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# Two-Body Scattering with Singular Potentials*


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The two-body scattering formalism is developed in a manner that makes it clear where the assumption of a "smooth" potential enters. Particular attention is paid to the modifications necessary if the scattering states do not form a complete set, as is the case for the pure hard-core (HC) potential and the pure (i.e., no external potential) boundary-condition model (BCM). As examples, the fully-off-shell $t$ matrices for HC and BCM are developed without treating them as the limits of finite-potential models. A general expression is derived for the fully-off-shell $t$ matrix, which can be applied to the general HC or BCM with external potential, and which involves only the solution to the Schrödinger equation in the external potential.


## I. INTRODUCTION

In all microscopic calculations on finite nuclei, nuclear matter, and other many-body problems that use a potential model to represent the free interaction between particles, one of the main difficulties is how to put in short-range effects. For example, the internucleon ($NN$) potential is highly repulsive at distances, roughly speaking, of less than about 0.5 fm.[1] Meson-theoretic calculations indicate that this is a region of enormous complexity, where multimeson exchange processes and a host of other manifestly nonlocal processes all contribute.[2] Phenomenological fits to $NN$ scattering data at low energies (up to a few hundred MeV) also indicate that a local potential in this region cannot be made to fit the experimental data.[1] The attempts to simulate this highly nonlocal region have thus concentrated on inserting either a very repulsive short-range local potential (so-called "soft core") of some given shape,[3] or such simple nonlocal devices as the (infinite) hard core[1] or its more general form, the boundary-condition model.[4] Adding in suitable attractive tails, each of these forms can be made to yield a phenomenological model of the $NN$ interaction that fits all the low-energy scattering data. The two-body data are, however, not sensitive to the off-shell behavior of the models, and only by going to systems of three or more particles can they be distinguished. In such systems involving more than two particles we must therefore learn how to include such singular interactions as the hard core. Just as in the Faddeev formulation[5] of the three-body problem, so in the Green's-function formulation of the nuclear matter problem[6-8] the (possibly singular) two-body potential can be totally eliminated in favor of the (well-behaved) fully-off-shell free two-body scattering $t$ matrix. It is worth pointing out here that many of the results applicable to "smooth" potentials are incorrect when applied to singular potentials, and mistakes have been made in the past. As an example, in investigating the properties of the ground state of a collection of hard-sphere fermions, Galitskii[6] showed how to eliminate the hard-core potential, using the $t$ matrix instead. His expression for the fully-off-shell $t$ matrix in terms of the half-off-shell quantity, while correct for well-behaved potentials, breaks down for the hard-core interaction. Galitskii was interested in expansions of the ground-state properties in powers of the hard-core radius $a$. He carried the expansions only to $O(a^2)$, in which case his results are certainly correct.

However, straightforward use of his expression for the $t$ matrix to higher orders[8] would have led to incorrect results. This point is elaborated in Sec. II, where the correct expression for this case is derived.

In the next section, we describe the free two-body scattering formalism, considering general potential scattering and the modifications necessary for singular potentials. In Sec. III we deal with the special problems involved with such singular potentials as the hard-core and the pure boundary-condition model. We derive closed exact expressions for the fully-off-shell $t$ matrices in both cases.

The general expression for the fully-off-shell $t$ matrix that is derived in Sec. II can equally well be applied to the more general and more realistic situation where there is an external potential (attractive tail) outside the core region of either the pure hard-core or the pure boundary-condition model. In this case, our method involves only the solution to the Schrödinger equation for two-particle scattering with an interaction potential equal to the external potential, fitted to the boundary condition at the core radius. It is demonstrated explicitly that the solution obtained by our method for the $t$ matrix for the boundary-condition model with external potential (BCME) satisfies the integral equation employed in the usual method, and hence provides the unique solution.

## II. GENERAL TWO-PARTICLE SCATTERING

The Schrödinger equation adequately describes the low-energy potential scattering region as

$$\left(-\frac{1}{2\mu}\vec{\nabla}^2+V(\vec{x})\right)\psi_{\vec{k}}^{+}(\vec{x})=\frac{k^2}{2\mu}\psi_{\vec{k}}^{+}(\vec{x}), \tag{2.1}$$

where $\mu$ is the reduced mass of the two particles, and $\vec{k}$ is their relative momentum. Equation (2.1) is augmented by the outgoing-wave boundary condition. As usual, Eq. (2.1) with this boundary condition can be converted into the Lippmann-Schwinger integral equation (2.2) for the wave function:

$$\psi_{\vec{k}}^{+}(\vec{p})=(2\pi)^3\delta(\vec{p}-\vec{k})+\frac{1}{k^2-p^2+i\epsilon}\tilde{f}(\vec{p},\vec{k}), \tag{2.2}$$

where the scattering amplitude $\tilde{f}(\vec{p},\vec{k})$ is defined by

$$\tilde{f}(\vec{p},\vec{k})\equiv\int\frac{d\vec{q}}{(2\pi)^3}2\mu V(\vec{q})\psi_{\vec{k}}^{+}(\vec{p}-\vec{q}). \tag{2.3}$$

Equations (2.2) and (2.3) yield the integral equation (2.4) for the scattering amplitude,

$$\tilde{f}(\vec{p},\vec{p}\,')=u(\vec{p}-\vec{p}\,')-\int\frac{d\vec{q}}{(2\pi)^3}u(\vec{p}-\vec{q})\frac{1}{q^2-p'^2-i\epsilon}\tilde{f}(\vec{q},\vec{p}\,'), \tag{2.4}$$

where $u(\vec{r})=2\mu V(\vec{r})$.

Equation (2.4) can be extended to yield a "fully-off-shell" scattering amplitude or $t$ matrix, $t(\vec{p},\vec{p}\,';s)$, defined by the solution to the integral equation (2.5) as

$$t(\vec{p},\vec{p}\,';s)=u(\vec{p}-\vec{p}\,')-\int\frac{d\vec{q}}{(2\pi)^3}u(\vec{p}-\vec{q})\frac{1}{q^2-s-i\epsilon}t(\vec{q},\vec{p}\,';s). \tag{2.5}$$

Thus, we shall call $t(\vec{p},\vec{p}\,';s)$ the fully-off-shell $t$ matrix; $\tilde{f}(\vec{p},\vec{p}\,')\equiv t(\vec{p},\vec{p}\,';p'^2)$ the half-off-shell $t$ matrix; and $t(p)\equiv\tilde{f}(\vec{p},\vec{p}\,')$, $p'^2=p^2$, the on-shell $t$ matrix. Equation (2.5) is written in operator notation as

$$t(s)=u-ug_0(s)t(s)=u-tg_0u, \tag{2.5$'$}$$

where

$$g_0(\vec{p},\vec{p}\,';s)\equiv\langle\vec{p}|g_0(s)|\vec{p}\,'\rangle=(2\pi)^3\delta(\vec{p}-\vec{p}\,')\frac{1}{p^2-s-i\epsilon}. \tag{2.6}$$

By comparison with Eq. (2.3) an off-shell wave function $\chi(\vec{p},\vec{p}\,';s)$ can be defined by

$$t(s)=u\chi(s), \tag{2.7}$$

where from Eq. (2.5′) $\chi(s)$ satisfies

$$\chi(s)=1-g_0(s)t(s) \tag{2.8a}$$

$$=1-g_0(s)u\chi(s)=1-\chi(s)g_0(s)u. \tag{2.8b}$$

It is worth noting at this point that $t(s)$ and $\chi(s)$ are related by the two equations (2.7) and (2.8a). Using the latter of these relations, we need never explicitly use the potential $u$ again. This will turn out to be important in the case of singular potentials, as we shall see below.

Time-reversal invariance, or Eq. (2.5′) directly, implies the first equality of Eq. (2.9),

$$t(\vec{p},\vec{p}\,';s)=t(-\vec{p}\,',-\vec{p};s)=t(\vec{p}\,',\vec{p};s), \tag{2.9}$$

where the second equality follows from the fact that $t(\vec{p}\,',\vec{p};s)$ is a function only of the variables $p^2$, $p'^2$, $\vec{p}\cdot\vec{p}\,'$, and $s$.

From Eq. (2.5′), assuming a *real* scattering potential ($u=u^\dagger$), the unitarity condition expressed by Eq. (2.10) is readily shown:

$$t-t^\dagger=t^\dagger(g_0^\dagger-g_0)t=t(g_0^\dagger-g_0)t^\dagger. \tag{2.10}$$

Just as unitarity imposes the restriction expressed by Eq. (2.10) on the $t$ matrix, so completeness and orthonormality of the scattering wave functions can be used to impose restrictions on $\tilde{f}(\vec{p},\vec{p}\,')$. In general, the scattering states can be orthonormalized by

$$\int d\vec{r}\,\psi_{\vec{k}}(\vec{r})\psi^*_{\vec{q}}(\vec{r}) = (2\pi)^3\delta(\vec{k}-\vec{q})\,. \tag{2.11}$$

Substituting for both wave functions in Eq. (2.11) from Eq. (2.2) yields

$$\frac{1}{(p^2-p'^2-i\epsilon)}[\tilde{f}(\vec{p},\vec{p}\,')-\tilde{f}^*(\vec{p}\,',\vec{p})] = \int\frac{d\vec{k}}{(2\pi)^3}\,\frac{\tilde{f}(\vec{k},\vec{p}\,')\tilde{f}^*(\vec{k},\vec{p})}{(k^2-p^2+i\epsilon)(k^2-p'^2-i\epsilon)}\,. \tag{2.12}$$

The general completeness relation can be written

$$\int\frac{d\vec{k}}{(2\pi)^3}\psi_{\vec{k}}(\vec{r})\psi^*_{\vec{k}}(\vec{r}\,') = \delta(\vec{r}-\vec{r}\,') - P(\vec{r},\vec{r}\,') \tag{2.13a}$$

or, in operator notation,

$$|\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}| = 1-P\,, \tag{2.13b}$$

where the integration over $\vec{k}$ is understood, where $|\psi_{\vec{k}}\rangle$ is a scattering eigenstate, and where $P$ is a projection operator ($P^2=P$) if the eigenstates $|\psi_{\vec{k}}\rangle$ are orthonormal. If the scattering states by themselves form a complete set, then $P$ is identically zero. For a normal "smooth" potential, $P=|i\rangle\langle i|$ where the index $i$ labels the normalized bound-state eigenfunctions. For a "pathological" potential as the hard core, $P$ can be nonzero even in the absence of bound states, as we shall see in the next section. Substituting twice from Eq. (2.2) into Eq. (2.13a) yields

$$\frac{1}{p^2-p'^2-i\epsilon}[\tilde{f}(\vec{p},\vec{p}\,')-\tilde{f}^*(\vec{p}\,',\vec{p})] = \int\frac{d\vec{k}}{(2\pi)^3}\,\frac{\tilde{f}(\vec{p},\vec{k})\tilde{f}^*(\vec{p}\,',\vec{k})}{(k^2-p^2+i\epsilon)(k^2-p'^2-i\epsilon)} + P(\vec{p},\vec{p}\,')\,. \tag{2.14}$$

If we define the partial-wave decomposition of the general operator $B(\vec{p},\vec{p}\,';s)$ by

$$B(\vec{p},\vec{p}\,';s) = \sum_l(2l+1)B_l(p,p';s)P_l(\hat{p}\cdot\hat{p}')\,,$$

Eqs. (2.9), (2.10), (2.12), and (2.14) can be rewritten as follows:

$$t_l(p,p';s) = t_l(p',p;s)\,, \tag{2.9$'$}$$

$$\mathrm{Im}\,t_l(p,p';s) = -\frac{\kappa}{4\pi}\tilde{f}_l(p',\kappa)\tilde{f}^*_l(p,\kappa) = -\frac{\kappa}{4\pi}\tilde{f}_l(p,\kappa)\tilde{f}^*_l(p',\kappa)\,, \tag{2.10$'$}$$

$$\tilde{f}_l(p,p')-\tilde{f}^*_l(p',p) = \int_0^\infty\frac{k^2dk}{2\pi^2}\tilde{f}_l(k,p')\tilde{f}^*_l(k,p)\left(\frac{1}{k^2-p^2+i\epsilon}-\frac{1}{k^2-p'^2-i\epsilon}\right), \tag{2.12$'$}$$

$$\tilde{f}_l(p,p')-\tilde{f}^*_l(p',p) = \int_0^\infty\frac{k^2dk}{2\pi^2}\tilde{f}_l(p',k)\tilde{f}^*_l(p,k)\left(\frac{1}{k^2-p^2+i\epsilon}-\frac{1}{k^2-p'^2-i\epsilon}\right)+(p^2-p'^2)P_l(p,p')\,, \tag{2.14$'$}$$

where

$$\kappa \equiv +s^{1/2}\,.$$

Putting $p=p'=\kappa$ in Eq. (2.10′) gives

$$t_l(\kappa) \equiv \tilde{f}_l(\kappa,\kappa) = -\frac{4\pi}{\kappa}e^{i\delta_l(\kappa)}\sin\delta_l(\kappa) \tag{2.15}$$

as a means of parametrizing $t_l(\kappa)$. The function $\delta_l(\kappa)$ is then identified as the phase shift of the $l$th partial wave, since examination of the large $r$ limit of the $l$th partial wave in the decomposition of the Fourier transform of Eq. (2.2) yields

$$\psi^l_k(r) \underset{r\to\infty}{\longrightarrow} i^l e^{i\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l\, n_l(kr)]\,. \tag{2.16}$$

In general, the easiest way to find $\tilde{f}(\vec{p},\vec{k})$ for a given potential $V(\vec{r})$ is to solve the Schrödinger (differential) equation (2.1) for the wave function $\psi_{\vec{k}}(\vec{r})$ and then use Eq. (2.2), rather than solve the integral equation (2.4) directly. By comparison, the fully-off-shell $t$ matrix can be obtained from the off-shell wave function $\chi(s)$, which can in turn be obtained from the solution to Eq. (2.8b). This equation is then easily cast in the form of a differential equation[9] if one so wishes. This approach to finding the $t$ matrix has been used by several authors to treat the boundary-condition model.[10] However, instead of solving Eq. (2.8b) directly, we shall now derive several equations relating $t(\vec{p}, \vec{p}'; s)$ to $\tilde{f}(\vec{p}, \vec{p}')$.

The resolvent $g_0(s)$ of the equation (2.1) with no potential can be defined as $g_0(s) \equiv [2\mu H_0 - s - i\epsilon]^{-1}$, where $H_0$ is the kinetic energy operator. Similarly $g(s)$, the resolvent of the full equation, is defined as $g(s) \equiv [2\mu H_0 + u - s - i\epsilon]^{-1}$. These definitions immediately yield

$$g^{-1} - g_0^{-1} = u ,$$

or

$$g_0 - g = gug_0 = g_0 ug . \tag{2.17}$$

Comparison of Eqs. (2.8) and (2.17) then shows

$$\chi(s) g_0(s) = g(s) . \tag{2.18}$$

Premultiplication of Eq. (2.18) with the potential leads to the more familiar relation

$$t(s) g_0(s) = ug(s) ,$$

which is sometimes used as the defining equation for the $t$ matrix. Using the definitions of $g(s)$ and $g_0(s)$ above, and the completeness relation of Eq. (2.13b), Eq. (2.18) can be written as

$$\chi(\vec{p}, \vec{p}'; s) = (p'^2 - s - i\epsilon)\left( \int \frac{d\vec{k}}{(2\pi)^3} \frac{\psi_{\vec{k}}(\vec{p}) \psi^*_{\vec{k}}(\vec{p}')}{k^2 - s - i\epsilon} + \langle \vec{p} | P g(s) P | \vec{p}' \rangle \right) . \tag{2.18$'$}$$

In deriving this equation, we have made use of the fact that $P|\psi_{\vec{k}}\rangle = 0$, which follows directly from Eq. (2.13b) by operationally multiplying the equation by the scattering state $|\psi_{\vec{k}'}\rangle$ and using orthogonality. The derivation of Eq. (2.18′) was perfectly general, and it is valid for *all* potentials once the operator $P$ is given.

We now wish to specialize Eq. (2.18′) by dropping the second term in brackets on the right-hand side. This is certainly valid for ordinary potentials that have no bound eigenstates ($P = 0$ in this case). In the next section we shall show that for a hard-core potential, while $P \neq 0$, the combination $Pg(s) = 0$. Thus in this case also, the last term of Eq. (2.18′) can be dropped. This is the real motivation for ignoring this term from now on. Under this assumption, there are now several relations that can be derived, with Eq. (2.18′) as the starting point, that relate $t(\vec{p}, \vec{p}'; s)$ to $\tilde{f}(\vec{p}, \vec{p}')$.

In the first place, substituting $\psi_{\vec{k}}(\vec{p}')$ from Eq. (2.2) into Eq. (2.18′), we get

$$\chi(\vec{p}, \vec{p}'; s) = \psi_{\vec{p}'}(\vec{p}) + \int \frac{d\vec{k}}{(2\pi)^3} \psi_{\vec{k}}(\vec{p}) \tilde{f}^*(\vec{p}', \vec{k}) \left( \frac{1}{k^2 - p'^2 - i\epsilon} - \frac{1}{k^2 - s - i\epsilon} \right) . \tag{2.19}$$

By operationally premultiplying this equation by the potential $u$, and making use of Eqs. (2.3) and (2.7) to relate $\chi(s)$ to $t(s)$, we get[11]

$$t(\vec{p}, \vec{p}'; s) = \tilde{f}(\vec{p}, \vec{p}') + \int \frac{d\vec{k}}{(2\pi)^3} \tilde{f}(\vec{p}, \vec{k}) \tilde{f}^*(\vec{p}', \vec{k}) \left( \frac{1}{k^2 - p'^2 - i\epsilon} - \frac{1}{k^2 - s - i\epsilon} \right) \tag{2.20a}$$

$$= \tilde{f}^*(\vec{p}', \vec{p}) + \int \frac{d\vec{k}}{(2\pi)^3} \tilde{f}(\vec{p}, \vec{k}) \tilde{f}^*(\vec{p}', \vec{k}) \left( \frac{1}{k^2 - p^2 + i\epsilon} - \frac{1}{k^2 - s - i\epsilon} \right) + (p^2 - p'^2) P(\vec{p}, \vec{p}') , \tag{2.20b}$$

where Eq. (2.20b) follows from Eq. (2.20a) using the completeness relation of Eq. (2.14). We emphasize again that both Eqs. (2.20a) and (2.20b) were derived from the quite general relation of Eq. (2.19) by operational multiplication with the potential $u$. For nonsingular potentials this is a valid operation. However, for singular potentials like the hard core this is tantamount to multiplication of the wave function, which is zero inside the hard core, by the potential, which is infinite in the same region. The multiplication is not well defined, and Eqs. (2.20a) and (2.20b) thus fall under suspicion in the case of such singular potentials. In the next section we shall show explicitly that they lead to nonsensical results for the hard-core potential.

However, we can avoid using the potential again by using Eq. (2.8a) to relate $\chi(s)$ to $t(s)$. Using this relation, and substituting for both wave functions in Eq. (2.18′), leads to a third relation,

$$t(\vec{p}, \vec{p}'; s) = \frac{1}{p'^2 - p^2 + i\epsilon} [(s - p^2) \tilde{f}(\vec{p}, \vec{p}') - (s - p'^2) \tilde{f}^*(\vec{p}', \vec{p})] - (s - p'^2)(s - p^2) \int \frac{d\vec{k}}{(2\pi)^3} \frac{\tilde{f}(\vec{p}, \vec{k}) \tilde{f}^*(\vec{p}', \vec{k})}{(k^2 - s - i\epsilon)(k^2 - p'^2 - i\epsilon)(k^2 - p^2 + i\epsilon)} . \tag{2.20c}$$

To recapitulate, we have derived three relations that express the fully-off-shell $t$ matrix in terms of the half-off-shell quantity, which in turn can be found by solving the Schrödinger equation. Each of the relations was derived from Eq. (2.18′), which is absolutely general, by dropping the last term for convenience. In the cases of interest to us in the next section, we show that this term is zero. For the general class of nonsingular potentials sustaining no bound states, all three relations are valid and must lead to the same result for the $t$ matrix. For singular potentials (with no bound states) only the third relation, Eq. (2.20c), is valid. If in either case the potential is capable of supporting bound states, these can be included in a straightforward manner by keeping the last term in Eq. (2.18′).

The relation expressed in Eq. (2.20c) is the main result of this section. Decomposing the equation into partial waves, and using the unitarity relation (2.10′) with $\kappa = p$, gives

$$t_l(p, p'; s) = \frac{1}{p'^2 - p^2}\Big[(p'^2 - s)\tilde{f}_l(p', p) - (p^2 - s)\tilde{f}_l(p, p') - (p^2 - s)(p'^2 - s) \times \int_0^\infty \frac{k^2 dk}{2\pi^2} \frac{\tilde{f}_l(p, k)\tilde{f}_l^*(p', k)}{k^2 - s - i\epsilon}\left(\frac{1}{k^2 - p'^2 - i\epsilon} - \frac{1}{k^2 - p^2 - i\epsilon}\right)\Big], \tag{2.21}$$

in which form the right-hand side of the equation is manifestly symmetric under interchange of $p$ and $p'$.

In the next section, the results derived here are applied to two specific examples of singular potentials, viz., the hard-core potential and the pure boundary-condition model.

## III. SCATTERING FROM A SINGULAR POTENTIAL

In the last section we set up the formalism for free two-body potential scattering, and derived several relations for the fully-off-shell $t$ matrix in terms of the half-off-shell quantities. We now wish to specialize these results to the hard-core potential,

$$V(r) = \lim_{g \to \infty} g\theta(a - r), \tag{3.1}$$

where $\theta(x)$ is the unit-step function.

Many of the results of the last section used completeness, and our formalism was set up to indicate explicitly where this entered. We indicated that two conditions may arise to prevent the scattering states from forming a complete set: (i) The potential may be attractive enough to have bound eigenstates, and (ii) the potential may be "pathological." For the (repulsive) hard-core potential we need only concern ourselves with case (ii). With the potential of Eq. (3.1), we have the option of either performing all calculations with $g$ finite until the end, when the limit is taken, or taking the limit from the outset. Keeping $g$ finite throughout the calculations enables us to use any of Eqs. (2.20), for example. However, much of the simplicity inherent in the hard-core potential is lost in doing this, as the potential depends explicitly on another parameter. Several authors[9, 12] have used this method to find the fully-off-shell hard-core $t$ matrix. We shall adopt the alternative method of assuming $g$ infinite from the outset. In this case we have to consider the incompleteness problem of case (ii) above. The hard-core scattering wave functions in the coordinate-space representation are obviously zero inside the radius $a$. The completeness relation becomes

$$\int \frac{d\vec{k}}{(2\pi)^3}\psi_{\vec{k}}(\vec{r})\psi_{\vec{k}}^*(\vec{r}\,') = \delta(\vec{r} - \vec{r}\,')[1 - \theta(a - r)], \tag{3.2}$$

or in the operator notation of Eq. (2.13b), $P = \theta$ for this case, where the coordinate-space representation of the operator $\theta$ is

$$\langle \vec{r} \,|\, \theta \,|\, \vec{r}\,' \rangle \equiv \theta(r, r') = \delta(\vec{r} - \vec{r}\,')\theta(a - r). \tag{3.3}$$

These equations merely express the result that the hard-core wave functions form a complete set only over the partial range of $r$ for $a < r < \infty$.

From Eqs. (2.7) and (3.1), since $t(s)$ is finite (nonsingular), it is apparent that

$$\theta\chi(s) = 0, \tag{3.4}$$

and hence by premultiplying Eq. (2.18) with $\theta$, that

$$\theta g(s) = 0. \tag{3.5}$$

Equation (3.4) just expresses symbolically the fact that the wave function $\chi(s)$ vanishes inside the core. This last result of Eq. (3.5) is just the relation needed to drop the last term in Eq. (2.18′) in order to derive Eqs. (2.20).

The hard-core wave functions evidently take their asymptotic form *exactly* for all $r > a$, and hence from Eq. (2.16)

$$\psi_k^l(r) = \begin{cases} i^l e^{i\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l\, n_l(kr)], & r > a \\ 0, & r < a, \end{cases} \tag{3.6}$$

where, from continuity of the wave function at $r=a$,

$$\tan\delta_l(k) = j_l(ka)/n_l(ka). \tag{3.7}$$

From Eq. (2.2), we can calculate $\tilde{f}_l(p,k)$ immediately as

$$\tilde{f}_l(p,k) = 4\pi(k^2-p^2)\int_0^\infty r^2 dr\; i^{-l} j_l(pr)\psi_k^l(r),$$

or, using Eq. (3.6),

$$\tilde{f}_l(p,k) = 4\pi e^{i\delta_l}(k^2-p^2)\int_a^\infty r^2 dr\, j_l(pr)[\cos\delta_l\, j_l(kr) - \sin\delta_l\, n_l(kr)]. \tag{3.8}$$

Using the well-known relation

$$(p^2-k^2)r^2 u_l(kr)v_l(pr) = \frac{d}{dr}\left[r^2\left(v_l\frac{du_l}{dr} - u_l\frac{dv_l}{dr}\right)\right], \tag{3.9}$$

where $u_l(x)$ and $v_l(x)$ are arbitrary linear combinations of $j_l(x)$ and $n_l(x)$, and the Wronskian relation

$$j_l(x)n_l'(x) - j_l'(x)n_l(x) = x^{-2}, \tag{3.10}$$

the integration of Eq. (3.8) is easily performed to give

$$\tilde{f}_l(p,k) = \frac{j_l(pa)}{j_l(ka)}\tilde{f}_l(k,k) = \frac{4\pi j_l(pa)}{ikh_l^+(ka)}, \tag{3.11}$$

where we have used Eqs. (2.15) and (3.7). Thus, $\tilde{f}_l(p,k)$ is separable in $p$ and $k$. Using this explicit form for $\tilde{f}_l(p,p')$, the orthogonality and completeness relations of Eqs. (2.12′) and (2.14′) are easily checked, using Eqs. (A5) and (A6) from the Appendix and the explicit form for $\theta_l(p,p')$, which is readily evaluated, using Eq. (3.9), to be

$$\theta_l(p,p') = \frac{4\pi a^2}{p'^2-p^2}[p\,j_l(p'a)\,j_l'(pa) - p'j_l(pa)\,j_l'(p'a)]. \tag{3.12}$$

Using the explicit form for $\tilde{f}_l(p,k)$ derived above, we can use the results of Sec. II to find $t_l(p,p';s)$. We pointed out in the last section that while the three relations (2.20a)–(2.20c) are all valid for nonsingular potentials, the first two are not valid for singular potentials. It is easy to check at this point that these two relations, if used for the hard-core potential, both lead to expressions for $t_l(p,p';s)$ which are not even symmetric between $p$ and $p'$, and are thus obviously incorrect. These were, in fact, the relations used by Galitskii,[6] which we referred to in Sec. I. On the other hand, Eq. (2.20c) remains valid for singular potentials, and substituting from Eq. (3.11) leads to the following correct expressions for $t_l(p,p';s)$ after a little algebra:

$$t_l(p,p';s) = \frac{1}{p'^2-p^2}[(p'^2-s)\tilde{f}_l(p',\kappa)B_l(p,\kappa) - (p^2-s)\tilde{f}_l(p,\kappa)B_l(p',\kappa)] \tag{3.13a}$$

$$= (p'^2-s)\theta_l(p,p') + \tilde{f}_l(p,\kappa)B_l(p',\kappa), \tag{3.13b}$$

where

$$B_l(p,\kappa) = i\kappa a^2[p\,j_l'(pa)h_l^+(\kappa a) - \kappa j_l(pa)h_l^{+\prime}(\kappa a)]. \tag{3.14}$$

From the definition above, it is apparent that

$$B_l(\kappa,\kappa) = 1, \tag{3.15}$$

as needed. It is easy to see that $t_l(p,p';s)$ satisfies the symmetry and unitarity conditions of Eqs. (2.9′) and (2.10′). The result of Eqs. (3.13) is exactly the same (after a little manipulation to put it in the same form) as that derived by Brayshaw[12] by the entirely different method of starting with a finite repulsive square well and taking the hard-core limit at the end of the calculation. The expressions (3.13) can now be used as the starting point for calculations on three or more particle systems interacting via hard-core potentials. It is interesting to note that in the limit $s\to\infty$, the fully-off-shell $t$ matrix contains a term linear in $s$, whereas in this limit for ordinary potentials the $t$ matrix approaches the potential $u(\vec{p}-\vec{p}')$ and becomes independent of $s$.

For simplicity we have carried out the calculations above only for a pure hard-core potential. It is not difficult however to extend the calculations to the more general case of the so-called pure boundary-condition model (BCM). The most general boundary-condition model comprises a core interaction which gives rise to an energy-independent logarithmic derivative of the wave function at the core radius $a$, with a given local potential beyond this radius. We shall consider only the pure boundary-condition model (BCM), in which case the external potential is zero. The boundary condition is taken to be

$$\lim_{\delta\to 0}\frac{\psi_k^{l\,\prime}(a+\delta)}{\psi_k^l(a+\delta)}=\lambda_l\,. \tag{3.16}$$

It has been shown[13] that the BCM can be equivalently cast in the form of the limit of a potential model containing a repulsive square well and an attractive surface $\delta$-function potential,

$$u(r)=g\theta(a-r)-h\delta(r-a)\,, \tag{3.17}$$

where $g>0$, $h>0$ in the limit as $g\to\infty$, $h\to\infty$ such that the quantity

$$\lambda=\sqrt{g}-h-1/a$$

remains finite. The limit can obviously be taken separately in each partial wave. The HC potential is obviously just the special case of the BCM where $\lambda_l\to\infty$. It is then apparent that the BCM wave functions still obey Eq. (3.6), where to satisfy the boundary condition of Eq. (3.16) the phase shifts $\delta_l(k)$ are given by

$$\tan\delta_l(k)=\frac{\lambda_l j_l(ka)-kj_l'(ka)}{\lambda_l n_l(ka)-kn_l'(ka)}\,. \tag{3.18}$$

The scattering amplitude $\tilde{f}_l(p,k)$ is calculated exactly as before to give

$$\begin{aligned}\tilde{f}_l(p,k)&=\frac{\lambda_l j_l(pa)-pj_l'(pa)}{\lambda_l j_l(ka)-kj_l'(ka)}\tilde{f}_l(k,k)\\&=\frac{4\pi}{ik}\frac{\lambda_l j_l(pa)-pj_l'(pa)}{\lambda_l h_l^+(ka)-kh_l^{+\prime}(ka)}\,,\end{aligned} \tag{3.19}$$

which is still separable in $p$ and $k$. It is readily checked that the BCM wave functions obtained from this expression for $\tilde{f}_l(p,k)$ by Eq. (2.2) satisfy the defining condition Eq. (3.16), and are zero inside the radius $a$. Using the explicit form for $\tilde{f}_l(p,k)$, the BCM $t$ matrix is obtained from Eq. (2.21) as before. The necessary integral is evaluated in the Appendix as Eq. (A7), where we have assumed no bound states, to be compatible with the use of the formalism of Sec. II. After a lot of algebra, the remarkable result obtains that the BCM $t$ matrix is given in terms of the half-off-shell amplitude by exactly the same Eqs. (3.13) as for the HC potential. The actual expressions, of course, differ, since the functions $\tilde{f}_l(p,k)$ have different forms. The final expression agrees with that found by other authors.[12-14]

We have derived an exact analytic expression above for the pure BCM $t$ matrix (and have seen how the pure hard-core result can be obtained from it as a special case) by making use of our general expression (2.20c). This expression is also valid in the more general boundary-condition model (BCME) which contains an arbitrary (nonsingular) external potential $V_e(\vec{r})$ outside the core radius $a$. The procedure in this case is to first solve the two-particle Schrödinger equation for the interaction potential $V_e(\vec{r})$ for the wave function $\Psi_{\vec{k}}(\vec{r})$ in the range $a<r<\infty$, fitted to the boundary condition (3.16) at $r=a$. From the wave function, the scattering amplitude is derived from Eq. (2.2), and hence the $T$ matrix from Eq. (2.20c).

The procedure described above differs from the method generally employed, described briefly below (and in, e.g., Ref. 12), and it is instructive to compare the two methods and thereby verify our solution.

For general two-particle scattering with an interaction potential given by the sum of two terms

$$U=u+u_e\,,$$

we define a $T$ matrix by the solution to the integral equation

$$T=U-Ug_0T\,. \tag{3.20a}$$

Similarly $t(s)$ is defined to be the $t$ matrix with only the potential $u$ acting,

$$t=u-ug_0t\,. \tag{3.20b}$$

By subtracting these two equations, it is apparent that

$$(1+ug_0)(T-t)=u_e(1-g_0T)\,.$$

Premultiplication of this last equation with the factor $(1-tg_0)$ gives the result

$$T-t=(1-tg_0)u_e(1-g_0T)\,. \tag{3.21}$$

Using Eq. (2.8a), and a similar expression for the fully-off-shell wave function $X(s)$ corresponding to $T(s)$, gives immediately the equivalent equation

$$X=\chi-\chi g_0u_eX\,. \tag{3.22}$$

Since the potential $u$ has now been eliminated from Eqs. (3.21) and (3.22), we can specialize to the case where $u$ represents the pure BCM and $u_e$ the external potential of the BCME. Equation (3.21) can now be considered as an integral equation for $T(s)$, the BCME $T$ matrix, since the pure BCM $t$ matrix, $t(s)$, is known; this is the method generally used to solve for $T(s)$. Since we have been somewhat cavalier about taking the limit to the BCM in the integral equations (3.21) and (3.22), it is worthwhile to check that Eq. (3.22) does in fact lead to a BCME wave function $\Psi_{\vec{k}}(\vec{r}) \equiv \langle\vec{r}\,|X(k^2)|\vec{k}\rangle$ that satisfies the required boundary condition,

$$\frac{\Psi_k^{l\,\prime}(a)}{\Psi_k^l(a)} = \lambda_l \,.$$

Using our explicit expression for $t(s)$, the pure BCM $t$ matrix, this is easily verified from Eq. (3.22); it can also be shown[12] that Eqs. (3.21) and (3.22) have unique solutions if $u_e$ satisfies the usual asymptotic condition,

$$\lim_{r\to\infty} r u_e(r) = 0\,.$$

Thus, if we can now show that our general expression (2.18′), or equivalently (2.20c), satisfies Eq. (3.22), or equivalently Eq. (3.21), we are guaranteed that we have found the unique solution $T(s)$ of the BCME $T$ matrix with arbitrary external potential $u_e(\vec{r})$. The proof is given below.

The scattering wave functions $|\psi_{\vec{k}}\rangle$ and $|\Psi_{\vec{k}}\rangle$ of the pure BCM and BCME, respectively, both satisfy the same completeness relation of Eq. (2.13b),

$$|\Psi_{\vec{k}}\rangle\langle\Psi_{\vec{k}}| = |\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}| = 1-\theta\,, \qquad (3.23)$$

assuming no bound states in either case. The general projection operator $P$ of Sec. II can thus be identified with $\theta$ in both cases. Thus Eq. (3.5) holds for both the BCM and BCME, and hence the last term can be dropped from Eq. (2.18′) in both models to give

$$\chi(s) = \frac{|\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}|}{k^2-s-i\epsilon}\, g_0^{-1}\,, \qquad (3.24a)$$

$$X(s) = \frac{|\Psi_{\vec{k}}\rangle\langle\Psi_{\vec{k}}|}{k^2-s-i\epsilon}\, g_0^{-1}\,. \qquad (3.24b)$$

Substituting from Eqs. (3.24), the right-hand side of Eq. (3.22) becomes

$$\chi - \chi g_0 u_e X = \chi - \frac{|\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}|u_e|\Psi_{\vec{q}}\rangle\langle\Psi_{\vec{q}}|g_0^{-1}}{(k^2-s-i\epsilon)(q^2-s-i\epsilon)}\,. \qquad (3.25)$$

Using the Schrödinger equations

$$(2\mu H_0 + u + u_e)|\Psi_{\vec{q}}\rangle = q^2|\Psi_{\vec{q}}\rangle\,,$$

$$(2\mu H_0 + u)|\psi_{\vec{k}}\rangle = k^2|\psi_{\vec{k}}\rangle\,,$$

it is trivial to prove that

$$\langle\psi_{\vec{k}}|u_e|\Psi_{\vec{q}}\rangle = (q^2-k^2)\langle\psi_{\vec{k}}|\Psi_{\vec{q}}\rangle\,.$$

Using this result in Eq. (3.25) gives

$$\chi - \chi g_0 u_e X = \chi - |\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}|\Psi_{\vec{q}}\rangle\langle\Psi_{\vec{q}}|\left(\frac{1}{k^2-s-i\epsilon} - \frac{1}{q^2-s-i\epsilon}\right) g_0^{-1}\,.$$

The completeness relations of Eq. (3.23) can now be employed to give

$$\begin{aligned}\chi - \chi g_0 u_e X &= \chi - \left(\frac{|\psi_{\vec{k}}\rangle\langle\psi_{\vec{k}}|(1-\theta)}{k^2-s-i\epsilon} - \frac{(1-\theta)|\Psi_{\vec{q}}\rangle\langle\Psi_{\vec{q}}|}{q^2-s-i\epsilon}\right) g_0^{-1} \\ &= \chi - [\chi - X] = X\,,\end{aligned}$$

which is exactly Eq. (3.22). We have thus verified that the expression of Eq. (2.18′), or equivalently Eq. (2.20c), works equally well for the BCME as for the pure BCM, as originally asserted.

## IV. SUMMARY

We have obtained a general formula for the fully-off-shell two-body $t$ matrix in terms of the half-off-shell scattering amplitude, which can in turn be found from solving the Schrödinger equation. The derivation is valid for singular, as well as nonsingular potentials, and we discussed the care necessary in applying the completeness relation for the case of singular potentials. Since the real world probably contains no potentials which are strictly singular, such potentials are probably best treated as the limit of nonsingular potentials, since all relevant functions then depend on one parameter less. Our general formula for the $t$ matrix avoids the need for a separate final limiting process in each case.

The formalism was applied to the pure HC and pure BCM, and exact analytic expressions for the $t$ matrices were easily found in both cases. The formalism is also suitable for the more general BCME which includes an external potential outside the core region. Our expression for the $t$ matrix of this model was explicitly shown to be the unique solution to the integral equation of an alternative formalism in general use.

An expression for the two-body $t$ matrix in any model forms the starting point for calculations on systems involving more than two particles. This author has employed the expression for the pure hard-core $t$ matrix in calculations of the ground-state properties of an infinite system of fermions interacting via hard-core potentials.[8]

It is hoped that the examples of the pure HC potential and the pure BCM, as well as our discussion of the general BCME, demonstrate both the practicality of the formalism of Sec. II for other models involving singular potentials and how to apply the formalism in such cases.

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## APPENDIX

In this Appendix, the singular integrals occurring in Sec. III are evaluated. The integrals of interest can all be put in the form

$$I(x)=\frac{1}{\pi}\int_{-\infty}^{\infty}dx'\,\frac{v(x')}{x'-x-i\epsilon}, \tag{A1}$$

where $v(x)$ is a real function. Furthermore, in the cases of interest to us, we can define a function $f(z)$, analytic in the upper half complex plane, which goes to zero as $z$ approaches infinity along any direction in the upper half-plane, and has the property

$$f(x)=u(x)+i\,v(x), \tag{A2}$$

on the real axis. For such functions,

$$f(x)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}dx'\,\frac{f(x')}{x'-x-i\epsilon}=\frac{1}{2\pi i}\int_{-\infty}^{\infty}dx'\,\frac{f(x')}{x'-x}+\tfrac{1}{2}f(x), \tag{A3}$$

where an integral with no $\pm i\epsilon$ in the denominator is to be taken as a principal-value integral. Taking the real part of both sides of Eq. (A3), we get

$$u(x)=\frac{1}{\pi}\int_{-\infty}^{\infty}dx'\,\frac{v(x')}{x'-x},$$

and upon adding the quantity $iv(x)$ to both sides,

$$f(x)=\frac{1}{\pi}\int_{-\infty}^{\infty}dx'\,\frac{v(x')}{x'-x-i\epsilon}.$$

If $v(x)$ is also an even function of $x$, as in the three cases below, the last equation can be written as

$$f(x)=\frac{2x}{\pi}\int_{0}^{\infty}dx'\,\frac{v(x')}{x'^2-x^2-i\epsilon}. \tag{A4}$$

Equation (A4) is now specialized to the three cases of interest.

*Case (i).*

$$f(z)=i\,j_l(z)h_l^+(z)\,;\quad v(x)=j_l^{\,2}(x).$$

The conditions necessary for Eq. (A4) are all readily seen to be satisfied, and hence

$$i\,j_l(x)h_l^+(x)=\frac{2x}{\pi}\int_0^{\infty}dx'\,\frac{j_l^{\,2}(x')}{x'^2-x^2-i\epsilon},$$

which easily yields the desired integral,

$$\int_0^{\infty}k^2dk\,j_l^{\,2}(ka)\left(\frac{1}{k^2-p^2+i\epsilon}-\frac{1}{k^2-p'^2-i\epsilon}\right)=\tfrac{1}{2}\pi p[i\,j_l(pa)h_l^+(pa)]^*-\tfrac{1}{2}\pi p'[i\,j_l(p'a)h_l^+(p'a)]. \tag{A5}$$

*Case (ii).*

$$f(z)=h_l^{+\prime}(z)/h_l^+(z)\,;\quad v(x)=(x\,|\,h_l^+(x)\,|)^{-2},$$

where we have used the Wronskian relation Eq. (3.10) to evaluate the imaginary part. Both $h_l^+(z)$ and $h_l^{+\prime}(z)$ take all their zeros in the lower half-plane, and hence $f(z)$ is analytic in the upper half-plane as required. The function $f(z)$ actually approaches an imaginary constant as $z\to\infty$, which leads to an additional imaginary constant term in Eq. (A3) from the contribution to the contour integral from the infinite semicircle.

Since Eq. (A4) is obtained from Eq. (A3) by taking the real part, we may still use the equation to obtain

$$\frac{h_l^{+\prime}(x)}{h_l^+(x)}=\frac{2x}{\pi}\int_0^\infty \frac{dx'}{x'^2-x^2-i\epsilon}\,\frac{1}{x'^2|h_l^+(x')|^2},$$

from which the desired relation follows:

$$\int_0^\infty \frac{dk}{|h_l^+(ka)|^2}\left(\frac{1}{k^2-p^2+i\epsilon}-\frac{1}{k^2-p'^2-i\epsilon}\right)=\frac{1}{2}\pi a^2\left[p\left(\frac{h_l^{+\prime}(pa)}{h_l^+(pa)}\right)^*-p'\left(\frac{h_l^{+\prime}(p'a)}{h_l^+(p'a)}\right)\right]. \tag{A6}$$

*Case (iii).*

$$f(z)=h_l^{+\prime}(z)\left(\lambda_l h_l^+(z)-\frac{z}{a}h_l^{+\prime}(z)\right)^{-1};\quad v(x)=\lambda_l\left(x\left|\lambda_l h_l^+(x)-\frac{x}{a}h_l^{+\prime}(x)\right|\right)^{-2},$$

where we have again used the Wronskian relation (3.10) to evaluate $v(x)$. In general this function $f(z)$ need *not* be analytic in the upper half-plane. However, in the case of interest to us, there will be no poles in this region, since if there were, some would correspond to bound-state poles, as seen from Eq. (3.19), since bound states correspond to poles $k=i\kappa$ in $t_l(\kappa)=\tilde{f}_l(\kappa,\kappa)$. Since we exclude this possibility, the necessary conditions for Eq. (A4) are fulfilled, as it is readily verified that $v(x)$ is an even function. Thus we obtain

$$\frac{h_l^{+\prime}(x)}{\lambda_l h_l^+(x)-(x/a)h_l^{+\prime}(x)}=\frac{2x}{\pi}\int_0^\infty \frac{dx'}{x'^2-x^2-i\epsilon}\,\frac{\lambda_l}{x'^2|\lambda_l h_l^+(x')-(x'/a)h_l^{+\prime}(x')|^2},$$

from which follows immediately that

$$\int_0^\infty \frac{dk}{|B(k)|^2}\left(\frac{1}{k^2-p^2-i\epsilon}-\frac{1}{k^2-p'^2-i\epsilon}\right)=\frac{\pi a^2}{2\lambda_l}\left(p\,\frac{h_l^{+\prime}(pa)}{B(p)}-p'\,\frac{h_l^{+\prime}(p'a)}{B(p'a)}\right),$$

where

$$B(k)=\lambda_l h_l^+(ka)-kh_l^{+\prime}(ka)\,. \tag{A7}$$

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