Integral identities and bounds for scattering calculations and the Dirac formalism

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Integral identities that hold between ''desired'' and ''comparison'' solutions of the radial Dirac equations for scattering processes are considered. Applications of these identities are discussed, particularly the determination of bounds to variational calculations of *K*-matrix elements. [S1050-2947(99)09106-4]

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Relativistic effects in atomic scattering, and indeed in many quantum scattering processes, can usually be treated as small corrections, and handled by perturbation theory with respect to the nonrelativistic (Schrödinger) results. However, for some processes, such as the scattering of electrons by atoms and molecules, and for many nuclear scattering processes, it is often convenient or even necessary to use the Dirac equation directly. This is because the relativistic kinematics and spin effects are then automatically ''built in'' (see, for example, Refs. [1–3] and citations therein). In addition to this, relativistic corrections to the dynamics (i.e., corrections to the static potential) may need to be taken into account.

In the Dirac formalism, the description of the scattering of a fermion (such as an electron or positron) by a target (such as a neutral atom) is often reducible to the solution of the radial Dirac equations ($\hbar=c=1$)

$$f'(r)+\frac{\kappa}{r}f(r)=[E+m-V(r)]g(r)+X(r), \tag{1}$$

$$g'(r)-\frac{\kappa}{r}g(r)=-[E-m-V(r)]f(r)+Y(r), \tag{2}$$

where $f(r)$ and $g(r)$ are the usual reduced radial coefficients of the ''large'' and ''small'' components of the Dirac spinor for the incident fermion of mass m and energy E. The terms $X(r)$ and $Y(r)$ include exchange effects as may be applicable. We shall restrict our discussion to the class of potentials $V(r)$, and corresponding exchange terms $X(r),Y(r)$, such that the solutions $f(r),g(r)$ satisfy the following boundary conditions:

$$f_\kappa(r=0)=g_\kappa(r=0)=0, \tag{3}$$

$$f_\kappa(r\to\infty)\sim A_\kappa(k)\sin\left(kr-l\frac{\pi}{2}\right)+B_\kappa(k)\cos\left(kr-l\frac{\pi}{2}\right), \tag{4}$$

$$g_\kappa(r\to\infty)\sim\frac{f'_\kappa(r)}{E+m}=\frac{k}{E+m}\left[A_\kappa(k)\cos\left(kr-l\frac{\pi}{2}\right)-B_\kappa(k)\sin\left(kr-l\frac{\pi}{2}\right)\right], \tag{5}$$

where $k^2=E^2-m^2$, and $\kappa=j+\frac{1}{2}$ if $j=l-\frac{1}{2}$ (''spin down'') and $\kappa=-(j+\frac{1}{2})$ if $j=l+\frac{1}{2}$ (''spin up''). This means that the potentials are short range and not overly singular at the origin. Specifically, a sufficient condition is that the limit of $r^2V(r)$ be zero as $r\to\infty$ and as $r\to 0$. If the potential $V(r)$ is long range, i.e., if it contains a Coulombic contribution, then the sine and cosine functions in Eqs. (4) and (5) would be replaced by the corresponding Coulomb functions.

The asymptotic forms (4) and (5) can be written in the equivalent form

$$f_\kappa(r\to\infty)\sim C_\kappa(k)\sin\left(kr-l\frac{\pi}{2}+\eta_\kappa(k)\right), \tag{6}$$

$$g_\kappa(r\to\infty)\sim\frac{k}{E+m}C_\kappa(k)\cos\left(kr-l\frac{\pi}{2}+\eta_\kappa(k)\right), \tag{7}$$

where $\eta_\kappa(k)$ are the scattering phase shifts, while

$$A_\kappa(k)=C_\kappa(k)\cos\eta_\kappa(k)\quad\text{and}\quad B_\kappa(k)=C_\kappa(k)\sin\eta_\kappa(k). \tag{8}$$

The asymptotic normalization constants $C_\kappa(k)$ [or, equivalently, the constants $A_\kappa(k),B_\kappa(k)$] may be chosen to be anything that is convenient. Some common choices are $C_\kappa(k)=1$, $C_\kappa(k)=\sec\eta_\kappa(k)$, etc. The scattering cross sections or polarization parameters are then calculated from the phase shifts $\eta_\kappa(k)$ [1,2].

In nonrelativistic (Schrödinger) scattering theory, perturbative effects can be taken into account by using the integral identity between a ''given'' and ''comparison'' solution first obtained by Hulthén [4] and later elaborated by Kato [5] and others. This integral identity can also serve as the basis for approximate variational solutions to the scattering equations [4–7], and for determining bounds on approximate calculations of scattering parameters [8,9].

Evidently, analogous results can be written down in the Dirac formalism of scattering theory, as we now proceed to discuss. Thus, suppose $\overline{f}(r),\overline{g}(r)$ are solutions of a ''trial'' or ''comparison'' problem, corresponding to $\overline{X}(r)$, $\overline{Y}(r)$ and the potential $\overline{V}(r)$, namely

$$\overline{f}'(r)+\frac{\kappa}{r}\overline{f}(r)=[E+m-\overline{V}(r)]\overline{g}(r)+\overline{X}(r), \tag{9}$$

$$\overline{g}'(r)-\frac{\kappa}{r}\overline{g}(r)=-[E-m-\overline{V}(r)]\overline{f}(r)+\overline{Y}(r), \quad (10)$$

with

$$\overline{f}_\kappa(r\to\infty)\sim\overline{C}_\kappa(k)\sin\left(kr-l\frac{\pi}{2}+\overline{\eta}_\kappa(k)\right), \quad (11)$$

$$\overline{g}_\kappa(r\to\infty)\sim\frac{k}{E+m}\overline{C}_\kappa(k)\cos\left(kr-l\frac{\pi}{2}+\overline{\eta}_\kappa(k)\right). \quad (12)$$

Straightforward manipulations of Eqs. (1), (2), (9), and (10) result in the identity

$$\frac{d}{dr}(\overline{f}g-f\overline{g})=(V-\overline{V})(f\overline{f}+g\overline{g})+\overline{X}g-X\overline{g}+\overline{f}Y-f\overline{Y}. \quad (13)$$

Integration of Eq. (13) leads to the result

$$[\overline{f}(r)g(r)-f(r)\overline{g}(r)]_0^R=\int_0^R dr[(V-\overline{V})(f\overline{f}+g\overline{g})+\overline{X}g-X\overline{g}+Y\overline{f}-\overline{Y}f], \quad (14)$$

where $f=f(r)$, etc. in the integrand of Eq. (14). If we now make the replacements $f=\overline{f}+(f-\overline{f})$, etc., Eq. (14) can be rewritten in the form

$$\begin{aligned}\Delta=&\int_0^R dr[(V-\overline{V})(\overline{f}^2+\overline{g}^2)]\\&+\int_0^R dr(V-\overline{V})[(f-\overline{f})\overline{f}+(g-\overline{g})\overline{g}]\\&+\int_0^R dr[(\overline{X}-X)\overline{g}-(\overline{Y}-Y)\overline{f}]\\&+\int_0^R dr[\overline{X}(g-\overline{g})-\overline{Y}(f-\overline{f})],\end{aligned} \quad (15)$$

where

$$\begin{aligned}\Delta=[\overline{f}(r)g(r)-f(r)\overline{g}(r)]_0^R&\sim\frac{k}{E+m}C\overline{C}\sin(\overline{\eta}_\kappa-\eta_\kappa)\\&=\frac{k}{E+m}(\overline{B}A-\overline{A}B),\end{aligned} \quad (16)$$

and the symbol ''$\sim$'' indicates that R has been taken to be sufficiently large that the asymptotic forms (6), (7), (11), and (12) apply (we can take $R\to\infty$).

The integral identities (14) and (15) relate the phase shifts η_κ (or, more generally, functions of these, such as the K-matrix elements, $K_\kappa=\tan\eta_\kappa$, T-matrix elements, $T_\kappa=e^{i\eta_\kappa}\sin\eta_\kappa$, etc.) to the ''comparison'' phase shifts $\overline{\eta}_\kappa$ (or corresponding functions thereof). This is clear from the explicit form of Δ for a given choice of asymptotic normalization, that is, choice of A and B or alternatively C. For example, if $C=\overline{C}=1$, then $\Delta=[k/(E+m)]\sin(\overline{\eta}_\kappa-\eta_\kappa)$, or if $A=\overline{A}=1$, $B=\tan\eta_\kappa=K_\kappa$, and $\overline{B}=\tan\overline{\eta}_\kappa=\overline{K}_\kappa$, then $\Delta=[k/(E+m)](\overline{K}_\kappa-K_\kappa)$, etc.

The integral identities (14) or (15) can be used for various purposes, some of which we discuss briefly in what follows:

(i) Formal results. If we take $\overline{V}=0$, and the corresponding free incident wave solutions of Eqs. (9) and (10) for $\overline{f}_\kappa$ and $\overline{g}_\kappa$, then the identity (14) (with $A=\overline{A}=1$, $B=\tan\eta_\kappa=K_\kappa$, and $\overline{B}=0$) gives the well-known integral expression for the K-matrix elements,

$$K_\kappa=-\frac{E+m}{k}\int_0^R dr[V(f\overline{f}+g\overline{g})-X\overline{g}+Y\overline{f}]. \quad (17)$$

This is often used for extracting the phase shifts from numerical solutions of Eqs. (1) and (2).

(ii) Perturbative calculations. A not-infrequent situation is that the potential V can be written in the form $V=V_0+V_1$, where V_0 is a dominant (and/or easily solvable) interaction term (such as the electrostatic potential in atomic scattering), and V_1 is a small ''correction'' term. Then, obviously, if $\overline{V}=V_0$, $\overline{f}$ and $\overline{g}$ are known (or easily obtainable), while $V-\overline{V}=V_1$ can be handled perturbatively. Taking $f=\overline{f}$ and $g=\overline{g}$ in lowest order on the right-hand side of Eq. (15), one can use that equation to evaluate η_κ in terms of $\overline{\eta}_\kappa$ plus a lowest-order perturbative correction [which is given by the right-hand side of Eq. (15) with $f=\overline{f}$ and $g=\overline{g}$]. In general the perturbation may be in V only, or in X and Y, or both (see, for example, Ref. [10]).

(iii) Variational approximations. In some instances it may be useful or necessary to approximate the solutions of Eqs. (1) and (2) variationally. For example, one may wish to have analytic representations of the solutions [recall that, with rare exceptions, Eqs. (1) and (2) are not analytically solvable]. In such cases, one can use a variational approach, in which the desired (unknown) solutions $f(r),g(r)$ are approximated by analytic trial forms $\overline{f}(r),\overline{g}(r)$ that contain adjustable parameters α_j $(j=1,...,n_p)$. The identity (15) can be used to choose these parameters α_j in a variationally optimal way. We illustrate this in the case $X=Y=\overline{X}=\overline{Y}=0$, and normalization choice $C_\kappa=\overline{C}_\kappa=1$, in which case the identity (15) can be written as

$$\frac{k}{E+m}\sin(\overline{\eta}_\kappa-\eta_\kappa)=I[\overline{f},\overline{g}]+\mathcal{R}_2[f,g,\overline{f},\overline{g}], \quad (18)$$

where

$$I[\overline{f},\overline{g}]=\int_0^R dr(V-\overline{V})(\overline{f}^2+\overline{g}^2) \quad (19a)$$

$$=\int_0^R dr\left\{\overline{f}\left[\left(\frac{d}{dr}-\frac{\kappa}{r}\right)\overline{g}+(E-m-V)\overline{f}\right]-\overline{g}\left[\left(\frac{d}{dr}+\frac{\kappa}{r}\right)\overline{f}-(E+m-V)\overline{g}\right]\right\}, \quad (19b)$$

and where we have used the identities

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)\overline{f}(r)-[E+m-V(r)]\overline{g}(r)=[V(r)-\overline{V}(r)]\overline{g}(r), \tag{20}$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)\overline{g}(r)+[E-m-V(r)]\overline{f}(r)=-[V(r)-\overline{V}(r)]\overline{f}(r), \tag{21}$$

in rewriting Eq. (19a) in the form (19b). The term $\mathcal{R}_2$ is a ''remainder'' that is given by the expression

$$\mathcal{R}_2[f,g,\overline{f},\overline{g}]=\int_0^R dr(V-\overline{V})[(f-\overline{f})\overline{f}+(g-\overline{g})\overline{g}], \tag{22}$$

which is second order in the ''small'' quantities $f-\overline{f}$, $g-\overline{g}$, and $V-\overline{V}$. Usually we take $R\to\infty$ in these integrals, and this shall be done in the rest of this paper.

From Eq. (18), if we neglect $\mathcal{R}_2$, it follows that

$$\eta_\kappa(k)\simeq\overline{\eta}_\kappa(k)-\frac{E+m}{k}\sin^{-1}I[\overline{f},\overline{g}]=\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j), \tag{23}$$

where $\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)$ is the approximate value of $\eta_\kappa(k)$ for any given k and κ. Note that an explicit knowledge of the comparison potential $\overline{V}$ is not necessary to evaluate $\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)$, that is, it is only necessary to choose the trial functions $\overline{f},\overline{g}$. This is evident from Eq. (19b), in which, as can be seen, $\overline{V}$ does not appear explicitly. Of course, we want to choose the adjustable parameters α_j of $\overline{f}(r,\alpha_j)$ and $\overline{g}(r,\alpha_j)$ in such a way that $\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)$ is as close to $\eta_\kappa(k)$ as possible. In other words, we wish to minimize $|\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)|$ with respect to α_j. Since

$$\frac{\partial}{\partial\alpha_j}|\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)| =-\frac{(\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j))}{|\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)|}\frac{\partial}{\partial\alpha_j}\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j), \tag{24}$$

we see that a condition for a minimum of $|\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)|$ is that

$$\frac{\partial}{\partial\alpha_j}\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)=0, \tag{25}$$

as happens also in the corresponding Schrödinger theory. The resulting optimal values, α_j^{opt}, of the adjustable parameters α_j (which include the trial value $\overline{\eta}_\kappa$ of the phase shift, or of $\overline{K}_\kappa=\tan\overline{\eta}_\kappa$ if the normalization $\overline{A}=1$, $\overline{B}=\tan\overline{\eta}_\kappa$ is used, etc.), are then substituted into Eq. (23) to yield the optimal variational approximation, $\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j^{\mathrm{opt}})$, to $\eta_\kappa(k)$ [or $K_\kappa=\tan(\eta_\kappa)$, etc.], corresponding to a minimum value of $|\mathcal{R}_2|$. (Strictly speaking, minima of $|\eta_\kappa(k)-\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)|$ may occur at points in parameter space where $(\partial/\partial\alpha_j)\eta_\kappa^{(\mathrm{app.})}(k,\alpha_j)$ is undefined (i.e., cusps rather than smooth minima) or at boundary points of the domain of parameter space. Such possibilities must be kept in mind and investigated, if necessary.)

(iv) Bounds on scattering parameters. In approximate calculations of scattering parameters (phase shifts, K-matrix elements, etc.) neither the sign nor the magnitude of the difference between the (unknown) exact and approximate value is known. However, for the case $X=\overline{X}=Y=\overline{Y}=0$, if we write $\overline{V}=V+\delta V$, $\overline{f}=f+\delta f$, and $\overline{g}=g+\delta g$, where $\delta V,\delta f,\delta g\to 0$, then (with the choice of asymptotic normalization $C=1$) Eq. (14) implies that

$$\frac{k}{E+m}(\overline{\eta}_\kappa-\eta_\kappa)=-\int_0^\infty dr\ \delta V(\overline{f}^2+\overline{g}^2), \tag{26}$$

where we have kept only the first-order terms in infinitesimal quantities, and so set $\sin(\delta\eta)=\delta\eta$. Equation (26) shows that if $\overline{V}\to V$ from below, i.e., if $\delta V=\overline{V}-V<0$, then $\overline{\eta}_\kappa>\eta_\kappa$ and vice versa (as happens also in Schrödinger theory). This property can be used to set up a scheme in which approximate calculations of phase shifts approach the (unknown) exact values from above (or below), provided that the trial solutions are chosen so that the corresponding trial potentials approach the exact one from below (or above).

Although, as already stated, in general it is not possible to evaluate either the sign or the magnitude of the remainder term $\mathcal{R}_2$, Eq. (22), it is possible, in some cases, to determine calculable bounds $\mathcal{B}$ on $\mathcal{R}_2$ of the form

$$|\mathcal{R}_2[f,g,\overline{f},\overline{g}]|<\mathcal{B}[V,\overline{f},\overline{g}]. \tag{27}$$

This, together with Eq. (18) (or its equivalent with other asymptotic normalizations), leads to upper and lower bounds on the scattering parameters. We illustrate this on the potential scattering case ($X=Y=\overline{X}=\overline{Y}=0$), and the choice of asymptotic normalization $A=\overline{A}=1$, $B=\tan\eta_\kappa=K_\kappa$, $\overline{B}=\tan\overline{\eta}_\kappa=\overline{K}_\kappa$, whereupon Eq. (14) becomes

$$\frac{k}{E+m}(\overline{K}_\kappa-K_\kappa)=I[\overline{f},\overline{g}]+\mathcal{R}_2, \tag{28}$$

where $I[\overline{f},\overline{g}]$ is given in Eq. (19).

We write the remainder term, Eq. (22), in the form

$$\mathcal{R}_2=\mathcal{R}_{2L}+\mathcal{R}_{2S}, \tag{29}$$

where

$$\mathcal{R}_{2L}=\int_0^\infty dr\ \Delta V F(r)\overline{f}(r),\quad \mathcal{R}_{2S}=\int_0^\infty dr\ \Delta V G(r)\overline{g}(r), \tag{30}$$

with $\Delta V=V-\overline{V}$, $F=f-\overline{f}$, and $G=g-\overline{g}$. Then, using the Schwartz inequality $|(s,t)|^2\leqslant(s,s)(t,t)$, it follows from Eq. (29) that

$$|\mathcal{R}_{2L}|\leqslant a_F b_{\overline{f}},\quad |\mathcal{R}_{2S}|\leqslant a_G b_{\overline{g}}\ \text{ and so}$$

$$|\mathcal{R}_2|<a_F b_{\overline{f}}+a_G b_{\overline{g}}, \tag{31}$$

where

$$b_{\bar{f}}^2=\int_0^\infty dr\,\rho^{-1}(r)|\Delta V(r)\bar{f}(r)|^2,$$

$$b_{\bar{g}}^2=\int_0^\infty dr\,\rho^{-1}(r)|\Delta V(r)\bar{g}(r)|^2, \tag{32}$$

$$a_F^2=\int_0^\infty dr\,\rho(r)|F(r)|^2,\quad a_G^2=\int_0^\infty dr\,\rho(r)|G(r)|^2, \tag{33}$$

and $\rho(r)$ is an arbitrary, positive weight function (but such that all the indicated integrals exist). For example, $\rho(r)$ might be chosen to be $|\Delta V(r)|$, or some other positive function, possibly with adjustable parameters, such that the indicated integrals exist. For a given choice of trial functions $\bar{f},\bar{g}$, the expressions $b_{\bar{f}}$ and $b_{\bar{g}}$ of Eq. (32) are calculable [remember that $\bar{V}$ need not be known explicitly, in light of the identities (20) and (21)].

It remains now to determine bounds on a_F and a_G (which are not calculable since $F=f-\bar{f}$ and $G=g-\bar{g}$ are not known). One way that such bounds can be obtained is from the integral equations for the radial Dirac functions (written here for the present choice of asymptotic normalization $A=\bar{A}=1$ so that $B=K=\tan\eta$ and $\bar{B}=\bar{K}=\tan\bar{\eta}$):

$$f_\kappa(r)=u_1(r)+\int_0^\infty dr'U(r')[G_l^{11}(r,r')f_\kappa(r')+G_l^{12}(r,r')g_\kappa(r')], \tag{34}$$

$$g_\kappa(r)=u_2(r)+\int_0^\infty dr'U(r')[G_l^{21}(r,r')f_\kappa(r')+G_l^{22}(r,r')g_\kappa(r')], \tag{35}$$

where the Green functions G_l^{ab} are defined by

$$G_l^{ab}(r,r')=\frac{1}{k}v_a(kr)u_b(kr'),\quad r'<r$$

$$=\frac{1}{k}u_a(kr)v_b(kr'),\quad r'>r \tag{36}$$

and $U(r)=(E+m)V(r)$. The functions u_a,v_a are defined in terms of the usual Ricatti-Bessel and Ricatti-Neumann functions [11],

$$\hat{j}_l(kr)=krj_l(kr)\sim\sin\left(kr-l\frac{\pi}{2}\right)$$

and

$$\hat{n}_l(kr)=krn_l(kr)\sim-\cos\left(kr-l\frac{\pi}{2}\right), \tag{37}$$

namely

$$u_1(kr)=\hat{j}_l(kr),\quad v_1(kr)=\hat{n}_l(kr), \tag{38}$$

$$u_2(kr)=\sigma_\kappa\frac{k}{E+m}\hat{j}_{\bar{l}}(kr),\quad v_2(kr)=\sigma_\kappa\frac{k}{E+m}\hat{n}_{\bar{l}}(kr), \tag{39}$$

where $\bar{l}=l-\sigma_\kappa$ and $\sigma_\kappa=\kappa/|\kappa|$ is the sign of κ. Similar integral equations can be written down for $\bar{f}$ and $\bar{g}$, hence also for $F=f-\bar{f}$ and $G=g-\bar{g}$, specifically

$$F_\kappa(r)=\bar{F}_\kappa(r)+\int_0^\infty dr'U(r')[G_l^{11}(r,r')F_\kappa(r')+G_l^{12}(r,r')G_\kappa(r')], \tag{40}$$

$$G_\kappa(r)=\bar{G}_\kappa(r)+\int_0^\infty dr'U(r')[G_l^{21}(r,r')F_\kappa(r')+G_l^{22}(r,r')G_\kappa(r')], \tag{41}$$

where

$$\bar{F}_\kappa(r)=\int_0^\infty dr'[U(r')-\bar{U}(r')][G_l^{11}(r,r')\bar{f}_\kappa(r')+G_l^{12}(r,r')\bar{g}_\kappa(r')], \tag{42}$$

$$\bar{G}_\kappa(r)=\int_0^\infty dr'[U(r')-\bar{U}(r')][G_l^{21}(r,r')\bar{f}_\kappa(r')+G_l^{22}(r,r')\bar{g}_\kappa(r')]. \tag{43}$$

Note that $\bar{F}_\kappa(r),\bar{G}_\kappa(r)$ are known functions, for given trial functions $\bar{f}_\kappa$ and $\bar{g}_\kappa$, since $G_l^{ab}(r,r')$ are known. We stress that the explicit form of the trial potential $\bar{U}(r)$ need not be known in Eqs. (42) and (43) because of the identities (20) and (21). Thus, only the trial functions $\bar{f}_\kappa(r,\alpha_j)$ and $\bar{g}_\kappa(r,\alpha_j)$ need be specified.

Now, multiplying Eq. (42) by $\rho(r)F^*(r)$, integrating over r, and making repeated use of the Schwartz inequality gives the result

$$a_F\leqslant a_{\bar{F}}+a_Fg_{11}+a_Gg_{12}, \tag{44}$$

and similarly

$$a_G\leqslant a_{\bar{G}}+a_Fg_{21}+a_Gg_{22}, \tag{45}$$

where $a_{\bar{F}}$ and $a_{\bar{G}}$, defined as in Eq. (33), are calculable since $\bar{F}$ and $\bar{G}$ are known. The factors g_{ij} are given by

$$g_{ij}^2=\int_0^\infty\int_0^\infty dr\,dr'\rho(r)|G_l^{ij}(r,r')U(r')|^2\rho^{-1}(r'). \tag{46}$$

The generalized Schwartz inequality

$$\left| \int\int dr\, dr' s(r) Q(r,r') t(r') \right|^2 \leqslant \int dr |s(t)|^2 \int dr' |t(r')|^2 \int\int dr\, dr' |Q(r,r')|^2 \tag{47}$$

was used in obtaining the results (44)–(46).

From Eqs. (44) and (45), it follows that

$$a_F \leqslant \frac{1}{\mathcal{D}} [(1-g_{22}) a_{\bar{F}} + g_{12} a_{\bar{G}}] = B_F, \tag{48}$$

$$a_g \leqslant \frac{1}{\mathcal{D}} [(1-g_{11}) a_{\bar{G}} + g_{21} a_{\bar{F}}] = B_G, \tag{49}$$

provided that

$$g_{ii} < 1 \quad (i=1,2) \quad \text{and} \quad \mathcal{D} = (1-g_{11})(1-g_{22}) - g_{12} g_{21} > 0. \tag{50}$$

From the definition (46) of g_{ij}, and that of the Green functions (36), it is clear that the conditions (50) are, for given k (i.e., given energy of incidence), restrictions on the strength of the potential $V(r)$. That is, the potential must be sufficiently weak for the inequalities (50) to be met. Note, however, that since the Green functions contain the factor $1/k$, g_{ij} will generally decrease with increasing k. This means that a given potential $V(r)$ may be such that the inequalities (50) might not hold when k is small (low-energy scattering) but will hold for higher values of k.

Replacing the expressions a_F and a_G by their bounds (48) and (49) in Eq. (31) then leads to the inequality

$$|\mathcal{R}_2| < B_F b_{\bar{f}} + B_G b_{\bar{g}} = \mathcal{B}_2, \tag{51}$$

and hence to the following simultaneous upper and lower bounds on the (unknown) exact K-matrix element:

$$K_\kappa^{(\text{app.})} - \frac{E+m}{k} \mathcal{B}_2 < K_\kappa^{(\text{exact})} = \tan \eta_\kappa < K_\kappa^{(\text{app.})} + \frac{E+m}{k} \mathcal{B}_2, \tag{52}$$

where

$$K_\kappa^{(\text{app.})} = \bar{K} - \frac{E+m}{k} I[\bar{f}, \bar{g}]. \tag{53}$$

The definition (53) is the analog of that of Eq. (23) for the present choice of asymptotic normalization $A = \bar{A} = 1$. Note, again, that the bounds (52) hold provided that all the integrals that enter into the expressions for $K_\kappa^{(\text{app.})}$ and $\mathcal{B}_2$ exist, and that the inequalities (50) apply.

We stress that the bound $\mathcal{B}_2$ of Eq. (51) [with Eqs. (32), (48), and (49)] is expressible in terms of $V(r)$ and the trial functions $\bar{f}_\kappa(r, \alpha_j)$ and $\bar{g}_\kappa(r, \alpha_j)$, hence it is ultimately a function of the adjustable parameters, that is, $\mathcal{B}_2(\alpha_j)$. These parameters may be chosen in accordance with the variational prescription (25), or such that the upper and lower bounds are as close as possible, i.e., such that $\mathcal{B}_2(\alpha_j)$ is a minimum. These two prescriptions are not the same but, for sufficiently flexible trial functions, they will yield similar results. In practice, the prescription (25) is simpler to implement. In either case $\mathcal{B}_2$ can be made as small as desirable [in the domain where the conditions (50) hold], provided that $\bar{f}$ and $\bar{g}$ are sufficiently flexible.

To summarize, we have presented integral identities that hold between given and comparison (or ''trial'') solutions for scattering calculations in the Dirac formalism. Various applications of these integral identities have been discussed, including their use in approximate, variational solutions of the scattering parameters (phase shifts or functions thereof). In particular, we have used these integral identities to establish rigorous and calculable bounds on the difference between the exact and approximate K-matrix elements for a wide class of potentials. These bounds can be made as tight as necessary, if sufficiently flexible trial functions are used.

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