PHYSICAL REVIEW A VOLUME 12, NUMBER 6 DECEMBER 1975

Adiabatic optical potential and variational lower bounds on scattering parameters near threshold

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(Received 2 June 1975)

The exact elastic optical potential is compared with an analogous potential in the adiabatic approximation, which is shown to give a lower bound on the scattering length. A variational-bound procedure is formulated to estimate the scattering length and also the scattering phase shift near the elastic threshold.

For low-energy slow scattering by composite targets, the adiabatic approximation can often provide a useful estimate of the scattering parameters.[1] We present here an improved derivation of the lower bound on the scattering length at zero energy, based on a new representation of the scattering wave function in the adiabatic approximation. Extensions of the bound principle to a variational procedure and to energies above the threshold are also given.

(a) Consider the low energy scattering by a composite target, as described by the Hamiltonian

$$H=K(\vec{R})+H_T(\vec{r})+V(\vec{r},\vec{R}),$$

where K denotes the relative kinetic energy of the projectile, $H_T(\vec{r})$ describes the target system, and V is the projectile-target interaction. As usual, the undistorted target states $\psi_n(\vec{r})$ are generated by H_T, as $H_T\psi_n=e_n\psi_n$, while the adiabatic states $\phi_n(\vec{r},\vec{R})$ are obtained from $(H_T+V)\phi_n=\mathcal{E}_n(R)\,\phi_n$, in which the variable $\vec{R}$ appears as a parameter. As $R\to\infty$, we have

$$\phi_n\to\psi_n \quad\text{and}\quad \mathcal{E}_n(R)\equiv e_n+\mathcal{V}_n\to e_n\,. \tag{1}$$

The elastic scattering is conveniently described in terms of the optical potential U_0 in the equation

$$(K+U_0-E_0)u_0(\vec{R})=0\,, \tag{2}$$

where $E_0=E-e_0$ and

$$U_0=V_0+(\psi_0,VG^QV\psi_0). \tag{3}$$

In (3) we have used $G^Q=[Q(E-H)Q]^{-1}$, with $Q=1-P$ where P is the elastic channel projection operator $P=\psi_0\psi_0^*$. Obviously, $\psi_0(\vec{r})u_0(\vec{R})$ is the P projection of the total wave function Ψ, and $V_0=(\psi_0,V\psi_0)$. The standing-wave boundary conditions are assumed for u_0. It was shown earlier[1] that the adiabatic potential $\mathcal{V}_0$ can be written as

$$\mathcal{V}_0=V_0+(\psi_0,VG_a^QV\psi_0), \tag{4}$$

where

$$G_a^Q=[Q(\mathcal{E}_0-H_T-V)Q]^{-1}<0, \tag{5}$$

which is local in the $\vec{R}$ variable. Evidently, it is clear from Eqs. (3) and (5) that only those parts of the G^Q and G_a^Q which are within the range of V are relevant in the optical potentials and thus can affect the elastic amplitude.

(b) The potentials U_0 and $\mathcal{V}_0$ may be compared by examining the Green's functions G^Q and G_a^Q. For the zero-energy scattering with $E_0=0$, $\mathcal{V}_0$ may not support any bound states, in which case we have

$$t_0\equiv K+\mathcal{V}_0-E_0=K+\mathcal{V}_0\geq 0, \tag{6}$$

which in turn gives the inequalities

$$0>G^Q\geq G_a^Q \quad\text{and}\quad U_0\geq\mathcal{V}_0. \tag{7}$$

Therefore we have the desired bound on the exact scattering length A, as

$$A\geq A_a \tag{8}$$

(in the same cotanget branch[2]), where A_a is the scattering length obtained in the adiabatic approximation using the potential $\mathcal{V}_0$ in place of U_0 in Eq. (2). This is the derivation given earlier in Appendix A of Ref. 1, and is somewhat different from the result obtained with $t_0u_a=0$: The contents of the theory become quite different when their wave functions are compared and the error terms in the Kato identity are analyzed in detail. In the simple derivation presented above, we may assign the corresponding wave function by

$$\Psi_a=P\Psi_a+Q\Psi_a, \tag{9}$$

where

$$P\Psi_a=\psi_0(\vec{r})u_a(\vec{R}) \quad\text{and}\quad Q\Psi_a=G_a^QQVP\Psi_a\,. \tag{10}$$

The $Q\Psi_a$ part did not play any role in the previous formulation.[1] The adiabatic Hamiltonian is therefore not simply Pt_0P, but now[3]

$$\begin{aligned}H_a-E={}&P(H-E)P+PVQ+QVP\\&+Q(H_T+V-\mathcal{E}_0)Q\end{aligned} \tag{11}$$

and thus

$$H-H_a=Q(K+\mathcal{E}_0-E)Q=Qt_0Q\,.$$

We especially note that the asymptotic behavior of

$Q\Psi_a$ given in Eq. (10) in terms of G_a^Q differs from that of $Q\Psi$. That is, $Q\Psi$ decays rapidly as $R\to\infty$ in the elastic energy region, while $Q\Psi_a$ decays only as fast as the QVP. However, only those parts of $Q\Psi_a$ which lie inside the range of V are relevant for the amplitude, so that $Q\Psi_a$ should be regarded here as an auxiliary inelastic function simulating the $Q\Psi$.

(c) A variational procedure to improve the lower bound on A may be developed by examining the difference between U_0 and $\mathcal{V}_0$, or more directly between G^Q and G_a^Q. Using the operator identity for two Hermitian operators a and b,[4]

$$a^{-1}-b^{-1}=a^{-1}(b-a)b^{-1} = -[b+b(a-b)^{-1}b]^{-1}, \tag{12}$$

we have

$$g^Q \equiv G^Q - G_a^Q = d^{-1}, \tag{13}$$

where

$$d=d_0+d_0(Q/t_0)d_0 \tag{14}$$

with

$$d_0=Q(H_T+V-\mathcal{E}_0)Q \geq 0,$$

$$t_0=K+\mathcal{V}_0-E_0.$$

(The question of the spurious solutions in the Q-space will be discussed later.) With $t_0\geq 0$ by assumption, at $E_0=0$ we have $d>0$ and $g^Q>0$, which gives

$$U_0>\mathcal{V}_0 \tag{15}$$

as before. Furthermore, g^Q may be approximated variationally as

$$g^Q \geq g_S^Q = \frac{Q\chi_t)(Q\chi_t}{(Q\chi_t, dQ\chi_t)} \geq 0, \tag{16}$$

where $Q\chi_t$ is a trial function which is square integrable in both the variables $\vec{R}$ and $\vec{r}$. The use of a square-integrable function in Eq. (16) is justified in view of the earlier remark that both G^Q and G_a^Q are cut off at large values of R by the factors QVP and PVQ in the optical potential. A more general inequality of the form (16) with more than one $Q\chi_t$ is also possible. Defining the trial optical potential by

$$U_{0t}=\mathcal{V}_0+(\psi_0, Vg_s^QV\psi_0), \tag{17}$$

we have, under conditions similar to Eq. (8), the inequality

$$U_0 \geq U_{0t} \geq \mathcal{V}_0 \tag{18}$$

with the resulting bounds at zero energy ($E_0=0$)

$$A \geq A_t \geq A_a \tag{19}$$

if they are all in the same cotangent branch.[2] In Eq. (19), A_t is the scattering length calculated with U_{0t} replacing the exact U_0 in Eq. (2). A more detailed discussion of this result using the Kato identity for A will be given later in part (f).

(d) Extensions of the above formalism to the positive energy scattering and related bounds on the phase shift δ_l for each partial wave requires $g^Q>0$ at $E_0>0$. This is difficult to prove in general, but we have[1]

$$\frac{\partial g^Q}{\partial E_0}=\frac{\partial}{\partial E_0}(G^Q-G_a^Q)=-(G^Q)^2<0, \tag{20}$$

where $G^Q(<0)$ is assumed to be Hermitian. Therefore, if $g^Q\geq 0$ at $E_0=0$ and $G^Q<0$ for some $E_0>0$, we have a finite nonvanishing region of energy E_0 above the threshold in which $g^Q>0$. As E_0 increases further, g^Q will eventually become negative. Denoting this limit to be $E_0=E_c$, we have

$$\delta_l \leq \delta_{lt} \leq \delta_{la} \quad \text{for} \quad 0<E_0\leq E_c, \tag{21}$$

where δ_{lt} is the phase shift obtained with U_{0t}. Or, assuming that both δ_l and δ_{la} are in the same cotangent branch, we have

$$\cot\delta_l \geq \cot\delta_{lt} \geq \cot\delta_{la} \quad \text{for} \quad 0<E_0\leq E_c. \tag{22}$$

The precise value for E_c depends on the details of the dynamics, but Eqs. (21) and (22) are expected to be valid for E_0 in the region close to the threshold. Some indication of the magnitude of E_c may be obtained variationally; the lowest zero of $d(E_0)$ may be obtained by the equation

$$(Q\chi_t, d_0Q\chi_t)=-(Q\chi_t, d_0(Q/t_0)d_0Q\chi_t), \tag{23}$$

where t_0^{-1} involves the principal value integration. For a fixed E_0 in t_0, Eq. (23) should give an upper bound on E_c, which can be systematically improved by including more terms.

(e) The form for g^Q given by Eqs. (13) and (14) requires further discussion. Although the effect of t_0 is relevant only in the region where V is large, t_0 can, for $E_0\geq 0$, still generate a spurious asymptotic behavior in the Q-space since it is purely an R-dependent operator. This is obviously unphysical because, for E below the first excitation threshold, the Q space is closed. However, we show below that the appearance of t_0^{-1} in the operator d is entirely consistent with the asymptotic boundary condition of the original problem. Unlike in the earlier formulation of Ref. 1, the difficulty with the spurious solution does not appear in the present formulation with the operator d^{-1}; the Q-space wave function is always damped out by the factor QVP at large R.

For a single, elastic channel problem, G^Q and $Q\Psi=G^QQVP\Psi$ contain no outgoing waves, since they are in the Q space. As noted earlier, $Q\Psi_a$ also goes to zero asymptotically as fast as QVP does, although G_a^Q does not necessarily vanish at large R. Therefore, the function

$$Q\Psi_x \equiv Q\Psi - Q\Psi_a = d^{-1}QVP\Psi$$

should also vanish faster than R^{-1} at large R. That is, the asymptotic behavior of d^{-1} is similar to that of d_0^{-1} and the term $d_0 t_0^{-1} d_0$ in d does *not* alter the asymptotic behavior of d^{-1} in any essential way. In fact, $Q\Psi_x$ can be shown to satisfy a set of coupled equations

$$-Qd_0Q\Psi_x = -QVP\Psi - Qd_0Q\phi$$

$$Qt_0Q\phi = -Qd_0Q\Psi_x$$

where we have introduced an auxiliary function $Q\phi$ which carries the effect of $d_0t_0^{-1}d_0$. Evidently, by eliminating $Q\Psi_x$ from the $Q\phi$ equation and rearranging terms, we can show that $Q\phi = Q\Psi$. That is, $Q\Psi_x$ and $Q\phi$ both vanish asymptotically faster than R^{-1}. (They may go like R^{-2} in atomic problems, rather than decaying exponentially.)

Therefore the apparent inconsistency between the asymptotic behavior of t_0^{-1} in the operator d and the over-all boundary condition on $Q\Psi$ has been resolved; the difficulty of the spurious solution is not present if $Q\Psi_x$ is treated correctly. In view of the above discussion, a slightly more convenient form for the operator d may be obtained by repeating the use of Eq. (12) and writing

$$a^{-1} - b^{-1} = -\left(b + b\frac{1}{c}b - b\frac{1}{c + ce^{-1}c}b\right)^{-1}, \qquad (24)$$

where

$$a - b \equiv c + e.$$

The identity (24) gives[5]

$$g^Q = d^{-1} = [d_0 + d_0\bar{t}_0^{-1}d_0 - d_0(\bar{t}_0 + \bar{t}_0^2\bar{e}^{-1})^{-1}d_0]^{-1}, \qquad (25)$$

where we identified

$$b \equiv d_0 = Q(H_T + V - \mathcal{E}_0)Q,$$

$$c \equiv \bar{t}_0 = Q(K + \mathcal{V}_0 - E_0 + \bar{e})Q = Qt_0 + Q\bar{e},$$

$$e \equiv \bar{e} \lesssim e_1 - e_0.$$

The positivity of d is less clear in the form of Eq. (25), since we have the additional negative term involving $\bar{t}_0^2$. However, $\bar{t}_0^{-1}$ may be easier to use in practice than t_0^{-1}, since $\bar{t}_0^{-1}$ now decays asymptotically.

(f) Now we discuss the bound property using the Kato identity for the scattering parameter λ defined by (depending on the normalization of u)

$$\lambda \equiv k \cot\delta.$$

From Eq. (13) it is clear that the original scattering problem in the elastic region can be cast in a form suitable for the present purpose as a set of coupled equations; using the operator d given by (14), for example, we have the exact scattering equations[6]

$$P(K + \mathcal{V}_0 - E_0)P\Psi_x = -PVQ\Psi_x,$$
$$-Q(d_0 + d_0(Q/t_0)d_0)Q\Psi_x = -QVP\Psi_x. \qquad (26)$$

Note especially the negative sign on the left-hand side of the $Q\Psi_x$ equation. In Eq. (26), we could of course have used the form (25) for d with the improved asymptotic behavior in $\bar{t}_0^{-1}$. However, the main point of the discussion below will not be affected by this change.

To derive a useful Kato identity, we first solve formally for $P\Psi_x$ as

$$P\Psi_x = P\Psi_a^P + PG_a^PPVQ\Psi_x, \qquad (27)$$

where

$$P(K + \mathcal{V}_0 - E_0)P\Psi_a^P = 0,$$

$$P(K + \mathcal{V}_0 - E_0)PG_a^PP = -P. \qquad (28)$$

Substitution of Eq. (28) into the right hand side of the $Q\Psi_x$ equation gives

$$-QDQ\Psi_x \equiv -Q(d_0 + d_0(Q/t_0)d_0 - VG_a^PV)Q\Psi_x$$
$$= -QVP\Psi_a^P. \qquad (29)$$

Thus we have

$$\lambda = \lambda_a + (P\Psi_a^P, PVQ\Psi_x)$$
$$= \lambda_{Lt} + \tau, \qquad (30)$$

where

$$\lambda_{Lt} = \lambda_a + 2(P\Psi_a^P, PVQ\Psi_t) - (Q\Psi_t, QDQ\Psi_t),$$

$$\tau = (Q\Omega, QDQ\Omega),$$

and where $Q\Psi_t$ is a square-integrable trial function and $Q\Omega = Q\Psi_t - Q\Psi_x$ is the error function. Therefore, if we assume that

$$QDQ \geqslant 0, \qquad (31)$$

then the error term τ, which is quadratic in $Q\Omega$, is also positive,

$$\tau > 0,$$

and thus

$$\lambda \geqslant \lambda_{Lt}. \qquad (32)$$

This inequality (32) for the parameter λ should be completely equivalent to the earlier result [Eq. (22)] obtained with g_s^Q, except that a slightly different operator QDQ is now involved, which contains the adiabatic shift operator $QVPG_a^PPVQ$.

It is of interest to compare Eq. (32) with the earlier result on the upper variational-bound formulation for λ, as given by[7]

$$\lambda \leq \lambda_{Ut},$$

with

$$\lambda_{Ut} = \lambda^P + 2(P\Psi^P, PVQ\Psi_t) + (Q\Psi_t, [\mathcal{H} - E]Q\Psi_t), \tag{33}$$

provided

$$Q(\mathcal{H} - E)Q \equiv Q(H - E + VG^PV)Q \geq 0. \tag{34}$$

In Eq. (33), we have used the functions in the static approximation,

$$P(H-E)P\Psi^P = P(K + V_0 - E_0)P\Psi^P = 0,$$

$$P(H-E)PG^PP = -P,$$

and λ^P is the parameter obtained from the static solution $P\Psi^P$. As in Eq. (33) which requires Eq. (34), our variational lower bound Eq. (34) requires Eq. (31) for its validity.

(g) Our main result is contained in inequalities (19), (22), and (32). In the course of the derivation of these inequalities, we have neglected several important effects:

(i) When t_0 supports one or more bound states, then the inequalities such as (15) may be violated, and a certain number of "subtractions" are required. This is also connected with the question of δ_l and δ_{la} being in the same branch of the cotangent function. With the use of the variational-bound formulation, such as in (18), this problem may be avoided in practice for most cases.

(ii) We have not included the exchange effect in the case when the projectile is identical to the target particles. This effect seems to be difficult to incorporate simply because of the very nature of the adiabatic approximation in which the projectile particle is singled out. An exception to this may be in the heavy-particle collisions where the adiabatic picture is often very appropriate.

(iii) The formalism may be trivially extended to obtain a lower bound on the binding energy of the composite system of the projectile and the target. The resulting equation is similar to Eq. (23), without the Q operator and with E_0 replaced by the estimated binding energy.

(iv) A more systematic formulation[8] of the lower variational bound can be given in terms of the adiabatic energy gaps from the beginning of the theory, at the stage where the total Hamilonian is split into an adiabatic form and the correction. However, from a calculational point of view, the present treatment using the operator d, given by (14) or (25), is much simpler and straight-forward. The main drawback of d is of course the uncertainty in the estimate of E_c below which the bound property is valid. For E_0 not too far from the threshold, however, this causes less serious problem.

(h) The problem of formulating a variational lower bound has been considered previously,[9] which invariably involves the complicated operators H^2 and $(QHQ)^2$. The main distinguishing feature of the present formulation is the use of the adiabatic picture, which makes it possible to avoid such a complicated operator. In both Eqs. (18) and (30) only operators linear in d_0 appear.

Recently, a different formulation of the variational lower bound on the scattering length was given by Rosenberg and Spruch,[10] which also adopts the adiabatic approximation as a basis. It is not clear at present whether these two formulations are in any way related; this should be examined more closely. However, we simply make a few remarks here on their formulation of the zero-energy scattering. A bound on the error term in the Kato identity for the scattering length A was expressed there in terms of an operator C_t which satisfies the inequalities $H - E_0 - C_t \geq 0$ and $C_t \geq 0$. We suggest a choice for this operator,

$$C_t = K + \mathcal{E}_0 - E_0, \quad (E_0 = 0),$$

which can be inverted exactly and gives

$$A \geq A_t + (\Psi_t, [H - E_0]\Psi_t) - \left(\Psi_t, [H - E_0]\frac{1}{K + \mathcal{E}_0 - E_0}[H - E_0]\Psi_t\right). \tag{35}$$

(Another possibility, $C_t = H_t + V - \mathcal{E}_0$, is excluded because C_t cannot be inverted exactly.) Aside from the arbitrariness in C_t, the formulation of Ref. 10 emphasizes the role of the trial function Ψ_t. Alternatively, one may place more emphasis on the trial nature of the operator C_t itself, rather than on the trial wave function Ψ_t as with Eq. (35). From the Kato identity we may then obtain, with $H_t = H - C_t$,

$$A_t(H_t) = A + (\Psi, [H_t - E_0]\Psi) - (\Omega, [H_t - E_0]\Omega) \leq A, \tag{36}$$

where A_t is obtained from the exact solution of an approximate problem

$$(H_t - E_0)\Psi_t = 0,$$

and where

$$H_t = K + \mathcal{E}_0 - E_0 + d_s$$

with

$$d_s = (d_0\chi)(\chi, d_0\chi)^{-1}(\chi d_0)$$

and

$$d_0 \equiv H_t + V - \mathcal{E}_0.$$

Such d_s corresponds to the choice $C_t = d_0 - d_s \geq 0$, and thus $H - E_0 - C_t \geq 0$ if $H - E_0 \geq 0$ and $K + \mathcal{E}_0 - E_0 \geq 0$. Note that the role of d_0 in Eqs. (35) and (36) is interchanged. The solution Ψ_t with the above H_t may involve the difficulty of the spurious Q-space solutions discussed in Ref. 1, and a more consistent treatment may eventually require the formulation with the adiabatic energy gap operators.[8]

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[1]Y. Hahn and L. Spruch, Phys. Rev. A 9, 226 (1974). Many earlier references to works on the lower-bound and variational-lower-bound formulations may be found in this paper.

[2]The same cotangent branch here implies that both A and A_a are associated with the corresponding zero-energy wave functions with the same number of nodes.

[3]This is in fact the choice (3) for the adiabatic Hamiltonian discussed in Ref. 1. [See Eq. (3.9) of that paper.] We have studied the Kato identity using the Hamiltonian (11) and the error function $\Omega = \Psi_a - \Psi$ from (10), but a similar result can also be obtained more directly from (26).

[4]We assume that the inverse of a and b, as well as the inverse of their difference, exists.

[5]Because $\bar{e}$ is chosen to be a constant, the unfamiliar operator $(\bar{e}\bar{t}_0 + \bar{t}_0^2)^{-1}$ is introduced in (25). However, $\bar{t}_0$ is assumed to be Hermitian so that we do not expect any difficulty in evaluating it. The evaluation of g_s^Q of (16) using the form (25) for d can be carried out in any number of ways; for example, we can construct an auxiliary function $Q\omega_t$ from the equation $Q(\bar{t}_0 + \bar{e})Q\omega_t = \bar{t}_0^{-1} d_0 Q\chi_t$. Then $(Q\chi_t, dQ\chi_t) = (Q\chi_t, Q\omega_t)$ for the denominator of g_s^Q.

[6]The Q-space wave function $Q\Psi_x$ defined here may not be directly related to the exact $Q\Psi$, but, when put into (26), generates the right effect needed to have the exact $P\Psi$. In fact, the new scattering function Ψ_x differs from the exact Ψ by $Q\Psi_a$ given in (10).

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[8]Y. Hahn and L. Spruch (unpublished).

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