^{-1} , \end{aligned} \quad (48)$$

we find that

$$(1-I) M = \frac{1}{3} (1-I) M (1-I) . \quad (49)$$

Thus

$$\begin{aligned} \Delta T &= -\frac{1}{3} G_0^{-1} (1-I) M^- \Delta G_0 G_0^{-1} (1-I) M^+ , \\ &= -\frac{1}{3} T^- \Delta G_0 T^+ , \end{aligned} \quad (50)$$

where we have used the fact that I and G_0 commute. Note that the factor of $1/3$ appearing in Eq. (50) arises from triple counting due to our choice of intermediate states; Eq. (50) is exactly equivalent to the usual statement of three-particle unitarity.

We now turn to an analogous derivation based on Eq. (13). Defining

$$Y = (1 - G_0 \tilde{t} I Q)^{-1}, \quad (51)$$

so

$$M_e = Y(1 - G_0 \tilde{t}),$$

we have

$$\Delta Y = Y^-(1 - G_0 \tilde{t}^-) \Delta G_0 \tilde{t}^+ I Q Y^+, \quad (52)$$

where we have used Eq. (32). Thus

$$\begin{aligned} \Delta M_e &= M_e^- \Delta G_0 \tilde{t}^+ (I Q M_e^+ - 1), \\ &= M_e^- \Delta G_0 G_0^{-1} M_e^+. \end{aligned} \quad (53)$$

Furthermore, Eq. (51) implies that

$$M_e = 1 + Y G_0 \tilde{t} (I Q - 1), \quad (54)$$

and the form of Q implies that $I Q - 1 \propto 1 - I$;

thus

$$(1 - I) Q M_e = \frac{1}{3} (1 - I) Q M_e (1 - I). \quad (55)$$

Eqs. (45) and (46), plus the relation $M = Q M_e$,

then give us the result

$$\begin{aligned} \Delta T &= -\frac{1}{3} G_0^{-1} (1 - I) Q M_e^- \Delta G_0 G_0^{-1} (1 - I) M_e^+, \\ &= -\frac{1}{3} T^- \Delta G_0 T^+, \end{aligned} \quad (56)$$

having used $\Delta G_0 G_0^{-1} Q = \Delta G_0 G_0^{-1}$. Equation (56) thus establishes that Eq. (13) leads to the proper statement of three-particle unitarity with regard to the cut of type (1).

We next consider cuts of type (2), recalling that

$$t_{\alpha}(\vec{p}', \vec{p}; s) \xrightarrow{S \rightarrow \nu_{\alpha j}} \frac{2\ell+1}{4\pi} P_{\ell}(\hat{p}' \cdot \hat{p}) \frac{g_{\alpha j}(p') g_{\alpha j}(p)}{S - \nu_{\alpha j}}, \quad (57)$$

ℓ being the partial-wave in which the bound state occurs. It is helpful to define the operators $r_{\alpha j}$, $S_{\alpha j}$ such that

$$\begin{aligned} \langle \beta \vec{p}' \vec{q}' | r_{\alpha j} | \gamma \vec{p} \vec{q} \rangle &= \delta_{\beta\alpha} \delta_{\gamma\alpha} \delta(\vec{q}' - \vec{q}) \frac{(2\ell+1)}{4\pi} P_{\ell}(\hat{p}' \cdot \hat{p}) g_{\alpha j}(p') g_{\alpha j}(p), \\ \langle \beta \vec{p}' \vec{q}' | S_{\alpha j} | \gamma \vec{p} \vec{q} \rangle &= \delta_{\beta\alpha} \delta_{\gamma\alpha} \frac{\delta(\vec{p}' - \vec{p}) \delta(\vec{q}' - \vec{q})}{W - q^2/2M_{\alpha} - \nu_{\alpha j} + i\epsilon}. \end{aligned} \quad (58)$$

The cut of t arising from the bound state pole $\nu_{\alpha j}$ then has the discontinuity

$$\Delta t = r_{\alpha j} \Delta S_{\alpha j}. \quad (59)$$

Clearly, $\Delta S_{\alpha j} \propto \delta(q - q_{\alpha j})$, where

$$q_{\alpha j}^2 = 2 M_{\alpha} (W - \nu_{\alpha j}). \quad (60)$$

For the usual Faddeev theory it follows that

$$\begin{aligned} \Delta M &= \Delta Z(1 - G_0 t^+) - Z^- G_0 \Delta t, \\ &= Z^- G_0 \Delta t (IM^+ - 1); \end{aligned} \quad (61)$$

thus

$$\Delta T = -G_0^{-1} (1 - I) Z^- G_0 \Delta t (IM^+ - 1). \quad (62)$$

On the other hand, we note that the effect of the operator $\Delta S_{\alpha j} S_{\alpha j}^{-1}$ is to pick out the residue at the $\nu_{\alpha j}$ pole of the operator it acts on; hence

$$\Delta S_{\alpha j} S_{\alpha j}^{-1} t = \Delta S_{\alpha j} r_{\alpha j}, \quad (63)$$

for example. Therefore

$$\begin{aligned}
\Delta S_{\alpha j} S_{\alpha j}^{-1} T &= -\Delta S_{\alpha j} S_{\alpha j}^{-1} G_0^{-1} M, \\
&= -\Delta S_{\alpha j} S_{\alpha j}^{-1} G_0^{-1} (1-G_0 t + G_0 t IM), \\
&= -\Delta S_{\alpha j} r_{\alpha j} (IM-1), \\
&= -\Delta t (IM-1).
\end{aligned} \tag{64}$$

Similarly,

$$\begin{aligned}
TS_{\alpha j}^{-1} \Delta S_{\alpha j} &= -G_0^{-1} (1-I) Z (1-G_0 t) S_{\alpha j}^{-1} \Delta S_{\alpha j}, \\
&= G_0^{-1} (1-I) Z G_0 \Delta t.
\end{aligned} \tag{65}$$

We also note that $r_{\alpha j}^2 = \rho_{\alpha j} r_{\alpha j}$, where⁶

$$\rho_{\alpha j} = \int_0^{\infty} dp p^2 g_{\alpha j}^2(p). \tag{66}$$

Thus

$$\begin{aligned}
\Delta T &= -G_0^{-1} (1-I) Z^{-1} G_0 \frac{r_{\alpha j}}{\rho_{\alpha j}} \Delta t (IM^+ - 1), \\
&= G_0^{-1} (1-I) Z^{-1} G_0 \frac{r_{\alpha j}}{\rho_{\alpha j}} \Delta S_{\alpha j} S_{\alpha j}^{-1} T^+, \\
&= T^- S_{\alpha j}^{-1} \frac{\Delta S_{\alpha j}}{\rho_{\alpha j}} S_{\alpha j}^{-1} T^+.
\end{aligned} \tag{67}$$

Defining

$$\Delta_{\alpha j} = S_{\alpha j}^{-1} \frac{\Delta S_{\alpha j}}{\rho_{\alpha j}} S_{\alpha j}^{-1}, \tag{68}$$

we finally obtain

$$\Delta T = T^- \Delta_{\alpha j} T^+. \tag{69}$$

When Eq. (69) is inserted between the proper initial and final states one obtains the usual unitarity relations connecting the break-up, elastic scattering, and re-arrangement amplitudes.

Finally, considering the same cut for our singular core formalism, we have that

$$\Delta M_e = Y^- G_0 \Delta \tilde{t} (IQM_e^+ - 1), \quad (70)$$

thus

$$\Delta T = -G_0^{-1} (1-I) Q Y^- G_0 \Delta \tilde{t} (IQM_e^+ - 1). \quad (71)$$

Applying Eq. (12), we deduce that

$$G_0 \Delta t = (1-\tilde{V}) G_0 \Delta \tilde{t}. \quad (72)$$

Consequently, using the properties of Q given in Eq. (10) and Eq. (17), we find that

$$(1-I) Q Y \tilde{V} = (1-I) Q \tilde{V} = 0. \quad (73)$$

Thus

$$\begin{aligned} (1-I) Q Y^- G_0 \Delta \tilde{t} &= (1-I) Q Y^- (1-\tilde{V}) G_0 \Delta \tilde{t}, \\ &= (1-I) Q Y^- G_0 \Delta t. \end{aligned} \quad (74)$$

Similarly, we note that

$$\begin{aligned} (1-I) Q M_e &= (1-I) Q (1-\tilde{V}) M_e, \\ &= (1-I) Q [1 - G_0 t + (G_0 t - \tilde{V}) IQM_e^{-1}]; \end{aligned} \quad (75)$$

this implies that

$$\begin{aligned} \Delta S_{\alpha j} S_{\alpha j}^{-1} T &= -\Delta S_{\alpha j} S_{\alpha j}^{-1} G_0^{-1} (1-I) Q M_e \\ &= -\Delta S_{\alpha j} S_{\alpha j}^{-1} t (IQM_e^{-1}) \\ &= -\Delta t (IQM_e^{-1}). \end{aligned} \quad (76)$$

Hence

$$\begin{aligned} \Delta T &= -G_0^{-1} (1-I) Q Y^- G_0 \frac{r_{\alpha j}}{\rho_{\alpha j}} \Delta t (IQM_e^+ - 1), \\ &= G_0^{-1} (1-I) Q Y^- G_0 \frac{\Delta t}{\rho_{\alpha j}} S_{\alpha j}^{-1} T^+, \\ &= T^- \Delta_{\alpha j} T^+, \end{aligned} \quad (77)$$

the last relation following similarly to the above.

In concluding this section, it must be pointed out that the above proofs rest on the existence of the operator Y defined in Eq. (51). At present the author has not been able to prove this rigorously; however, the existence of Y has been confirmed by the direct calculations to be described in the next paper of this series. We also note the ease of the above proofs for the usual Faddeev formalism as a result of the algebraic formulation introduced in B1 and summarized in Section II.

IV. EVALUATION OF IQ

In order to apply our new formalism, Eq. (13), one must first evaluate the operator product IQ which appears in the kernel. This being a somewhat tedious process, we shall devote this section to an abbreviated derivation of the result. The procedure followed is greatly facilitated by introducing a "super-vector" notation to describe our operators. We shall thus find it convenient to represent the pair of three-vectors \vec{p} , \vec{q} by the "super-vector" $\vec{\eta}$,

$$\vec{\eta} = \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}, \quad (78)$$

represented as a two-component spinor, each component being a three-vector.

We also note that Eq. (1) can be shown to imply the following relations between the reduced masses:

$$\frac{\mu_\beta}{M_\alpha} = \frac{\mu_\alpha}{M_\beta}, \quad (79)$$

$$\frac{\mu_\alpha}{M_\beta} + \frac{\mu_\alpha \mu_\beta}{m_\gamma^2} = 1,$$

$$\frac{1}{M_\alpha} = \frac{1}{m_\alpha} + \frac{\mu_\alpha}{m_\beta m_\gamma}.$$

Defining the rotation matrices ($\alpha \neq \beta \neq \gamma$)

$$R_{\beta\alpha} = \begin{pmatrix} -\frac{\mu_\alpha}{m_\alpha} & 1 \\ -\frac{\mu_\beta}{M_\alpha} & -\frac{\mu_\beta}{m_\alpha} \end{pmatrix}, \quad (80)$$

Eq. (79) implies that $\det R_{\beta\alpha} = 1$,

$$R_{\beta\alpha}^{-1} = \begin{pmatrix} \frac{-\mu_\beta}{m_\gamma} & -1 \\ \frac{\mu_\alpha}{M_\beta} & \frac{-\mu_\alpha}{m_\gamma} \end{pmatrix}. \quad (81)$$

It is also easy to verify that

$$R_{\gamma\alpha} R_{\alpha\beta} R_{\beta\gamma} = 1. \quad (82)$$

In what follows we shall mean by $R_{\beta\alpha} \vec{\eta}$ the "super-vector" $\vec{\eta}'$, where

$$\vec{\eta}' = \begin{pmatrix} \frac{-\mu_\alpha}{m_\gamma} \vec{q} + \vec{p} \\ \frac{-\mu_\beta}{M_\alpha} \vec{q} - \frac{\mu_\beta}{m_\gamma} \vec{p} \end{pmatrix}. \quad (83)$$

The above conventions allow us to make representations such as

$$\mathcal{A}_\alpha(\vec{\eta}) = A_\alpha(\vec{p}, \vec{q}) = \langle A | \alpha \vec{p} \vec{q} \rangle, \quad (84)$$

$$\mathcal{B}_\alpha(\vec{\eta}) = B_\alpha(\vec{p}, \vec{q}) = \langle \alpha \vec{p} \vec{q} | B \rangle.$$

From the matrix elements of I given in Eq. (4) one can then show that

$$\langle A | I | \alpha \vec{p} \vec{q} \rangle = -\mathcal{A}_\gamma(R_{\gamma\alpha} \vec{\eta}) - \mathcal{A}_\beta(R_{\alpha\beta}^{-1} \vec{\eta}), \quad (85)$$

$$\langle \alpha \vec{p} \vec{q} | I | B \rangle = -\mathcal{B}_\beta(R_{\alpha\beta}^{-1} \vec{\eta}) - \mathcal{B}_\gamma(R_{\gamma\alpha} \vec{\eta}),$$

where $\alpha \beta \gamma$ are cyclic. Thus the operator I which connects the channels has the effect of a rotation on $\vec{\eta}$.

As shown in the Appendix, Q is of the form $Q = 1 + \tilde{V} B (I-1)$, where

$$\langle \alpha \vec{p}' \vec{q}' | B | \beta \vec{p} \vec{q} \rangle = \delta_{\alpha\beta} \left\{ \delta(\Delta \vec{p}) \delta(\Delta \vec{q}) - \frac{1}{2} \delta(\vec{q}_1) \tilde{V}_\sigma(\vec{q}_2) - \frac{1}{2} \delta(\vec{q}_2) \tilde{V}_\epsilon(\vec{q}_1) + \frac{1}{3} \tilde{V}_\epsilon(\vec{q}_1) \tilde{V}_\sigma(\vec{q}_2) \right\}, \quad (86)$$

$$\begin{aligned} \Delta \vec{p} &= \vec{p} - \vec{p}', \\ \Delta \vec{q} &= \vec{q} - \vec{q}', \\ \vec{q}_1 &= \Delta \vec{p} + \frac{\mu_\alpha}{m_\epsilon} \Delta \vec{q}, \\ \vec{q}_2 &= -\Delta \vec{p} + \frac{\mu_\alpha}{m_\sigma} \Delta \vec{q}, \quad \alpha\sigma\epsilon \text{ cyclic.} \end{aligned}$$

We thus observe that the above matrix element of B can be represented in the form

$\delta_{\alpha\beta} \mathcal{B}_\alpha(\vec{\Delta}; \vec{\eta}_1, \vec{\eta}_2)$, with $\vec{\Delta}, \vec{\eta}_1, \vec{\eta}_2$ the "super-vectors"

$$\begin{aligned} \vec{\Delta} &= \vec{\eta} - \vec{\eta}', \\ \vec{\eta}_1 &= R_{\alpha\sigma}^{-1} \vec{\Delta}, \\ \vec{\eta}_2 &= R_{\epsilon\alpha} \vec{\Delta}. \end{aligned} \quad (87)$$

Note that $\mathcal{B}_\alpha(\vec{\Delta}; \vec{\eta}_1, \vec{\eta}_2)$ only depends on $\vec{\Delta}$ and the upper components of $\vec{\eta}_1, \vec{\eta}_2$ (\vec{q}_1, \vec{q}_2). We take advantage of the fact that B and \tilde{V} commute to write $Q = 1 + B\tilde{V}(I-1)$; Eq. (85) and the above representation then imply that

$$\begin{aligned} \langle \alpha \vec{p}' \vec{q}' | IB | \beta \vec{p} \vec{q} \rangle &= \\ &- \delta_{\beta\sigma} \mathcal{B}_\sigma(\vec{\eta} - R_{\alpha\sigma}^{-1} \vec{\eta}'; R_{\alpha\epsilon}^{-1} \vec{\eta} - R_{\epsilon\alpha} \vec{\eta}', R_{\alpha\sigma} \vec{\eta} - \vec{\eta}') \\ &- \delta_{\beta\epsilon} \mathcal{B}_\epsilon(\vec{\eta} - R_{\epsilon\alpha} \vec{\eta}'; R_{\epsilon\alpha}^{-1} \vec{\eta} - \vec{\eta}', R_{\sigma\epsilon} \vec{\eta} - R_{\alpha\sigma}^{-1} \vec{\eta}'), \end{aligned} \quad (88)$$

with $\alpha\sigma\epsilon$ cyclic.

Comparing Eqs. (86) and (88), we can now make a key observation which greatly simplifies the subsequent analysis. That is, it is possible to represent IB in the form

$$IB = I + C + \tilde{V}D. \quad (89)$$

Hence, since $\tilde{t}\tilde{V} = 0$, and we shall only need the product $\tilde{t}IQ = \tilde{t}[I + IB\tilde{V}(I-1)]$ for our integral equation, e.g., Eq. (20), we do not have to evaluate D. In fact, one never needs D at all since neither the three-body wave-function⁷ nor the on-shell t-matrix require it (D does appear, however, in the off-shell three-body t-matrix). As an example of terms contributing to D, we note that \mathcal{B}_σ of Eq. (88) contains the terms

$$\tilde{V}_\alpha(\vec{q}_1) \left\{ -\frac{1}{2} \delta(\vec{q}_2) + \frac{1}{3} \tilde{V}_\epsilon(\vec{q}_2) \right\},$$

where

$$\vec{q}_1 = -\frac{\mu_\sigma}{m_\alpha} \vec{q} - \vec{p} + \frac{\mu_\alpha}{m_\sigma} \vec{q}' - \vec{p}', \quad (90)$$

$$\vec{q}_2 = -\frac{\mu_\sigma}{m_\epsilon} \vec{q} + \vec{p} - \vec{q}'.$$

The important point here is that \vec{q}_2 is independent of \vec{p}' . Recalling Eq. (9) then leads to the above conclusion. We observe in particular that all the double products of \tilde{V} in B go into D, greatly simplifying our subsequent expressions.

Collecting the terms which contribute to C, it is straight forward to show that

$$\begin{aligned} \langle \alpha \vec{p}' \vec{q}' | C | \beta \vec{p} \vec{q} \rangle &= \delta_{\beta\sigma} \frac{1}{2} \delta\left(\vec{p} + \frac{\mu_\sigma}{m_\alpha} \vec{q} + \vec{p}' - \frac{\mu_\alpha}{m_\sigma} \vec{q}'\right) \tilde{V}_\epsilon\left(\vec{q} + \vec{p}' + \frac{\mu_\alpha}{m_\epsilon} \vec{q}'\right) \\ &+ \delta_{\beta\epsilon} \frac{1}{2} \delta\left(\vec{p} - \frac{\mu_\epsilon}{m_\alpha} \vec{q} + \vec{p}' + \frac{\mu_\alpha}{m_\epsilon} \vec{q}'\right) \tilde{V}_\sigma\left(\vec{q} - \vec{p}' + \frac{\mu_\alpha}{m_\sigma} \vec{q}'\right), \end{aligned} \quad (91)$$

$\alpha\sigma\epsilon$ cyclic.

The delta-functions in C make the product $C\tilde{V}$ trivial to evaluate, and if we adopt the further notation $\mathcal{V}_\alpha(\vec{\eta}) = \tilde{V}_\alpha(\vec{q})$, the result is conveniently expressed as

$$\begin{aligned} \mathcal{F}_{\alpha\beta}(\vec{\eta}', \vec{\eta}) &\equiv \langle \alpha \vec{p}' \vec{q}' | C\tilde{V} | \beta \vec{p} \vec{q} \rangle, \quad (92) \\ &= \delta_{\beta\sigma} \frac{1}{2} \mathcal{V}_\sigma \left(-R_{\epsilon\alpha} \vec{\eta}' + R_{\sigma\epsilon}^{-1} \vec{\eta} \right) \mathcal{V}_\epsilon \left(\vec{\eta} - R_{\alpha\sigma}^{-1} \vec{\eta}' \right) \\ &+ \delta_{\beta\epsilon} \frac{1}{2} \mathcal{V}_\epsilon \left(R_{\alpha\sigma}^{-1} \vec{\eta}' - R_{\sigma\epsilon} \vec{\eta} \right) \mathcal{V}_\sigma \left(\vec{\eta} - R_{\epsilon\alpha} \vec{\eta}' \right). \end{aligned}$$

If we now write

$$IQ = I + \Omega_1 + \Omega_2 + \tilde{V}D', \quad (93)$$

where

$$\Omega_1 = C\tilde{V}(I-1),$$

$$\Omega_2 = I\tilde{V}(I-1),$$

Eqs. (85) and (92) imply that

$$\begin{aligned} \langle \beta \vec{p}' \vec{q}' | \Omega_1 | \alpha \vec{p} \vec{q} \rangle &= - \mathcal{F}_{\beta\alpha}(\vec{\eta}', \vec{\eta}) - \mathcal{F}_{\beta\epsilon}(\vec{\eta}', R_{\epsilon\alpha} \vec{\eta}) - \mathcal{F}_{\beta\sigma}(\vec{\eta}', R_{\alpha\sigma}^{-1} \vec{\eta}), \\ &= - \delta_{\alpha\beta} \tilde{V}_\tau \left(-\vec{p}' + \vec{p} + \frac{\mu_\beta}{m_\tau} [\vec{q} - \vec{q}'] \right) \tilde{V}_\rho \left(\vec{p} - \vec{p}' + \frac{\mu_\beta}{m_\rho} [\vec{q}' - \vec{q}] \right) \\ &- \delta_{\alpha\rho} \tilde{V}_\tau \left(\vec{p}' + \vec{q} + \frac{\mu_\beta}{m_\tau} \vec{q}' \right) \tilde{V}_\rho \left(\vec{p} + \vec{p}' + \frac{\mu_\rho}{m_\beta} \vec{q} - \frac{\mu_\beta}{m_\rho} \vec{q}' \right) \\ &- \delta_{\alpha\tau} \tilde{V}_\tau \left(\vec{p} + \vec{p}' + \frac{\mu_\beta}{m_\tau} \vec{q}' - \frac{\mu_\tau}{m_\beta} \vec{q} \right) \tilde{V}_\rho \left(-\vec{p}' + \vec{q} + \frac{\mu_\beta}{m_\rho} \vec{q}' \right), \quad (94) \end{aligned}$$

$\beta\rho\tau$ cyclic.

In order to evaluate Ω_2 we proceed similarly, letting

$$\langle \alpha \vec{p}' \vec{q}' | \tilde{V} | \beta \vec{p} \vec{q} \rangle = \delta_{\alpha\beta} \mathcal{N}_\alpha(\vec{\eta}', \vec{\eta}). \quad (95)$$

Equation (85) implies that

$$\langle \alpha \vec{p}' \vec{q}' | I \tilde{V} | \beta \vec{p} \vec{q} \rangle = -\delta_{\beta\sigma} \mathcal{N}_\sigma \left(R_{\alpha\sigma}^{-1} \vec{\eta}', \vec{\eta} \right) - \delta_{\beta\epsilon} \mathcal{N}_\epsilon \left(R_{\epsilon\alpha} \vec{\eta}', \vec{\eta} \right),$$

$\alpha\sigma\epsilon$ cyclic. Again applying Eq. (85), we obtain

$$\begin{aligned} \langle \beta \vec{p}' \vec{q}' | \Omega_2 | \alpha \vec{p} \vec{q} \rangle = & \quad (96) \\ & \delta_{\alpha\beta} \left[\mathcal{N}_\tau \left(R_{\tau\beta} \vec{\eta}', R_{\tau\beta} \vec{\eta} \right) + \mathcal{N}_\rho \left(R_{\beta\rho}^{-1} \vec{\eta}', R_{\beta\rho}^{-1} \vec{\eta} \right) \right] \\ & + \delta_{\alpha\rho} \left[\mathcal{N}_\rho \left(R_{\beta\rho}^{-1} \vec{\eta}', \vec{\eta} \right) + \mathcal{N}_\tau \left(R_{\tau\beta} \vec{\eta}', R_{\rho\tau}^{-1} \vec{\eta} \right) \right] \\ & + \delta_{\alpha\tau} \left[\mathcal{N}_\tau \left(R_{\tau\beta} \vec{\eta}', \vec{\eta} \right) + \mathcal{N}_\rho \left(R_{\beta\rho}^{-1} \vec{\eta}', R_{\rho\tau} \vec{\eta} \right) \right], \end{aligned}$$

$\beta\rho\tau$ cyclic. Finally, using the definition of \mathcal{N}_α given in Eq. (95), we arrive at the result

$$\begin{aligned} \langle \beta \vec{p}' \vec{q}' | \Omega_2 | \alpha \vec{p} \vec{q} \rangle = & \quad (97) \\ & \delta_{\alpha\beta} \left\{ \delta \left(\vec{p}' - \vec{p} + \frac{\mu_\beta}{m_\tau} (\vec{q}' - \vec{q}) \right) \tilde{V}_\rho(\vec{q}' - \vec{q}) + \delta \left(\vec{p}' - \vec{p} + \frac{\mu_\beta}{m_\rho} (\vec{q} - \vec{q}') \right) \tilde{V}_\tau(\vec{q}' - \vec{q}) \right\} \\ & + \delta_{\alpha\rho} \left\{ \delta \left(\vec{p}' + \frac{\mu_\beta}{m_\tau} \vec{q}' + \vec{q} \right) \tilde{V}_\rho \left(\vec{q}' + \frac{\mu_\rho}{m_\tau} \vec{q} - \vec{p} \right) + \delta \left(\vec{p}' - \frac{\mu_\beta}{m_\rho} \vec{q}' + \vec{p} + \frac{\mu_\rho}{m_\beta} \vec{q} \right) \tilde{V}_\tau \left(\vec{q}' - \vec{p} + \frac{\mu_\rho}{m_\tau} \vec{q} \right) \right\} \\ & + \delta_{\alpha\tau} \left\{ \delta \left(\vec{p}' + \frac{\mu_\beta}{m_\tau} \vec{q}' + \vec{p} - \frac{\mu_\tau}{m_\beta} \vec{q} \right) \tilde{V}_\rho \left(\vec{q}' + \vec{p} + \frac{\mu_\tau}{m_\rho} \vec{q} \right) + \delta \left(\vec{p}' - \frac{\mu_\beta}{m_\rho} \vec{q}' - \vec{q} \right) \tilde{V}_\tau \left(\vec{q}' + \vec{p} + \frac{\mu_\tau}{m_\rho} \vec{q} \right) \right\}. \end{aligned}$$

With Eq. (93) and the above explicit formulas we can now proceed with the evaluation of our kernel.

V. KERNEL EVALUATION FOR THE PURE BCM

The simplest example of our formalism is realized when the pair interactions are specified by the BCM alone (pure BCM). In this section we shall consider the explicit evaluation of our kernel for this special case. Aside from not having to specify a particular external potential, this choice is motivated by several considerations. In the first place, this model in itself is not totally uninteresting. For example, it contains as a special case the proper quantum - mechanical formulation for a system of three hard spheres. Moreover, as a consequence of Eq. (24), the kernel is separable in each partial-wave, and hence the problem is particularly easy to solve. It is thus quite practical to explore the consequences of this model (and a generalization to be discussed in the next section) as a first approximation to the interactions in three-body systems of more direct physical interest, such as the triton system.

Aside from these areas of immediate application, however, the expressions which we shall obtain for the pure BCM play a special role in the more general problem of BCM plus external potential. This is due to the fact that if we write our general $\tilde{t} = \tilde{t}^{BC} + \Delta \tilde{t}$ as suggested by Eq. (30), the most singular part of the kernel arises from \tilde{t}^{BC} . In fact, as we shall see, the pure BCM contribution to the kernel is sufficiently singular as to require special treatment.

In what follows we will use the separability of \tilde{t}^{BC} to obtain a coupled set of integral equations in one vector variable, the kernel of which we shall determine in some detail. Coupled one-dimensional equations can be derived from this set by projecting onto states of total angular momentum; since this is totally analogous to the reduction of the usual Faddeev equations with separable t-matrices⁸ we shall only sketch this step. In concluding this section we shall take advantage of the simplicity of the pure BCM to investigate the relationship between our calculated amplitudes and the corresponding three-body wave-function.

It will be advantageous to define the states $|\alpha lm\vec{q}\rangle$ and $\langle\alpha lm\vec{q}|$ such that

$$\langle\beta\vec{p}'\vec{q}'|\alpha lm\vec{q}\rangle = \delta_{\alpha\beta} \delta(\vec{q}-\vec{q}') \frac{Y_{lm}(\hat{p}') G_l^\alpha(p', s_\alpha)}{D_l^\alpha(\kappa_\alpha)}, \quad (98)$$

$$\langle\alpha lm\vec{q}|\beta\vec{p}'\vec{q}'\rangle = \delta_{\alpha\beta} \delta(\vec{q}-\vec{q}') Y_{lm}^*(\hat{p}) g_l^\alpha(p).$$

Here

$$\begin{aligned} s_\alpha &= W - q^2/2 M_\alpha, \\ \kappa_\alpha &= (2\mu_\alpha s_\alpha)^{1/2}; \end{aligned} \quad (99)$$

while G_l^α , g_l^α , D_l^α are the quantities defined in Eqs. (24) and (33) with a particle index α added. It then follows that \tilde{t}^{BC} may be represented in the form

$$\tilde{t}^{BC} = \sum_{\alpha lm} \int d\vec{q} |\alpha lm\vec{q}\rangle \langle\alpha lm\vec{q}|. \quad (100)$$

Defining the amplitudes

$$X_{lm}^\alpha(\vec{q}) = \langle\alpha lm\vec{q}|\text{IQM}_e|\phi\rangle, \quad (101)$$

$$Z_{lm}^\alpha(\vec{q}) = \langle\alpha lm\vec{q}|\text{IQ}(1 - G_0\tilde{t})|\phi\rangle,$$

in which we suppress the parameters characterizing the plane-wave state $|\phi\rangle$, Eq. (13) and the above imply that $X_{lm}^\alpha(\vec{q})$ satisfies the coupled equations

$$X_{lm}^\alpha(\vec{q}) = Z_{lm}^\alpha(\vec{q}) + \sum_{\beta l'm'} \int d\vec{q}' K_{lm;l'm'}^{\alpha\beta}(\vec{q}, \vec{q}') X_{l'm'}^\beta(\vec{q}'),$$

with

$$K_{lm;l'm'}^{\alpha\beta}(\vec{q}, \vec{q}') = \langle\alpha lm\vec{q}|\text{IQG}_0|\beta l'm'\vec{q}'\rangle. \quad (102)$$

Employing the results of the preceding section as to the form of IQ, we now proceed to evaluate explicitly the matrix elements of this kernel. Introducing the cyclic set $\alpha\sigma\epsilon$, we begin with the diagonal element ($\beta=\alpha$). Recalling

Eq. (93), we observe that there are contributions to this element from Ω_1 and Ω_2 , so that

$$K_{lm;l'm'}^{\alpha\alpha}(\vec{q}',\vec{q}) = \frac{2\mu_\alpha}{D_{l',(\kappa_\alpha)}^\alpha} \int d\vec{p}' Y_{lm}^*(\hat{p}') g_l^\alpha(p') \int \frac{d\vec{p} Y_{l'm'}(\hat{p})}{p^2 - \kappa_\alpha^2} G_{l'}^\alpha(p, s_\alpha) \times \\ \times \langle \alpha \vec{p}' \vec{q}' | \Omega_1 + \Omega_2 | \alpha \vec{p} \vec{q} \rangle. \quad (103)$$

Equation (94) implies that the contribution of Ω_1 to the above double integral is

$$- \int d\vec{P}' Y_{lm}^*(\hat{p}') g_l^\alpha(p') \int \frac{d\vec{p} Y_{l'm'}(\hat{p})}{p^2 - \kappa_\alpha^2} G_{l'}^\alpha(p, s_\alpha) \tilde{V}_\epsilon \left(\vec{P}' + \frac{\mu_\alpha}{m_\epsilon} \vec{\Delta} \right) \tilde{V}_\sigma \left(\vec{P}' - \frac{\mu_\alpha}{m_\sigma} \vec{\Delta} \right), \quad (104)$$

where we have made the change of variable $\vec{p}' = \vec{P}' + \vec{p}$ and introduced $\vec{\Delta} = \vec{q}' - \vec{q}$.

We now substitute for \tilde{V}_ϵ and \tilde{V}_σ their Fourier transforms, e. g.,

$$\tilde{V}_\epsilon(\vec{Q}) = \frac{1}{(2\pi)^3} \int d\vec{x} e^{i\vec{x} \cdot \vec{Q}} \theta(a_\epsilon - x), \quad (105)$$

while $\tilde{V}_\sigma(\vec{Q})$ involves the coordinate \vec{y} and range a_σ .

Making the subsequent change of variables

$$\vec{u} = \vec{x} + \vec{y}, \\ \vec{v} = \vec{y} - \vec{x}, \\ d\vec{x} d\vec{y} = d\vec{u} d\vec{v}, \quad (106)$$

Eq. (104) becomes

$$- \frac{i\kappa_\alpha}{16\pi^2} i^{\ell' - \ell} \int d\vec{v} e^{i\vec{v} \cdot \vec{\Delta}} \int d\vec{u} h_{l',(\mu\kappa_\alpha)}^{\Lambda\alpha}(u) Y_{l'm'}(\hat{u}) Y_{lm}^*(\hat{u}) \times \\ \times \theta \left(a_\epsilon - \left| \vec{v} - \frac{\mu_\alpha}{m_\sigma} \vec{u} \right| \right) \theta \left(a_\sigma - \left| \vec{v} + \frac{\mu_\alpha}{m_\epsilon} \vec{u} \right| \right). \quad (107)$$

Here we have made use of the representation

$$e^{i\vec{x}\cdot\vec{q}} = 4\pi \sum_{\ell m} i^\ell j_\ell(xq) Y_{\ell m}(\hat{x}) Y_{\ell m}^*(\hat{q}) \quad (108)$$

and the properties of $G_{\ell'}^\alpha(p, s_\alpha)$ which follow from Eq. (25) to deduce that

$$\int \frac{d\vec{p}}{p^{2-\kappa_\alpha}} Y_{\ell'm'}(\hat{p}) G_{\ell'}^\alpha(p, s_\alpha) e^{i\vec{u}\cdot\vec{p}} = 2\pi^2 i^{\ell'+1} \kappa_\alpha h_{\ell'}(u\kappa_\alpha) Y_{\ell'm'}(\hat{u}), \quad (109)$$

while Eq. (37) and the relation

$$\int_0^\infty dp p^2 j_\ell(up) j_\ell(rp) = \frac{\pi}{2} \frac{\delta(u-r)}{r^2} \quad (110)$$

imply that

$$\int d\vec{p}' Y_{\ell m}^*(\hat{p}') g_\ell^\alpha(p') e^{-i\vec{u}\cdot\vec{p}'} = 2\pi^2 i^{-\ell} g_\ell^\alpha(u) Y_{\ell m}^*(\hat{u}). \quad (111)$$

We now introduce a partial-wave expansion for the product of two theta-functions,

$$\theta\left(a_\epsilon - \left|\vec{v} - \frac{\mu_\alpha}{m_\sigma} \vec{u}\right|\right) \theta\left(a_\sigma - \left|\vec{v} + \frac{\mu_\alpha}{m_\epsilon} \vec{u}\right|\right) = \sum_{LM} \theta_L^\alpha(u, v) Y_{LM}(\hat{u}) Y_{LM}^*(\hat{v}); \quad (112)$$

hence

$$\theta_L^\alpha(u, v) = 2\pi \int_{-1}^1 dz P_L(z) \theta\left(a_\epsilon - \left|\vec{v} - \frac{\mu_\alpha}{m_\sigma} \vec{u}\right|\right) \theta\left(a_\sigma - \left|\vec{v} + \frac{\mu_\alpha}{m_\epsilon} \vec{u}\right|\right), \quad (113)$$

$$z = \hat{u} \cdot \hat{v}.$$

Defining

$$\tilde{Z}_M = \frac{a_\sigma^2 - v^2 - \frac{\mu_\alpha^2}{m_\epsilon^2} u^2}{2 \frac{\mu_\alpha}{m_\epsilon} u v} , \quad (114)$$

$$\tilde{Z}_L = \frac{a_\epsilon^2 - v^2 - \frac{\mu_\alpha^2}{m_\sigma^2} u^2}{-2 \frac{\mu_\alpha}{m_\sigma} u v} ,$$

it is easy to see that

$$\theta_L^\alpha(u, v) = 2\pi \int_{Z_L}^{Z_M} dZ P_L(Z) , \quad (115)$$

$$Z_M = \min(1, \tilde{Z}_M) , \quad Z_L = \max(-1, \tilde{Z}_L) ,$$

where the integral is taken to vanish if $Z_M < -1$, $Z_L > 1$, or $Z_L > Z_M$.

Adopting the notation

$$\begin{aligned} \mathcal{I}_{Mm'm}^{Ll'l} &\equiv \int d\hat{u} Y_{l'm'}(\hat{u}) Y_{LM}(\hat{u}) Y_{lm}^*(\hat{u}) , \\ &= \left[\frac{(2l'+1)(2L+1)}{4\pi(2l+1)} \right]^{1/2} C(Ll'l; Mm'm) C(Ll'l; 000), \end{aligned} \quad (116)$$

for the integral of three spherical harmonics,⁹ and employing the expression for $g_\ell^\alpha(u)$ given in Eq. (37), Eq. (107) becomes

$$-\frac{i\kappa_\alpha}{4\pi} \sum_{LM} i^{L+l'-l} \mathcal{J}_{Mm'm}^{Ll'l} Y_{LM}^*(\hat{\Delta}) \int_0^\infty dv v^2 j_L(v\Delta) J_{Ll'l}^\alpha(v, \kappa_\alpha), \quad (117)$$

where

$$J_{Ll'l}^\alpha(v, \kappa_\alpha) = \left[(a_\alpha \lambda_\ell^\alpha - l') h_{l, (a_\alpha \kappa_\alpha)} + a_\alpha \kappa_\alpha h_{l+1, (a_\alpha \kappa_\alpha)} \right] \theta_L^\alpha(a_\alpha, v) - a_\alpha h_{l, (a_\alpha \kappa_\alpha)} \theta_L^{\alpha'}(a_\alpha, v).$$

We next note that the contribution of Ω_2 to the double integral in Eq. (103) is given by

$$\int \frac{d\vec{p}}{p^2 - \kappa_\alpha^2} Y_{l'm, (\hat{p})} G_{l'}^\alpha(p, s_\alpha) \left\{ \tilde{V}_\sigma(\vec{\Delta}) \left[Y_{lm}^*(\hat{p}') g_\ell^\alpha(p') \right]_{\vec{p}' = \vec{p} - (\mu_\alpha/m_\epsilon) \vec{\Delta}} + \tilde{V}_\epsilon(\vec{\Delta}) \left[Y_{lm}^*(\hat{p}') g_\ell^\alpha(p') \right]_{\vec{p}' = \vec{p} + (\mu_\alpha/m_\sigma) \vec{\Delta}} \right\}. \quad (118)$$

Making use of the relation

$$Y_{lm}^*(\hat{p}') j_\ell(rp') = \frac{i^{-l}}{4\pi} \int d\hat{r} Y_{lm}^*(\hat{r}) e^{i\vec{r} \cdot \vec{p}'}, \quad (119)$$

we observe that

$$\int d\hat{p} Y_{l'm, (\hat{p})} Y_{lm}^*(\hat{p}') g_\ell^\alpha(p') = 4\pi \sum_{LM} i^{L+l'-l} \mathcal{J}_{Mm'm}^{Ll'l} Y_{LM}^*(\hat{Q}) \times \int_0^\infty dr r^2 g_\ell^\alpha(r) j_L(rQ) j_{l'}(rp) \quad (120)$$

for $\vec{p}' = \vec{p} + \vec{Q}$, where we have used Eqs. (37) and (116). Employing this

relation in Eq. (118), and performing the dp-integration as in Eq. (109), we find that the Ω_2 contribution becomes

$$\frac{i\kappa_\alpha}{4\pi} \sum_{LM} i^{L+l'-l} \mathcal{J}_{Mm'm}^{Ll'l} Y_{LM}^*(\hat{\Delta}) \left\{ \left[(a_\alpha \lambda_l^\alpha - l') h_{l',(a_\alpha \kappa_\alpha)} + a_\alpha \kappa_\alpha h_{l'+1,(a_\alpha \kappa_\alpha)} \right] \times \right. \\ \left. \times N_L^\alpha(\Delta, a_\alpha) - a_\alpha h_{l',(a_\alpha \kappa_\alpha)} N_L^{\alpha'}(\Delta, a_\alpha) \right\}, \quad (121)$$

where

$$\frac{N_L^\alpha(\Delta, v)}{(2\pi)^3} = \tilde{V}_\sigma(\Delta) (-1)^L j_L(v \frac{\mu_\alpha}{m_\epsilon} \Delta) + \tilde{V}_\epsilon(\Delta) j_L(v \frac{\mu_\alpha}{m_\sigma} \Delta).$$

In adding the two contributions exhibited in Eqs. (117) and (121), it is helpful to represent them in somewhat similar form. It is clear that if we write

$$N_L^\alpha(\Delta, u) = \int_0^\infty dv v^2 j_L(v\Delta) \rho_L^\alpha(u, v), \quad (122)$$

we can express Eq. (121) in the form of Eq. (117) with an integral $\tilde{J}_{Ll'l}^\alpha(v, \kappa_\alpha)$ defined as in the second part of Eq. (117), but with θ_L^α replaced by ρ_L^α . To determine the latter we apply Eq. (110) to obtain

$$\rho_L^\alpha(u, v) = \frac{2}{\pi} \int_0^\infty dq q^2 j_L(vq) N_L^\alpha(q, u). \quad (123)$$

Given the explicit form of N_L^α , the integral can be evaluated with the aid of the expression

$$j_\ell(vq) j_\ell(\sigma q) = \frac{1}{2} \int_{-1}^1 dz P_\ell(z) j_0(rq), \quad (124)$$

$$r = (v^2 + \sigma^2 - 2v\sigma z)^{1/2},$$

invoking a standard property of the spherical Bessel functions, as well as the formula

$$\tilde{V}_\alpha(q) = \frac{1}{2\pi^2} \int_0^\infty dx x^2 j_0(xq) \theta(a_\alpha - x), \quad (125)$$

which follows from Eq. (105). We thus obtain

$$\rho_L^\alpha(u, v) = 2\pi \int_{-1}^1 dz P_L(z) \left\{ \theta\left(a_\sigma - \left| \vec{v} + \frac{\mu_\alpha}{m_\epsilon} \vec{u} \right| \right) + \theta\left(a_\epsilon - \left| \vec{v} - \frac{\mu_\alpha}{m_\sigma} \vec{u} \right| \right) \right\}. \quad (126)$$

If we now compare this expression to the definition of θ_L^α given in Eq. (113) it is clear that

$$\frac{\rho_L^\alpha(u, v)}{2\pi} = \int_{-1}^{z_M} dz P_L(z) + \int_{z_L}^1 dz P_L(z), \quad (127)$$

with z_M, z_L defined as in Eq. (115). Defining

$$\sum_L^\alpha(u, v) = \rho_L^\alpha(u, v) - \theta_L^\alpha(u, v), \quad (128)$$

it follows that

$$\begin{aligned} \sum_L^\alpha(u, v) &= 4\pi \delta_{L0} \theta(z_M - z_L) + \theta(z_L - z_M) \rho_L^\alpha(u, v), \\ &= 4\pi \delta_{L0} \theta(z_M - z_L) + 2\pi \delta_{L0} \theta(z_L - z_M) \left[\theta(1+z_M) + \theta(1-z_L) \right] \\ &\quad + \frac{2\pi \theta(z_L - z_M)}{2L+1} \left[P_{L+1}(z) - P_{L-1}(z) \right]_{z_L}^{z_M}. \end{aligned} \quad (129)$$

Here one takes $P_{-1} \equiv 1$ and, as above, $P_n(z)$ is taken to vanish if $|z| > 1$.

Recalling Eq. (114), it is straightforward to show that

$$\theta(z_L - z_M) = \theta\left(v - v_0^\alpha(u)\right),$$

with

$$v_0^\alpha(u) = \left\{ \frac{m_\epsilon a_\sigma^2 + m_\sigma a_\epsilon^2 - \mu_\alpha u^2}{m_\epsilon + m_\sigma} \right\}^{1/2}. \quad (130)$$

Similarly, the conditions $|z| \leq 1$ restricts v to being less than a finite upper bound depending on the mass ratios and core radii, i. e., $v < v_{\text{MAX}}$.

To complete our evaluation of the diagonal element we introduce the definite integral

$$R_L^\alpha(\Delta, u) = \frac{1}{4\pi} \int_0^{v_{\text{MAX}}} dv v^2 j_L(v\Delta) \sum_L^\alpha(u, v). \quad (131)$$

Recalling Eqs. (34) and (103) we obtain

$$\begin{aligned} K_{lm; l'm'}^{\alpha\alpha}(\vec{q}', \vec{q}) &= \frac{2}{\pi} \sum_{LM} i^{L+l'-l} \mathcal{S}_{Mm'm}^{Ll'l} Y_{LM}^*(\hat{\Delta}) R_L^\alpha(\Delta, a_\alpha) \\ &+ 2\mu_\alpha i a_\alpha \kappa_\alpha \frac{h_{l'}(a_\alpha \kappa_\alpha)}{D_{l'}^\alpha(\kappa_\alpha)} \sum_{LM} i^{L+l'-l} \mathcal{S}_{Mm'm}^{Ll'l} Y_{LM}^*(\hat{\Delta}) \left\{ (\lambda_\ell^\alpha - \lambda_{\ell'}^\alpha) R_L^\alpha(\Delta, a_\alpha) \right. \\ &\quad \left. - R_L^{\alpha'}(\Delta, a_\alpha) \right\}. \quad (132) \end{aligned}$$

Here we note that $R_L^{\alpha'}$ means the derivative with respect to u ; Eq. (131) is to be evaluated with u regarded as infinitesimally close to a_α (these integrals are in fact elementary). For a given l and l' , due to the Clebsch-Gordan coefficients contained in $\mathcal{S}_{Mm'm}^{Ll'l}$, the diagonal element of the kernel is a finite sum of functions which can be expressed in closed form.

Turning now to the off-diagonal elements, we first note that

$$\langle \alpha \vec{p}' \vec{q}' | I | \sigma \vec{p} \vec{q} \rangle = -\delta \left(\vec{p} - \frac{\mu_\sigma}{m_\epsilon} \vec{q} - \vec{q}' \right) \delta \left(\vec{p}' + \vec{q} + \frac{\mu_\alpha}{m_\epsilon} \vec{q}' \right), \quad (133)$$

$$\langle \alpha \vec{p}' \vec{q}' | I | \epsilon \vec{p} \vec{q} \rangle = -\delta \left(\vec{p} + \frac{\mu_\epsilon}{m_\sigma} \vec{q} + \vec{q}' \right) \delta \left(\vec{p}' - \vec{q} - \frac{\mu_\alpha}{m_\sigma} \vec{q}' \right),$$

$\alpha \sigma \epsilon$ cyclic, where we have used Eqs. (4) and (79). We will also need the integral

$$\begin{aligned} \int \frac{d\vec{p}}{p^2 - \kappa_\sigma^2} Y_{\ell m}(\hat{p}) G_\ell^\sigma(p, s_\sigma) \tilde{V}_\sigma(\vec{p} - \vec{Q}) \\ = \frac{Y_{\ell m}(\hat{Q})}{Q^2 - \kappa_\sigma^2} \left[G_\ell^\sigma(Q, s_\sigma) - f_\ell(Q, a_\sigma, \kappa_\sigma) \right], \end{aligned} \quad (134)$$

where we have used the partial-wave expansion

$$\tilde{V}_\sigma(\vec{p} - \vec{Q}) = \sum_{\ell m} \tilde{V}_\ell^\sigma(p, Q) Y_{\ell m}(\hat{Q}) Y_{\ell m}^*(\hat{p}), \quad (135)$$

and Eq. [39] of B2. Given the above, it is straightforward to show that

$$\begin{aligned} \frac{K_{\ell m; \ell' m'}^{\alpha \sigma}(\vec{q}', \vec{q})}{2\mu_\sigma [D_{\ell'}^\sigma(\kappa_\sigma)]^{-1}} = - \frac{Y_{\ell m}^*(\hat{P}'_{\alpha \epsilon}) g_\ell^\alpha(P'_{\alpha \epsilon}) Y_{\ell' m'}(\hat{P}'_{\sigma \epsilon}) f_{\ell'}(P_{\sigma \epsilon}, a_\sigma, \kappa_\sigma)}{P_{\sigma \epsilon}^2 - \kappa_\sigma^2} \\ + \int \frac{d\vec{p}}{p^2 - \kappa_\sigma^2} Y_{\ell' m'}(\hat{p}) f_{\ell'}(p, a_\sigma, \kappa_\sigma) \tilde{V}_\epsilon(\vec{p} - \vec{P}'_{\sigma \epsilon}) Y_{\ell m}^*(\hat{p}') g_\ell^\alpha(p'), \end{aligned} \quad (136)$$

with $\vec{p}' = \vec{\Delta}_{\alpha\sigma} - \vec{p}$. Here we have introduced the quantities

$$\begin{aligned}\vec{P}'_{\alpha\beta} &= (\pm) \left(\vec{q} + \frac{\mu_\alpha}{m_\beta} \vec{q}' \right), \\ P_{\alpha\beta} &= (\pm) \left(\frac{\mu_\alpha}{m_\beta} \vec{q} + \vec{q}' \right), \\ \vec{\Delta}_{\alpha\beta} &= (\pm) \left(\frac{\mu_\alpha}{m_\beta} \vec{q}' - \frac{\mu_\beta}{m_\alpha} \vec{q} \right),\end{aligned}\tag{137}$$

where the upper (lower) sign pertains if $\alpha\beta$ is cyclic (anticyclic). By employing methods similar to those discussed above in the evaluation of the diagonal element, the integral term in Eq. (136) can be expressed as

$$4\pi \sum_{\substack{LL'L'' \\ MM'M''}} i^{L''-L-l} \mathcal{S}_{m'MM'}^{l'LL'} \mathcal{S}_{mMM''}^{lLL''} Y_{L''M''}^* (\hat{\Delta}_{\alpha\sigma}) Y_{L'M'} (\hat{P}_{\sigma\epsilon}) F_{\ell\ell';LL'L''}^{\alpha\sigma}(P_{\sigma\epsilon}, \Delta_{\alpha\sigma}, \kappa_\sigma).\tag{138}$$

Here we have defined

$$F_{\ell\ell';LL'L''}^{\alpha\sigma}(P, \Delta, \kappa) = \int_0^\infty \frac{dp p^2}{p^2 - \kappa^2} f_{\ell'}(p, a_\sigma, \kappa) \tilde{V}_{L'}^\epsilon(p, P) M_{\ell LL''}^\alpha(p, \Delta),\tag{139}$$

where

$$\begin{aligned}M_{\ell LL''}^\alpha(p, \Delta) &= (a_\alpha \lambda_\ell^\alpha - L - L'') j_L(a_\alpha p) j_{L''}(a_\alpha \Delta) \\ &+ a_\alpha p j_{L+1}(a_\alpha p) j_{L''}(a_\alpha \Delta) + a_\alpha \Delta j_L(a_\alpha p) j_{L''+1}(a_\alpha \Delta).\end{aligned}$$

We note that the summation over L in Eq. (138) is over all integers, while for fixed L the other indices have a finite range. In practice, the $F_{\ell\ell';LL'L''}^{\alpha\sigma}$ integral falls off rapidly as L increases and the sum may be safely truncated; this integral is complicated but can be performed analytically. The $K^{\alpha\epsilon}$ element can be obtained from the above expressions for $K^{\alpha\sigma}$ by simply exchanging σ and ϵ .

We have thus obtained explicit expressions for the kernel of Eq. (102), involving at most one infinite (and rapidly converging) sum of elementary functions. We note that, as anticipated in section II., our kernel does not contain any reference to the ambiguous quantity $G_\ell^\alpha(p, s)$, i. e., the kernel is invariant with respect to allowed changes in \tilde{t} . It is also worth noting that although $\tilde{t}_\ell^\beta(p', p; s_\beta)$ blows up exponentially like $e^{-ia_\beta \kappa_\beta}$ as $q \rightarrow \infty$, the effect of integrating \tilde{t} with $IQ G_0$ is to explicitly cancel this divergence. Thus, the divergent quantity $\left[D_{\ell'(\kappa_\beta)}^\beta \right]^{-1}$ only occurs in the above expressions multiplied by either $f_{\ell'}(p, a_\beta, \kappa_\beta)$ or $h_{\ell'}(a_\beta \kappa_\beta)$, which contain the explicit factor $e^{ia_\beta \kappa_\beta}$.

In order to reduce Eq. (102) to a set of coupled one-dimensional equations one proceeds in the usual way, defining the functions

$$X_{\ell\lambda}^{\alpha;JM}(q) = \sum_{m\mu} C(\ell\lambda J; m\mu M) \int d\hat{q} Y_{\lambda\mu}^*(\hat{q}) X_{\ell m}^\alpha(\vec{q}), \quad (140)$$

which satisfy

$$X_{\ell\lambda}^{\alpha;JM}(q) = Z_{\ell\lambda}^{\alpha;JM}(q) + \sum_{\beta\ell'\lambda'} \int_0^\infty dq' q'^2 K_{\ell\lambda;\ell'\lambda'}^{\alpha\beta;JM}(q, q') X_{\ell'\lambda'}^{\beta;JM}(q'). \quad (141)$$

Here the driving term is given by Eq. (140) with X replaced by Z; the kernel is

$$K_{\ell\lambda;\ell'\lambda'}^{\alpha\beta;JM}(q, q') = \sum_{\substack{m\mu \\ m'\mu'}} C(\ell\lambda J; m\mu M) C(\ell'\lambda' J; m'\mu' M) \int d\hat{q} Y_{\lambda\mu}^*(\hat{q}) \int d\hat{q}' Y_{\lambda'\mu'}(\hat{q}') K_{\ell m;\ell' m'}^{\alpha\beta}(\vec{q}, \vec{q}'). \quad (142)$$

By employing standard tricks with rotation functions, the double integral in Eq.

(142) can be reduced to a single integration over $\hat{q} \cdot \hat{q}'$.

In concluding this section, we consider the relation of our amplitudes $X_{lm}^\alpha(\vec{q})$ to the three-body wave-function. Recalling that

$$|\Psi\rangle = (1 - I) Q M_e |\phi\rangle, \quad (143)$$

it is straightforward to show that

$$\begin{aligned} \langle \alpha \vec{x} \vec{y} | \Psi \rangle &= \langle \alpha \vec{x} \vec{y} | Q M_e | \phi \rangle \\ &+ \langle \beta, -\frac{\mu_\alpha}{m_\gamma} \vec{x} + \vec{y}, -\frac{\mu_\alpha}{M_\beta} \vec{x} - \frac{\mu_\beta}{m_\gamma} \vec{y} | Q M_e | \phi \rangle \\ &+ \langle \gamma, -\frac{\mu_\alpha}{m_\beta} \vec{x} - \vec{y}, \frac{\mu_\alpha}{M_\gamma} \vec{x} - \frac{\mu_\gamma}{m_\beta} \vec{y} | Q M_e | \phi \rangle, \end{aligned} \quad (144)$$

$\alpha \beta \gamma$ cyclic.

As we have discussed previously, the effect of Q is to guarantee that the wave-function vanishes when any pair of particles are within their respective core radius, i. e., $\langle \alpha \vec{x} \vec{y} | \Psi \rangle$ is zero except in the exterior region defined by¹⁰

$$\begin{aligned} x &> a_\alpha, \\ \left| \frac{\mu_\alpha}{m_\gamma} \vec{x} - \vec{y} \right| &> a_\beta, \\ \left| \frac{\mu_\alpha}{m_\beta} \vec{x} - \vec{y} \right| &> a_\gamma. \end{aligned} \quad (145)$$

Given the form of $Q = 1 + \tilde{V} B (I-1)$, Eq. (144) then implies that the wave-function in this exterior region is given by

$$\psi^{\text{ext}}(\vec{x}, \vec{y}) = \langle \alpha \vec{x} \vec{y} | (1-I) M_e | \phi \rangle. \quad (146)$$

Defining the exterior channel wave-functions

$$\psi_{\alpha}^{\text{ext}}(\vec{x}, \vec{y}) = \langle \alpha \vec{x} \vec{y} | M_e | \phi \rangle, \quad (147)$$

and substituting Eq. (13) for M_e , it is easy to show that

$$\begin{aligned} \psi_{\alpha}^{\text{ext}}(\vec{x}, \vec{y}) &= \langle \alpha \vec{x} \vec{y} | 1 - G_0 \tilde{t} | \phi \rangle \\ &+ 4\pi^2 \mu_{\alpha} \sum_{\ell m} i^{\ell+1} Y_{\ell m}(\hat{x}) \int \frac{d\vec{q} e^{i\vec{y} \cdot \vec{q}}}{D_{\ell}^{\alpha}(\kappa_{\alpha})} \kappa_{\alpha} h_{\ell}(\kappa_{\alpha} x) X_{\ell m}^{\alpha}(\vec{q}). \end{aligned} \quad (148)$$

We note that the first term in this equation is simply the product of a plane-wave for particle α and the usual BCM wave-function for particles β and γ .

Finally, using the relations

$$\nabla_{\vec{y}}^2 e^{i\vec{y} \cdot \vec{q}} = -q^2 e^{i\vec{y} \cdot \vec{q}}, \quad (149)$$

$$\nabla_{\vec{x}}^2 \left\{ Y_{\ell m}(\hat{x}) h_{\ell}(\kappa x) \right\} = -\kappa^2 Y_{\ell m}(\hat{x}) h_{\ell}(\kappa x),$$

Eq. (148) implies that

$$-\left(\frac{\nabla_{\vec{x}}^2}{2\mu_{\alpha}} + \frac{\nabla_{\vec{y}}^2}{2M_{\alpha}} \right) \psi_{\alpha}^{\text{ext}}(\vec{x}, \vec{y}) = W \psi_{\alpha}^{\text{ext}}(\vec{x}, \vec{y}), \quad (150)$$

or

$$(H_0 - W) \psi_{\alpha}^{\text{ext}}(\vec{x}, \vec{y}) = 0.$$

Since I and H_0 commute this explicitly verifies that

$$(H_0 - W) \Psi^{\text{ext}}(\vec{x}, \vec{y}) = 0. \quad (151)$$

Thus, as the nature of the model requires, Ψ^{ext} is a superposition of eigenfunctions of the kinetic energy operator, the superposition being taken to impose the boundary conditions at the core radii and the unitarity relation asymptotically.

VI. DISCUSSION

In the preceding sections we have considered in some detail a specific prescription for introducing singular cores into the three-body problem. It is important to note that we have made the explicit assumption that our three-body wave-function must vanish whenever any pair of particles are within their core radius. This is equivalent to assuming that the BCM is present in each two-body partial-wave, i. e. , that there is some minimum radius r_0 within which all two-body partial-waves vanish. However, it is quite possible to introduce models in which the hard core or BCM appears in only a finite number of partial-waves. Our proof that the usual Faddeev formalism does not yield a unique solution does not apply to this case; on the other hand, the Faddeev kernel is not square-integrable, and hence one cannot prove the existence of solutions. Of course, this does not mean that such solutions do not exist, and numerical solutions have in fact been obtained for the case of hard core plus square-well (two-body s-waves only) by Kim and Tubis.¹¹ Due to the centrifugal barrier, it does not appear likely that one will be able to distinguish between these two possibilities from the experimental information contained in higher partial-waves; their relative usefulness will hinge on the nature of the three-body predictions generated and the ease of calculation they afford. From the latter point of view, our approach has the advantage that the pure BCM part of the interaction reduces to an equation in only a single vector variable, a simplification analogous to that occurring in the usual Faddeev formalism for separable interactions.

As we have stated previously, our formalism shares the lack of square-integrability noted above. To see this one need only observe that the first term of Eq. (132) involves only the difference $\vec{q} - \vec{q}'$. Thus, if we were to Fourier-transform the equation the kernel would contain a piece proportional to $\delta(\vec{x} - \vec{x}')$,

proving the assertion. This property is reflected in our integral equation by a slow rate of convergence at infinity, a consequence of which is that Gaussian quadrature is ruled out as a method of solution. It was thus necessary to develop special numerical techniques which we shall describe in subsequent papers. It should be emphasized that this is true only for the pure BCM part of the kernel for "normal" external potentials.¹² To solve Eq. (13) for the general case, one would substitute $\tilde{t} = \tilde{t}^{BC} + \Delta$,

$$M_e = (1 - G_0 \tilde{t}^{BC} I Q)^{-1} R, \quad (152)$$

and solve the equation

$$R = 1 - G_0 \tilde{t} + G_0 \Delta I Q (1 - G_0 \tilde{t}^{BC} I Q)^{-1} R \quad (153)$$

for R. Here one could solve Eq. (153) by standard Gaussian methods, computing $(1 - G_0 \tilde{t}^{BC} I Q)^{-1}$ by the special technique as in the case of BCM alone.

In order to solve our equations, e. g., Eq. (102), in practice, it is necessary to truncate the sum over ℓ by restricting the number of partial-waves in the two-body channels. It is important to keep in mind the difference between this procedure and the alternate approach discussed above. In our case this is merely a numerical approximation, good to some degree of accuracy. At each stage of approximation (number of partial-waves kept) the basic conditions on the wave-function (vanishing in the interior, unitarity) are satisfied, and the limit as we take more partial-waves should exist. If, on the other hand, one assumes from the start that only a finite number of partial-waves contribute and employs the usual Faddeev formalism, one is committed to this viewpoint. Our proof indicates that the solutions obtained in this fashion should diverge as more and more partial-waves are retained.

Calculations are now underway which exploit the relative simplicity of the equations for BCM alone. Aside from direct applications such as the third virial

computation described above, these calculations should provide some insight into the type of solutions one can obtain from this new class of possibilities. Furthermore, it is this part of the more general interaction that presents the major difficulties in computation and which will be input into the general problem as outlined above. Once having established the required techniques for this special case the full range of models will be calculable.

Finally, one additional possibility is being explored which is of potential interest. The key observation is that by putting a particular type of energy-dependence into the logarithmic parameters λ_ℓ , one can maintain two- and three-particle unitarity while putting in "exact" two-body phase-shifts. That is, by taking $\lambda_\ell(\kappa^2)$ to be a meromorphic function of κ^2 , chosen to fit the experimental phase-shift in partial-wave ℓ , all of the above formalism goes through. This may be regarded as a kind of "asymptotic model" in the sense that the two-body asymptotic behavior sets in immediately exterior to the core. The effect of this model would be to generate a three-body wave-function based on interactions which are physically correct at both very short and long range. In turn, this would be a useful tool with which to probe the sensitivity of various characteristics of the "physical" wave-function to the dynamical region in which the particles are fairly close together. This program is quite practical in two important aspects: (1) it is not difficult to convince oneself that rather excellent fits to the nucleon-nucleon phase shifts can be obtained in this way; (2) this model possesses the same computational advantages as the ordinary pure BCM.

APPENDIX: CONSTRUCTION OF Q

In this appendix we derive an explicit form for the operator Q employed in the text. We want Q to be of the form

$$Q = 1 + \tilde{V}B(1-I) , \quad (A1)$$

where \tilde{V} and B commute, and Q satisfies the properties summarized in Eq. (10).

We first observe that it is sufficient that B satisfies

$$\tilde{V}(1-I)\tilde{V}B(1-I) = \tilde{V}(1-I) , \quad (A2)$$

and is diagonal in the coordinate representation. Since \tilde{V} is also diagonal the commutivity follows trivially, while

$$\tilde{V}(1-I)Q = \tilde{V}(1-I) [1 - \tilde{V}B(1-I)] = 0; \quad (A3)$$

hence

$$(1-\tilde{V}I)Q = (1-\tilde{V})Q = 1-\tilde{V}.$$

Also, it is easy to verify that $I^T = I$; thus, taking the transpose of Eq. (A2),

$$(1-I)\tilde{V} = (1-I)\tilde{V}B(1-I)\tilde{V}. \quad (A4)$$

This implies that

$$(1-I)Q\tilde{V} = (1-I)\tilde{V} [1 - B(1-I)\tilde{V}] = 0, \quad (A5)$$

while the remaining properties of Eq. (10) follow trivially.

Therefore, it is only necessary to find a diagonal operator B such that Eq. (A2) is satisfied. To do so it is convenient to make the double Fourier transformation $\vec{p} \rightarrow \vec{x}$, $\vec{q} \rightarrow \vec{y}$ and to consider Eq. (A2) in coordinate space. It is also convenient to utilize the "supervector" notation introduced in section IV, such that

$$\vec{\rho} = \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} ; \quad (A6)$$

$$\begin{aligned} \delta_{\alpha\beta} F(\vec{\rho}, \vec{\eta}) &= \langle \alpha \vec{x} \vec{y} | \beta \vec{p} \vec{q} \rangle, \\ &= \delta_{\alpha\beta} e^{-i\vec{x} \cdot \vec{p}} e^{-i\vec{y} \cdot \vec{q}} . \end{aligned}$$

One can then easily verify that

$$\begin{aligned}
\langle \alpha \vec{x} \vec{y} | I | \beta \vec{p} \vec{q} \rangle &= 0, \quad \alpha = \beta; \\
&= -F(R_{\beta\alpha} \vec{p}, \vec{\eta}), \quad \alpha\beta \text{ cyclic}; \\
&= -F(R_{\alpha\beta}^{-1} \vec{p}, \vec{\eta}), \quad \beta\alpha \text{ cyclic}.
\end{aligned} \tag{A7}$$

Similarly, representing

$$\langle \alpha \vec{x} \vec{y} | B | \beta \vec{x}' \vec{y}' \rangle = \delta_{\alpha\beta} \delta(\vec{x} - \vec{x}') \delta(\vec{y} - \vec{y}') B_{\alpha}(\vec{\rho}), \tag{A8}$$

it follows that

$$\begin{aligned}
\langle \alpha \vec{x} \vec{y} | \tilde{V}(1-I)\tilde{V}B | \beta \vec{x}' \vec{y}' \rangle & \\
&= \theta(a_{\alpha} - x) \langle \alpha \vec{x} \vec{y} | (1-I) | \beta \vec{x}' \vec{y}' \rangle \theta(a_{\beta} - x') B_{\beta}(\vec{\rho}').
\end{aligned} \tag{A9}$$

Using Eqs. (A7) and (A9), one can easily show that

$$\begin{aligned}
\langle \alpha \vec{x} \vec{y} | \tilde{V}(1-I)\tilde{V}B(1-I) | \gamma \vec{p} \vec{q} \rangle & \\
&= \left[\theta(a_{\alpha} - x) B_{\alpha}(\vec{\rho}) + \theta\left(a_{\sigma} - \left| \frac{\mu_{\alpha}}{m_{\epsilon}} \vec{x} - \vec{y} \right| \right) B_{\sigma}(R_{\sigma\alpha} \vec{\rho}) \right. \\
&\quad \left. + \theta\left(a_{\epsilon} - \left| \frac{\mu_{\alpha}}{m_{\sigma}} \vec{x} + \vec{y} \right| \right) B_{\epsilon}\left(R_{\alpha\epsilon}^{-1} \vec{\rho}\right) \right] \times \langle \alpha \vec{x} \vec{y} | \tilde{V}(1-I) | \gamma \vec{p} \vec{q} \rangle,
\end{aligned} \tag{A10}$$

with $\alpha \sigma \epsilon$ cyclic.

Comparing this result to Eq. (A2), it is clear that our purpose can be achieved if we choose $B_{\alpha}(\vec{\rho})$ such that the bracket in Eq. (A11) is unity for $x < a_{\alpha}$. To do so, we consider in turn four separate domains.

Suppose first that

$$\begin{aligned}
x &< a_{\alpha}, \\
\left| \frac{\mu_{\alpha}}{m_{\epsilon}} \vec{x} - \vec{y} \right| &> a_{\sigma}, \\
\left| \frac{\mu_{\alpha}}{m_{\sigma}} \vec{x} + \vec{y} \right| &> a_{\epsilon};
\end{aligned} \tag{A11}$$

let us call this region I_α . In this region the last two theta-functions in the bracket vanish and we may obviously choose

$$B_\alpha(\vec{\rho}) = 1, \quad \vec{\rho} \in I_\alpha. \quad (\text{A12})$$

We next consider region Π_α , defined by

$$\begin{aligned} x &< a_\alpha, \\ \left| \frac{\mu_\alpha}{m_\epsilon} \vec{x} - \vec{y} \right| &< a_\sigma, \\ \left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| &> a_\epsilon. \end{aligned} \quad (\text{A13})$$

For this case the first two terms in the bracket contribute, but we must be careful in handling $B_\sigma(R_{\sigma\alpha}\vec{\rho})$ since its argument lies in a different domain. Letting $\vec{\rho}' = R_{\sigma\alpha}\vec{\rho}$, we have that

$$\begin{aligned} \left| \frac{\mu_\sigma}{m_\alpha} \vec{x}' - \vec{y}' \right| &= \left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| > a_\epsilon, \\ \left| \frac{\mu_\sigma}{m_\epsilon} \vec{x}' + \vec{y}' \right| &= \left| \vec{x} \right| < a_\alpha, \end{aligned} \quad (\text{A14})$$

for $\vec{\rho} \in \Pi_\alpha$. Hence, defining region III_α to be the domain

$$\begin{aligned} x &< a_\alpha, \\ \left| \frac{\mu_\alpha}{m_\epsilon} \vec{x} - \vec{y} \right| &> a_\sigma, \\ \left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| &< a_\epsilon, \end{aligned} \quad (\text{A15})$$

it is straightforward to verify that for $\vec{\rho} \in \Pi_\alpha$, $R_{\sigma\alpha}\vec{\rho} \in \text{III}_\sigma$. Similarly, one finds that for $\vec{\rho} \in \text{III}_\alpha$, $R_{\alpha\epsilon}^{-1}\vec{\rho} \in \Pi_\epsilon$. Therefore, we can satisfy our requirement

in the regions II_α and III_α by taking

$$B_\alpha(\vec{\rho}) = \frac{1}{2}, \quad \vec{\rho} \in \text{II}_\alpha, \quad (\text{A16})$$

$$\text{or } \vec{\rho} \in \text{III}_\alpha.$$

Finally, we consider region IV_α , defined by

$$x < a_\alpha,$$

$$\left| \frac{\mu_\alpha}{m_\epsilon} \vec{x} - \vec{y} \right| < a_\sigma, \quad (\text{A17})$$

$$\left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| < a_\epsilon.$$

Here all three terms in the bracket contribute, but one can show that for $\vec{\rho} \in \text{IV}_\alpha$, $R_{\sigma\alpha}\vec{\rho} \in \text{IV}_\sigma$ and $R_{\alpha\epsilon}^{-1}\vec{\rho} \in \text{IV}_\epsilon$. Thus all of the B-functions are in the same relative domain and we may simply take

$$B_\alpha(\vec{\rho}) = \frac{1}{3}, \quad \vec{\rho} \in \text{IV}_\alpha. \quad (\text{A18})$$

The above requirements on B_α may be summarized in the explicit formula

$$\begin{aligned} B_\alpha(\vec{\rho}) = & 1 - \frac{1}{2} \theta\left(a_\sigma - \left| \frac{\mu_\alpha}{m_\epsilon} \vec{x} - \vec{y} \right| \right) - \frac{1}{2} \theta\left(a_\epsilon - \left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| \right) \\ & + \frac{1}{3} \theta\left(a_\sigma - \left| \frac{\mu_\alpha}{m_\epsilon} \vec{x} - \vec{y} \right| \right) \theta\left(a_\epsilon - \left| \frac{\mu_\alpha}{m_\sigma} \vec{x} + \vec{y} \right| \right). \end{aligned} \quad (\text{A19})$$

(Since B only occurs multiplied by \tilde{V} one need not put in the explicit factor $\theta(a_\alpha - x)$).

We have thus demonstrated the existence of our Q operator by actual construction. Given Eq. (A19), it is straightforward to perform the Fourier transform to derive Eq. (86) of the text.

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3. A particular example is the ^3H charge form factor, discussed by J. A. Tjon, B. F. Gibson and J. S. O'Connell, Phys. Rev. Letters 25, 540 (1970); however, this calculation is in apparent conflict with a more recent paper by S. N. Yang and A. D. Jackson (Stony Brook preprint). One may nevertheless point to the gap between calculation and experiment for as basic a quantity as the triton binding energy.
4. See, for example, T. D. Lee and C. N. Yang, Phys. Rev. 113, 1165 (1959); also A. Pais and G. E. Uhlenbeck, Phys. Rev. 116, 250 (1959).
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6. The introduction of $\rho_{\alpha j}$ is merely a formal convenience. It is possible that the definite integral defining it does not converge in some cases, but this in no way affects the results as it explicitly cancels when one evaluates Eq. (69).
7. The operator D does appear in the wave-function as part of the projection operator Q. However, in the region where the wave-function is non-vanishing (exterior to the cores), one does not require D explicitly, as we later show at the end of section V.
8. See, for example, M. Stingl and A. S. Rinat, Nucl. Phys. A154, 613 (1970).

9. This formula and our convention for the Clebsch-Gordan coefficients have been taken from M. E. Rose, Elementary Theory of Angular Momentum, John Wiley & Sons, Inc.; New York (1957).
10. Note that the physical interpretation of the vectors \vec{x} , \vec{y} is governed by the index α . Thus \vec{x} corresponds to the coordinate difference of particles β and γ , while \vec{y} is the position of particle α relative to the $\beta\gamma$ c.m.
11. Y. E. Kim and A. Tubis, Phys. Rev. C2, 2118 (1970); also recent preprint C00-1746-52 by the same authors.
12. By "normal" we mean, for example, potentials which fall off faster than $1/r$ at large r .