Off-Energy-Shell t-Matrix Elements for Local Potentials **Containing Hard Cores***

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A method is presented for calculating the off-energy-shell two-body reaction matrix elements for a local potential that contains a hard core. An analytic expression is presented for the matrix elements, t(k',k;s), for the special case of a hard-core potential with no other interaction. Graphs are presented showing the effects of the hard core for negative values of the energy parameter s and l=0 relative-angular-momentum states, using a potential of exponential shape and parameters chosen to approximate the nucleon-nucleon interaction.

I. INTRODUCTION

NOWLEDGE of the nuclear interaction has increased impressively in the past few years.¹ The elastic on-shell S matrix for the two-nucleon system now appears to be well known² and there exist several potential models³ that are quantitatively accurate over the elastic energy range.

For many problems of interest, however, knowledge of the on-shell S matrix, however complete, does not suffice. Thus in nearly every nuclear problem (excepting only free two-nucleon scattering) off-energy-shell matrix elements play an important role, e.g., p-p bremsstrahlung, nuclear matter, deuteron stripping, etc. Appreciation of the importance of realistic off-shell behavior has become well known only quite recently, after the invention of the Faddeev⁴ equations and the consequent renewed interest in the three-body problem.⁵

While the Faddeev equations give a mathematically correct and technically solvable system of equations, it is not possible in practice to obtain a solution with a realistic local potential such as is used to fit the on-shell S matrix. Presently available computers are not yet large or fast enough. For this reason, attention has been focused on the rather unusual separable⁶ interactions.

Although the on-shell behavior of a separable potential may duplicate that of a local potential, the off-shell behavior may be substantially different. It is therefore important, when using a separable potential, to determine whether the off-shell behavior is reasonable. At present there is almost no information at all on the behavior of off-shell elements. The technique most often used to go off-shell is through calculations that use a local potential that has been fitted to the on-shell data. Whether this technique is correct or not can only be determined by comparing the results obtained with observation.

The use of a separable potential to determine off-shell matrix elements is an even more hazardous technique because of the lack of physical justification for the separable form. However, the simplicity of this technique has gained for it very widespread use. Not only should the separable potential be fitted to the on-shell elements but its off-shell behavior should approximate that of a local potential (or at least there should be an awareness of the differences). The first step in this direction was taken by Mitra,⁷ who determined the form a separable potential must have if its S matrix is to have the same analytic properties on-shell as a superposition of Yukawa potentials. Noves8 and Kowalski9 attempted to improve this work through consideration of the off-shell behavior. Mongan¹⁰ obtained a potential with the correct on-shell analyticity properties but with a discontinuity in the off-shell elements between the bound-state and scattering regions. In addition Mongan presented numerical results for the positive energy on-shell elements. Wong and Zambotti¹¹ were the first to present numerical results for off-shell elements

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¹ For an excellent review of the present situation see the Proceedings of the International Conference on the Nucleon-Nucleon Interaction, Gainesville, Florida, 1967, edited by A. E. S. Green, M. H. MacGregor, and R. Wilson [Rev. Mod. Phys. 39, 495 (1967)

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where

although they confined their attention to negative energies and used a monotonic local potential.

In this work we extend the previous calculations to include the more realistic case of a potential that contains a hard core.

In Sec. II we review the t matrix and define our notation. In Sec. III the t matrix is obtained for a local potential containing a hard core. In Sec. IV we present results that compare the t-matrix elements for "similar" potentials with and without hard cores. Only negative energies (for which the t matrix is real) and S waves are considered. Section V gives our conclusions.

II. TWO-BODY t MATRIX

We define the two-body t operator, a function of the (complex) "energy" parameter s, by

$$t(s) = v + v [1/(s - H_0)]t(s), \qquad (1)$$

where v is the (Hermitian) potential operator and H_0 the kinetic energy operator. \mathbf{p}_{op} is the relative-momentum operator whose complete set of eigenfunctions are the normalized plane waves. The units are such that h=1=2m:

$$\mathbf{p}_{\rm op} \, | \, \mathbf{k} \rangle = \mathbf{k} \, | \, \mathbf{k} \rangle ,$$
$$\int d^3 k \, | \, \mathbf{k} \rangle \langle \mathbf{k} | = \mathbf{1}_{\rm op} \,, \qquad (2)$$

and

$$\langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/(2\pi)^{3/2}$$

The matrix representing t(s) in the momentum space defined by Eq. (2) is then

$$\langle \mathbf{k}' | t(s) | \mathbf{k} \rangle = \langle \mathbf{k}' | v | \mathbf{k} \rangle + \int d^3 q \frac{\langle \mathbf{k}' | v | \mathbf{q} \rangle \langle \mathbf{q} | t(s) | \mathbf{k} \rangle}{s - q^2} \,. \tag{3}$$

The integral in (3) is well defined except at real positive values of s. There we choose the usual definition that corresponds to outgoing scattered waves:

$$t(k_0^2) \equiv \lim_{\epsilon \to 0} t(k_0^2 + i\epsilon).$$
(4)

If the potential is central, one can effect a partialwave decomposition as follows:

$$\langle \mathbf{k}' | t(s) | \mathbf{k} \rangle = \sum_{l=0}^{\infty} (2l+1) t_l(k',k;s) P_l(\mathbf{k}',\mathbf{k}), \quad (5)$$

with a similar expression for the potential. Inserting (5) into (3), one obtains

$$t_{l}(k',k;s) = v_{l}(k',k) + \int d^{3}q \ v_{l}(k',q)t_{l}(q,k;s)/(s-q^{2}).$$
(6)

For a very general class of potentials¹² (not including those having hard cores) Eq. (6) can readily be solved by matrix inversion techniques¹¹ to obtain the t matrix. Note that with the above definition the positive energy on-shell elements can be related to the phase shifts,

$$t_{l}(k_{0},k_{0};k_{0}^{2}) = -\sin\delta(k_{0})e^{i\delta(k_{0})}/(2\pi^{2}k_{0}),$$

and for s negative $t_l(k',k;s)$ is real if $v_l(k',k)$ is real.

III. POTENTIALS CONTAINING HARD CORES

We consider here the solution of Eq. (3) for (local) central potentials having a hard core, i.e.,

$$\langle \mathbf{r} | v | \mathbf{r}' \rangle = V(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}'),$$
 (7)

$$V(r) = +\infty, \quad r < c$$
$$= v(r), \quad r > c.$$

It is clear that Eq. (3) cannot be attacked directly¹³ using the potential of (7) since the potential matrix elements are infinite. For this reason we seek to transform (3) into a differential equation. Thus we define the operator $\Omega(s)$ by

$$t(s) = v\Omega(s). \tag{8}$$

From (1), one sees that

$$\Omega(s) = 1 + [1/(s - H_0)] v \Omega(s).$$
⁽⁹⁾

Multiplying by $s - H_0$ and rearranging we find

$$(H_0 + v - s)\Omega(s) = (H_0 - s).$$
(10)

If one defines the ket $|\Psi_k(s)\rangle$ by

$$|\Psi_{\mathbf{k}}(s)\rangle \equiv \Omega(s) |\mathbf{k}\rangle, \qquad (11)$$

then it is clear that

$$\langle \mathbf{k}' | t(s) | \mathbf{k} \rangle = \langle \mathbf{k}' | v | \Psi_{\mathbf{k}}(s) \rangle.$$
 (12)

Operating with (10) onto $|\mathbf{k}\rangle$ gives

$$(H_0+v-s)|\Psi_k(s)\rangle = (H_0-s)|k\rangle.$$
(13)

Upon projecting into configuration space and defining the representative of $|\Psi_k(s)\rangle$ to be $\Psi_k(\mathbf{r}; s)$, one has

$$\begin{bmatrix} -\nabla^2 + V(\mathbf{r}) - \mathbf{s} \end{bmatrix} \Psi_{\mathbf{k}}(\mathbf{r}; \mathbf{s}) = (k^2 - s)e^{i\mathbf{k}\cdot\mathbf{r}}/(2\pi)^{3/2}, \quad (14)$$

and, finally, a partial-wave decomposition yields

$$\{ \frac{d^2}{dr^2} + [s - V(r) - l(l+1)/r^2] \} u_{l,k}(r;s)$$

= $(s - k^2) r j_l(kr)$, (15)

where

$$\Psi_{k}(\mathbf{r};s) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1)i^{l}P_{l}(\hat{k},\hat{r})u_{l,k}(r;s)/r. \quad (16)$$

¹² Steven Weinberg, Phys. Rev. 133, B232 (1964).

¹³ This is not to say that the integral equation cannot be used to obtain these results. K. L. Kowalski and D. Feldman [J. Math Phys. 2, 499 (1961); 4, 507 (1963)] have shown how the Lippman-Schwinger equation may be modified for use with hard-core potentials.

Equation (15) is an inhomogeneous, ordinary secondorder differential equation that can be solved for $u_{l,k}(\mathbf{r}; s)$ [abbreviated to $u_l(\mathbf{r})$ in the following] subject to the appropriate boundary conditions, which must be determined so that the resulting t(s)-matrix elements satisfy Eq. (3). Let us first consider the case of a hard core only, i.e., $v(\mathbf{r}) = 0$.

A. Hard Core Only

For simplicity we shall consider only S waves here, but the results are easily extended to higher partial waves. Then (15) becomes (for the hard core alone)

$$u'' + su(r) = V(r)u(r) + (s - k^2)(\sin kr)/k, \quad r < c$$

= $(s - k^2)(\sin kr)/k, \quad r > c.$ (17)

The solution that satisfies the boundary conditions required by (3) is

$$u(r) = 0, \qquad r < c$$

$$=\frac{\sin kr}{k}-\frac{\sin kc}{k}e^{i(\sqrt{s})(r-c)}, \quad r>c$$
(18)

where one chooses that branch of \sqrt{s} that has a positive imaginary part. Although u vanishes inside the core region, the product of V by u does not vanish, but is given by

$$V(r)u(r) = u'(c+)\delta(r-c) + (k^2 - s)(\sin kr)/k, \ r \le c$$

=0, r>c (19)

where u'(c+) designates the right-hand limit of the derivative of u. The derivative is easily evaluated from (18). Using (12) one can now evaluate the S-wave contribution to the t matrix.¹⁴ One finds

$$(2\pi^{2})t_{0}(k',k;s) = \frac{\sin k'c}{k'} \left(\cos kc - i\frac{\sqrt{s}}{k} \sin kc \right) + \frac{(k^{2}-s)}{kk'} \left(\frac{\sin(k'-k)c}{k'-k} - \frac{\sin(k'+k)c}{k'+k} \right). \quad (20)$$

Certain special cases may be noted: the half-off-shell element $t_0(k',k;k^2) = \sin k'c \ e^{-ikc}/(2\pi^2k')$ and the onshell element $t_0(k,k;k^2) = \sin kc \ e^{-ikc}/(2\pi^2k)$. Also one should note that $t_0(k',k;s)$ is symmetric with respect to the interchange of k and k' although this is not obvious as Eq. (20) is written.

Note that the second term in (20) is the contribution from within the core region while the coefficient of $(\sin k'c)/k'$ in the first term is just u'(c+). These features persist even when other interactions outside the core are allowed. The limits for large k, k' and s are of interest. One sees

$$\lim_{k'\to\infty}t_0(k',k;s)=0$$

as 1/k' and, by the symmetry,

$$\lim_{k\to\infty} t_0(k',k;s)$$

also vanishes as 1/k. On the other hand, the *t*-matrix element does not vanish as |s| grows:

$$\lim_{|s|\to\infty}t_0(k',k;s)\to\infty$$

as s. These limits have treated the three variables independently. Other limits may also be of interest, such as the diagonal element $t_0(k,k;s)$, for which

$$\lim_{k\to\infty} t_0(k,k;s) = c/4\pi^2$$

and does not vanish. Thus some special import of the diagonal elements for all values of s must be inferred.

B. Hard Core Plus Interaction

The results of Sec. III A are readily extended to include the potential of (7) in Eq. (15). Using Eq. (19) for the effect of the hard core, we have

$$u'' + su = u'(c+)\delta(r-c), \qquad r \le c = v(r)u + (s-k^2)(\sin kr)/k, \quad r > c. \quad (21)$$

If the form of v(r) is given, these equations can be easily solved, using a computer, subject to the appropriate boundary conditions:

$$u(r) = 0, \quad r < c$$

$$u(r) \xrightarrow[r \to \infty]{} (\sin kr)/k + Ae^{i(\sqrt{s})r}, \quad (22)$$

where A is a constant that, along with u'(c+), is determined by (21) and (22). Once u(r) is known, the *t*-matrix element is readily constructed:

$$2\pi^{2}t_{0}(k',k;s) = \frac{\sin k'c}{k'}u'(c+) + \frac{k^{2}-s}{2kk'} \times \left(\frac{\sin (k-k')c}{k-k'} - \frac{\sin (k+k')c}{k+k'}\right) + \int_{c}^{\infty} dr \frac{\sin k'r}{k'}v(r)u(r). \quad (23)$$

IV. NUMERICAL CALCULATIONS

In this section we investigate the effects of the hard core on the S-wave off-shell t matrix for negative (real) values of the energy parameter s, only. To this end we define two potentials to be "equivalent" if they have the

¹⁴ These results have been previously obtained by Brander using the integral-equation approach of Kowalski and Feldman (Ref. 13). O. Brander, Arkiv Fysik 24, 439 (1963).

same effective range and scattering length (i.e., the same low-energy on-shell properties) and the same shape differing only in that one has a hard core while the other does not. In order to be able to choose the potential parameters easily we have used an exponential radial dependence.¹⁵ So that our results will have meaning for nucleon-nucleon interactions, we choose the scattering length to be infinite and the effective range to be 2.5 F. Such a potential is a reasonable approximation¹⁶ for an average singlet-triplet interaction and, if a hard-core radius of 0.4 F is used, the resulting potential also gives satisfactory results for nuclear matter.¹⁷ More specifically

$$V(\mathbf{r}) = +\infty, \qquad \mathbf{r} < c$$

= $-v_0 e^{-\mu(\mathbf{r}-c)}, \quad \mathbf{r} > c$ (24)

where $\mu = 3.5412/(b-2c)$ F⁻¹ and $v_0 = 1.4458\mu^2$. Also b = 2.5 F and we consider both c = 0 and c = 0.4 F.



FIG. 1. S-wave part of the off-energy-shell *t*-matrix elements, $2\pi^2 t_0(k/k; s)$, for two "equivalent" potentials of exponential shape, in the low-energy region. One has a hard core of radius c=0.4 F. The "energy" parameter is s=-0.2 F⁻².



FIG. 2. S-wave part of the off-energy-shell *t*-matrix elements, $2\pi^2 t_0(k',k;s)$, for two "equivalent" potentials of exponential shape, in the high-energy region. One has a hard core of radius c=0.4 F. The "energy" parameter is s=-0.2 F⁻².

Figure 1 presents the results obtained from Eq. (23) using the potential of (24) for s=0.2 F⁻². One should note that the two t matrices are nearly equal when k', k, and s are all small. This results from choosing the effective ranges and scattering lengths of both potentials to be equal, along with the analyticity properties imposed by the defining equations. If any of the variables k', k, s differ appreciably from zero, then effects of the hard core may be seen. In particular, for large values of k or k' the hard-core t matrix changes sign while the zero-core t matrix does not.

Figure 2 is similar to Fig. 1 except that very large values of k are shown. It can be seen that, while the no-core elements are negligibly small for k larger than 4 F⁻¹, the core elements still have significant size. This may be expected to manifest itself in the three-body bound states, by, perhaps, giving a somewhat smaller binding energy and larger mean radius.

Figure 3 shows the behavior of the diagonal element t(k,k;s). In particular, the asymptotic limit $c/4\pi^2$ is evident, while Fig. 4 shows the *s* dependence of these matrix elements. Only a single value of *s* is shown in the first three figures because the curves for other values of *s* are quite similar.

The *t*-matrix elements in the form presented in this section are not really useful for attacking the three-nucleon problem because of the complexity of the

¹⁵ For this shape, T. Kikuta, M. Morita, and M. Yamada [Progr. Theoret. Phys. (Kyoto) 15, 222 (1956)] have shown how to obtain the parameters for a potential containing a hard core if those of the "equivalent" potential are known. ¹⁶ For the experimental values, see Richard Wilson, *The Nucleon*-

 ¹⁶ For the experimental values, see Richard Wilson, *The Nucleon-Nucleon Interaction* (Interscience Publishers, Inc., New York, 1963), p. 37.
 ¹⁷ S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) 11,

¹⁷ S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) 11, 65 (1960).



FIG. 3. Diagonal element of the S-wave part of the off-energyshell t-matrix, $2\pi^2 t_0(k,k;s)$, for two "equivalent" potentials of exponential shape, one having a hard core of radius c=0.4 F. The "energy" parameter is s=-0.2 F⁻².

resulting equations. However, if a separable approximation can be found, then the resulting Faddeev equations are tractable. The usual approach has been to define a separable potential that fits the positive energy on-shell matrix elements (by matching phase shifts) and then to use the results to extrapolate to the desired region. If one is interested in three-body bound states, then only matrix elements for negative values of s occur, and the necessary extrapolation from positive to negative energies has not been shown to be reliable.¹⁸ For the bound-state problem, it would seem preferable to use a local potential to compute the *t*-matrix elements for negative values of s and then to approximate the results obtained with a suitable separable form. A preliminary attempt to do this with a sum of two separable terms has been carried out by the authors but with little success. Although it appears that the matrix elements for the c=0 case can indeed be approximated by sums of separable terms, the more complicated behavior of the hard-core matrix elements has made a quantitative approximation much more difficult to achieve. The separable approximation can be made for low values of k, k', where the core has not yet manifested itself, but we have not yet been successful in developing a formula that will be valid over a large



FIG. 4. S-wave part of the off-energy-shell *t*-matrix elements, $2\pi^2 l_0(k',k;s)$, as a function of s for two "equivalent" potentials of exponential shape, one having a hard core of radius c=0.4 F.

range of the variables (k',k;s). This problem is being investigated extensively at present.

V. SUMMARY

We have presented off-energy-shell *t*-matrix elements for S waves at negative values of the "energy" s using a potential having a hard core. The results have been compared with those for an "equivalent" potential having no core. There were substantial differences apparent at large values of k, k', or -s. It was not found possible to approximate quantitatively the hard-core matrix elements by a sum of two separable terms although a single term, equivalent to the effective range approximation, worked well for small values of k', k, and -s. Further attempts to find a separable-type approximation, at least for the regions of interest in the threebody bound-state problem, are now underway. It is felt that this procedure-using a local potential to compute the off-shell t-matrix elements in the region of interest and then approximating them with sums of separable terms-is more reliable than the usual technique of fitting phase shifts with sums of separable potentials and then using these to extrapolate to negative energies.

This paper has developed a method for computing off-shell *t*-matrix elements for potentials that contain a

¹⁸ This point is currently under investigation.

hard core. Using this method, several problems should be considered. An evaluation of the aforementioned phase-shift fitting and extrapolation procedure should be made. An investigation of the sensitivity of the threebody bound state to various features of the hard-core elements should be carried out and attempts to impose a separable approximation should be pursued. Perhaps an extension of the separable approximation to higher partial waves is worthwhile. Positive energies have not been considered in this paper, but they occur in scattering problems such as *n*-*d* scattering. It would be of great interest to compare the off-shell behavior of the usual separable approximation with the results of the local potential containing a hard core at positive energies.

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Hamiltonian Operator for Velocity-Dependent Potentials

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The Hamiltonian operator for a class of velocity-dependent potentials is studied. It is shown that the Hamiltonian and the energy of the system are not simply related, and while the former is a constant of motion and does not depend on time explicitly, the latter quantity is time-dependent, and the Heisenberg equation of motion is not satisfied.

ELOCITY-DEPENDENT nuclear forces have been used by many authors to explain the strong short-range repulsion of the two-nucleon interaction at high energies. Phenomenologically the velocity-dependent interaction arises from the expansion of a nonlocal operator by Taylor series.¹ To the lowest order in powers of $\mathbf{p} = -i\boldsymbol{\nabla}$ one finds

$$K(\mathbf{r}, -i\nabla)\psi(\mathbf{r}, \mathcal{E}) = \mathcal{E}\psi(\mathbf{r}, \mathcal{E})$$
(1)

as the Schrödinger equation and

$$K(\mathbf{r},\mathbf{p}) = (1/2m)\mathbf{p} \cdot f(\mathbf{r})\mathbf{p} + v(\mathbf{r})$$
(2)

for the Hamiltonian operator. Here f(r) is a smooth function of r having third derivative and approaching unity as r becomes larger than the range of nuclear forces. The constants in Eq. (1) are determined by fitting the resulting phase shifts, cross sections, and bound-state energies to the empirical values.² While the Hamiltonian (2) satisfies the general requirements of Hermiticity, rotational and time-reversal invariance, and the invariance under reflection in space, it is not a proper quantum-mechanical Hamiltonian. By a proper Hamiltonian $H(\mathbf{p},\mathbf{r})$ we mean the operator that describes the development of the system in time, or the operator with the property that for any dynamical variable $F(\mathbf{r},\mathbf{p},t)$ the relation

$$dF/dt = \partial F/\partial t - i[F,H]$$
(3a)

is satisfied. The operator $H(\mathbf{p},\mathbf{r})$ is closely related to the energy of the system. If we eliminate \mathbf{p} between H and $\dot{\mathbf{r}} = \partial H / \partial \mathbf{p}$ while preserving the order of factors we find the energy operator $E(\mathbf{r}, \dot{\mathbf{r}})$. Then by expressing F in terms of \mathbf{r} and $\mathbf{\dot{r}}$ we can write Eq. (3a) as

$$dF/dt = \partial F/\partial t + i[E,F].$$
(3b)

The operator $K(\mathbf{r},\mathbf{p})$ is a constant of motion that gives the correct equation of motion when it is used in Hamilton's canonical equations:

$$\dot{\mathbf{r}} = \partial K / \partial \mathbf{p}, \qquad (4a)$$

$$\dot{\mathbf{p}} = -\partial K / \partial \mathbf{r}. \tag{4b}$$

From Eqs. (2), (4a), and (4b) we can calculate the equation of motion, and from the equation of motion we can construct the energy operator. Knowing the equation of motion, the energy operator, and the definition of the time derivative [Eq. (3b)] we can obtain the commutation relation between $\dot{\mathbf{r}}$ and \mathbf{r} and also between \mathbf{p} and \mathbf{r} .³ For a Hamiltonian that can be written as the sum of two terms, one depending only on momentum and the other being a function of position, the operator equation (3b) is consistent with the usual commutation relation between **p** and **r**. Now we want to show that if: (a) the equation of motion is

^{*} E. W. R. Steacie Fellow. ¹ See, for instance, N. F. Mott and H. S. Massey, *The Theory* of *Atomic Collisions* (Oxford University Press, New York, 1949),

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⁸ E, P, Wigner, Phys. Rev. 77, 711 (1950).