Role of near-degeneracy in the scattering of composite neutral systems

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(Received 25 February 1987)

We study the elastic scattering of two neutral composite systems, both of which have states nearly degenerate with the initial state. A novel consequence of the degeneracy is the appearance of a term in the scattering amplitude f, coming from the second Born approximation, which behaves as $i(Q^2/p)\ln(Q^2/p^2)$ for small momentum transfer Q and fixed momentum p. This term strongly affects the behavior of the partial-wave amplitudes f_l for $l>1$. Possible applications to experiment, especially to the scattering of excited-state positronium from molecules, are indicated.

I. INTRODUCTION

There has been extensive study of the effects of two-photon exchange in the interaction of two neutral systems[1] or of a neutral and a charged system.[2] In most of these analyses it was assumed that the initial state of the neutral system has no accidental degeneracy. Recently the effects of two-photon exchange in the scattering of an electron from a neutral atom were discussed for the case where the initial atomic state is nearly degenerate.[3] It was found that, in the limit of exact degeneracy, the leading term in the scattering amplitude at small momentum transfer $\mathbf{Q}=\mathbf{p}'-\mathbf{p}$ is imaginary and strongly dependent on both energy and angle, with a logarithmic divergence of the form $i(\ln Q)/p$ for $Q\to 0$ and p fixed. This singularity arises completely from double Coulomb exchange, with transverse photons giving only a small correction in the nonrelativistic regime.

In the present paper we extend this work by examining the scattering of two neutral systems, each of which may have an accidental near degeneracy. We find that if only one system is degenerate then the relevant part of the scattering amplitude at small Q is real and behaves as Q^3, corresponding to the familiar R^{-6} London potential. Furthermore, in the limit of exact degeneracy, transverse photons again only give a small correction; this is unlike the case of two nondegenerate systems, where there is a cancellation between transverse-photon and Coulomb exchange, leaving a residual term which behaves as $Q^4\ln Q$, corresponding to the Casimir-Polder R^{-7} potential.[4]

When both systems are degenerate the dominant contribution at small Q, again given by double Coulomb exchange, is imaginary and behaves as $i(Q^2/p)\ln Q$ for fixed p.

The derivation of these results is given below, in Sec. II. Concluding remarks are made in Sec. III.

II. ANALYSIS

A. Preliminaries

We consider a neutral target atom A and neutral projectile B and work in the c.m. of the combined systems. For simplicity we specialize to the case where both A and B are hydrogenlike, but allow the masses of the positively charged constituents to differ. The generalization to more complex systems is straightforward.

With $\mathbf{r}_1$ and $\mathbf{r}_2$ the coordinates of the electron and core of A, $\mathbf{r}_3$ and $\mathbf{r}_4$ those of the electron and core of B, the electrostatic interaction between A and B takes the form

$$U=e^2(|\mathbf{r}_1-\mathbf{r}_3|^{-1}+|\mathbf{r}_2-\mathbf{r}_4|^{-1} -|\mathbf{r}_1-\mathbf{r}_4|^{-1}-|\mathbf{r}_2-\mathbf{r}_3|^{-1}) .$$

With spin and exchange neglected, the wave function of the initial state is given by

$$\phi_I=\exp(i\mathbf{p}_A\cdot\mathbf{R}_A)\phi_{A;a}(\mathbf{r})\exp(i\mathbf{p}_B\cdot\mathbf{R}_B)\phi_{B;b}(\mathbf{r}') .$$

Here $\mathbf{p}_A$, $\mathbf{R}_A$, and $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ denote the initial momentum, c.m. coordinate, and relative coordinate, respectively, associated with A; the vectors $\mathbf{p}_B$, $\mathbf{R}_B$, and $\mathbf{r}'=\mathbf{r}_3-\mathbf{r}_4$ are similarly associated with B.

The second-order transition amplitude for elastic scattering to a final state ϕ_F with momenta $\mathbf{p}'_A$ and $\mathbf{p}'_B$ but unchanged internal quantum numbers a and b is given by

$$T=\langle \mathbf{p}';a,b\,|\,U(W_0+p^2/2M_{AB}-H_0+i\epsilon)^{-1}U\,|\,\mathbf{p};a,b\rangle , \tag{1a}$$

where $\mathbf{p}$ and $\mathbf{p}'$ are the initial and final momenta of B in the overall c.m. system and H_0 is the Hamiltonian in the c.m. system,

$$H_0=h_A+h_B+\mathbf{P}_{\rm op}^2/2M_{AB} . \tag{1b}$$

Here h_A and h_B are the internal Hamiltonians of A and B, $W_0=W_a+W_b$ is the sum of the binding energies of A and B, $M_{AB}=M_AM_B/(M_A+M_B)$ is the reduced mass of the combined system, and $\mathbf{P}_{\rm op}=-i\partial/\partial\mathbf{R}$, with $\mathbf{R}=\mathbf{R}_B-\mathbf{R}_A$ the coordinate vector of B relative to A.

On inserting a complete set of eigenstates $|\,\mathbf{k};m,n\,\rangle$ of H_0 into (1.2) we get

$$T=\sum_{m,n}T_{mn},\quad T_{mn}=(2\pi)^{-3}\int_0^\infty dk\,k^2I_{mn}\ , \tag{2}$$

where

$$I_{mn}=\int d\Omega\frac{\langle\mathbf{p}';a,b\,|\,U\,|\,\mathbf{k};m,n\,\rangle\langle\mathbf{k};m,n\,|\,U\,|\,\mathbf{p};a,b\,\rangle}{[D_{mn}(p,k)+i\epsilon]} \tag{3a}$$

with

$$D_{mn}(p,k)=(W_a-W_m)+(W_b-W_n)+(p^2-k^2)/2M_{AB}\ . \tag{3b}$$

The integration in (3) is over the angles of the vector $\mathbf{k}$. On use of the Fourier representation

$$x^{-1}=(1/2\pi^2)\int d\mathbf{y}\exp(i\mathbf{x}\cdot\mathbf{y})/y^2$$

one finds that the numerator matrix elements may be written in the form

$$\begin{aligned}\langle\mathbf{k};m,n\,|\,U\,|\,\mathbf{p};a,b\,\rangle&=(4\pi e^2/q^2)F_{mn;ab}(\mathbf{q})\ ,\\ \langle\mathbf{p}';a,b\,|\,U\,|\,\mathbf{k};m,n\,\rangle&=(4\pi e^2/q'^2)F_{ab;mn}(\mathbf{q}')\ ,\end{aligned} \tag{4}$$

with

$$\mathbf{q}=\mathbf{k}-\mathbf{p},\quad \mathbf{q}'=\mathbf{p}'-\mathbf{k}\ .$$

The F's are sums of products of transition form factors,

$$\begin{aligned}&F_{mn;ab}(q)\\ &=\{[\langle m\,|\,\exp(ia_2\mathbf{q}\cdot\mathbf{r})\,|\,a\,\rangle\langle n\,|\,\exp(-ib_2\mathbf{q}\cdot\mathbf{r}')\,|\,b\,\rangle]\\ &\quad+(a_2\to-a_1,b_2\to-b_1)\\ &\quad-(b_2\to-b_1)-(a_2\to-a_1)\}\ ,\end{aligned} \tag{5}$$

where a_i and b_i are mass ratios defined by

$$a_1=m_1/M_A,\quad a_2=m_2/M_A,$$
$$b_1=m_3/M_B,\quad b_2=m_4/M_B\ .$$

B. Computation

Let us regard T as a function of the relative momentum p and the squared momentum transfer t in the c.m. system,

$$t=-Q^2,\quad \mathbf{Q}=\mathbf{p}'-\mathbf{p}\ . \tag{6}$$

For fixed p we expect T to have the form

$$T=A(p)+B(p)t+C(p,t)\ , \tag{7}$$

where C is analytic in a cut t plane, with a singularity at $t=0$, and decreasing for large $|t|$. This singularity arises from the long-range character of the Coulomb interaction, whereas the polynomial $A+Bt$ also gets contributions from short distances. In the spirit of our earlier work[2] we concentrate on the calculation of the singularity at $t=0$, but in contrast to Ref. 3 we find it convenient this time to make use of dispersion theory techniques, as in Ref. 2 and Ref. 4.

We note first that the analyticity properties of T are closely tied to those of the partial summands I_{mn} which occur as integrands in (2). Let us define

$$J_{mn}=\sum_{\rm deg}I_{mn}\ , \tag{8}$$

where the sum is over a complete set of product states degenerate in energy with $\phi_{A;m}\phi_{B;n}$. Because of the rotational invariance of U and because the definition (3) includes an integration over the angles of the intermediate-state relative momentum k, the function J_{mn} is also rotationally invariant and can therefore be regarded as a function of t, p, and k. For our purpose it is sufficient to study the function J_{mn} in the dipole approximation. In this approximation we have

$$\begin{aligned}F_{mn;ab}&\to\langle m\,|\,\mathbf{r}\cdot\mathbf{q}\,|\,a\,\rangle\langle n\,|\,\mathbf{r}'\cdot\mathbf{q}\,|\,b\,\rangle\ ,\\ F_{ab;mn}&\to\langle a\,|\,\mathbf{r}\cdot\mathbf{q}'\,|\,m\,\rangle\langle b\,|\,\mathbf{r}'\cdot\mathbf{q}'\,|\,n\,\rangle\ .\end{aligned} \tag{9a}$$

The numerator in the expression for J_{mn} then reduces to the form

$$\sum_{\rm deg}\langle a\,|\,\mathbf{r}\cdot\mathbf{q}'\,|\,m\,\rangle\langle m\,|\,\mathbf{r}\cdot\mathbf{q}\,|\,a\,\rangle\sum_{\rm deg}\langle b\,|\,\mathbf{r}'\cdot\mathbf{q}'\,|\,n\,\rangle\langle n\,|\,\mathbf{r}'\cdot\mathbf{q}\,|\,b\,\rangle. \tag{9b}$$

For $|\,a\,\rangle$ and $|\,b\,\rangle$ both S states (the states $|\,m\,\rangle$ and $|\,n\,\rangle$ are then necessarily P states) this further reduces to the form

$$(\mathbf{q}'\cdot\mathbf{q}/3)(G_{ma})^2(\mathbf{q}'\cdot\mathbf{q}/3)(G_{nb})^2\ , \tag{9c}$$

where the G's denote the matrix element of r taken between radial wave functions. It follows that, in the dipole approximation and *with initial S states*,

$$J_{mn}\to J_{mn}^{\rm dip}=A_{mn}[D_{mn}(p,k)+i\epsilon]^{-1}K\ , \tag{10a}$$

where

$$A_{mn}=(4\pi e^2/3)^2(G_{ma}G_{nb})^2 \tag{10b}$$

and

$$K=\int d\Omega(\mathbf{q}'\cdot\mathbf{q})^2/q^2q'^2\ . \tag{11}$$

Since

$$\mathbf{Q}=\mathbf{q}+\mathbf{q}'$$

we have

$$\mathbf{q}'\cdot\mathbf{q}=(Q^2-q^2-q'^2)/2\ . \tag{12}$$

On substituting (12) into (11) we see that K has the form

$$K=K'+K''\ , \tag{13}$$

where

$$K'=(t/2)^2\int d\Omega/q^2q'^2 \tag{14}$$

arises from the square of the first term on the right-hand side of (12). The quantity K'' in (13) represents the contribution of the remaining terms which, as is readily shown, give just a first-degree polynomial in t,

$$K''=C_1 t+C_0 \tag{15}$$

with the C's functions of p and k. Although both K' and $C_1 t$ decrease rapidly enough for large k to give convergent integrals if (10a) is used in (2), the term C_0 in K'' does not; its contribution, while formally independent of t, is linearly divergent. However, the dipole approximation is not valid for the short distances to which large values of k correspond. If this approximation is not made, the analogue of the C_0 term gives a convergent contribution to T_{mn} which, while not independent of t, is not singular in the neighborhood of $t=0$. We can therefore concentrate on K'.

Let J'_{mn} denote the part of J_{mn} coming from K' and T'_{mn} the corresponding part of T_{mn},

$$T'_{mn}=(2\pi)^{-3}\int_0^\infty dk\, k^2 J'_{mn}\ . \tag{16}$$

Analysis shows that the quantity T'_{mn} is an analytic function of t with a branchpoint singularity at $t=0$. We will study the behavior of T'_{mn} in the neighborhood of $t=0$ by the techniques of dispersion theory. This leads us to consider the discontinuity across the cut, taken from 0 to plus infinity, which is given by

$$[T'_{mn}]_t=(2\pi)^{-3}\int_0^\infty dk\, k^2[J'_{mn}]_t\ , \tag{17}$$

where

$$[J'_{mn}]_t=A_{mn}\{D_{mn}(p,k)+i\epsilon\}^{-1}[K']_t\ ,$$

and $[K']_t$ is the discontinuity of K' across a cut extending from a branchpoint t_1 (which depends on k) to infinity. On combining the denominators in (14) by a Feynman parameter and carrying out the angular integration, one finds that

$$K'=(2\pi)(t/2)^2\int_{-1}^{1} du\ 1/k^2 F\ ,$$

where

$$F=t_1-(1-u^2)t,\quad t_1=(p^2-k^2)^2/k^2\ .$$

It follows that

$$[K']_t=(4i\pi^2)(t/2)^2\int_{-1}^{1} du\ \delta(F)/k^2\ . \tag{18}$$

On substituting (18) into (17) we get, on reversing the integration order,

$$[T'_{mn}]_t=(i/\pi)M_{AB}A_{mn}(t/2)^2 \times\int_{-1}^{1} du\int_0^\infty dk\,(k_0^2-k^2+i\epsilon)^{-1}\delta(F)\ , \tag{19}$$

where

$$k_0^2=p^2-\Delta,\quad \Delta=-(2M_{AB})(W_a-W_m+W_b-W_m)\ .$$

The integrations over k and u can then be carried out. With the quantities t_0 and C_{mn} defined by

$$t_0=\Delta^2/|k_0^2|,\quad C_{mn}=(M_{AB}A_{mn}t_0^{1/2})/8\Delta$$

we find the following result: for $p^2>\Delta$,

$$[T'_{mn}]_t=iC_{mn}t^{3/2}[(t_0-t)^{-1/2}\Theta(t_0-t) +i(t-t_0)^{-1/2}\Theta(t-t_0)]\ , \tag{20a}$$

and for $p^2<\Delta$,

$$[T'_{mn}]_t=-iC_{mn}t^{3/2}(t+t_0)^{-1/2}\ . \tag{20b}$$

The amplitude T'_{mn} in the physical region ($t<0$) is given, apart from an additive polynomial in t, by an integral of the form

$$(2\pi i)^{-1}\int_0^\infty dt'[T'_{mn}(t')]_t/(t'-t)\ ;$$

subtractions necessary for convergence are not explicitly indicated. We are now ready to consider in turn the special cases of interest to us.

(a) $p^2\gg\Delta$, $-t=Q^2\gg\Delta$. For $\Delta\to 0$, the first term in (20a) vanishes and the second term reduces to the form

$$\text{const}(t/p)\theta(t)\ ,$$

which yields a T'_{mn} proportional to

$$i(t/p)\ln(-t)\ . \tag{21a}$$

This situation applies when the states $|m\rangle$ and $|n\rangle$ are both degenerate, with the states $|a\rangle$ and $|b\rangle$, respectively, i.e., to the case of double degeneracy. We have thus shown that in this case the scattering amplitude behaves, for small t, as a polynomial plus a term proportional to (21a).

(b) $p^2\ll\Delta$ and $Q^2\ll\Delta$. In this case $t_0\sim\Delta$, $k_0\sim\Delta^{1/2}$, and (21a) reduces to the form

$$\text{const}(t^{3/2}/\Delta)\ . \tag{21b}$$

T'_{mn} itself then behaves for small t as (21b) plus an additive polynomial. This situation applies if only one of the intermediate states is degenerate while the excitation energy of the other is large compared to $p^2/2M_{AB}$; the behavior found corresponds to what one would get from the London potential.[5] It is easy to verify that the corresponding London constant is proportional to the electric polarizability α_E of the nondegenerate system.[6]

C. Transverse photon contribution

In this section we will show that if we consider only the excitation of states degenerate with the initial state, the exchange of transverse photons makes a negligible contribution to the scattering amplitude.

There are two types of transverse-photon contributions to T, those in which two transverse photons are exchanged and those in which one transverse photon and one "Coulomb photon" are exchanged. Consider first the exchange of two transverse photons. A typical degenerate-state contribution to T will contain a factor which also enters the Compton amplitude for photon scattering from system A, which we assume to be the one with degenerate states. This factor is given, in the dipole approximation, by

$$\langle a|\boldsymbol{\epsilon}'\cdot\mathbf{p}_{\text{op}}|d\rangle\langle d|\boldsymbol{\epsilon}\cdot\mathbf{p}_{\text{op}}|a\rangle\ ,$$

where $|d\rangle$ is a state almost degenerate with $|a\rangle$. Upon use of the usual commutator identity for $\mathbf{p}_{op}$ we see that this factor is proportional to the square of the energy difference $W_d - W_a$ between $|a\rangle$ and $|d\rangle$. It therefore vanishes in the limit of exact degeneracy. Similarly, if one transverse photon and a Coulomb photon are exchanged the corresponding factor is

$$\langle a|\mathbf{r}\cdot\mathbf{r}'|d\rangle\langle d|\boldsymbol{\epsilon}\cdot\mathbf{p}_{op}|a\rangle ,$$

which is proportional to $W_d - W_a$. It follows that if we do not make the adiabatic approximation (so that none of the accompanying energy denominators vanishes) these contributions all vanish in the limit of exact degeneracy.

III. DISCUSSION

A. Further remarks on photon exchange

In the preceding section we have isolated the dominant contribution to T from the degenerate states. Of course, other, nondegenerate states will give contributions to transverse photon exchange and to double Coulomb exchange. These combine to give that part of the scattering amplitude that arises from the Casimir-Polder potential. The latter amplitude behaves as $t^2 \ln t$ for small t,[4] and so should be substantially smaller than that arising from the degenerate states.

If the degeneracy is not exact, then the transverse photon contributions of the nearly degenerate states will not vanish exactly. In that case, at sufficiently small t the total long-range (i.e., nonanalytic) part of T will always be given by the Casimir-Polder potential. The relevant value of t is given by $t' \sim M_{AB}\Delta$. If $M_{AB} \sim m_e$ and Δ is much less than the usual atomic excitation energies, then t' will correspond to very small angles and the amplitude arising from double Coulomb exchange can be used in most of the region of physical interest.

B. Possible application to experiment

To orient ourselves about the approximate magnitude of the scattering amplitude and the domain of validity of the second Born approximation we estimate the degenerate-state contribution f' to the scattering amplitude f in the doubly degenerate case. Using $f = -(M_{AB}/2\pi)T$ and Eq. (21a) we get

$$f' \sim iM_{AB}\alpha^2 a^4 (M_{AB} t/p)\ln(t/p^2) , \tag{22}$$

where a is a length of atomic dimensions. This can be rewritten in the form

$$f' \sim a(M_{AB}/m_e)^2 (pa) g(\theta) , \tag{23}$$

where

$$g(\theta) = (1-\cos\theta)\ln(1-\cos\theta) . \tag{24}$$

TABLE I. Order of magnitude of various contributions to partial wave amplitudes f_l, for small values of l.

l	f_l'/a	f_l''/a	$f_l'^{nd}/a$
0	pa	1	$(pa)^3$
1	pa	pa	$(pa)^3$
2	pa	$(pa)^2$	$(pa)^3$

The amplitude f' contains all partial wave amplitudes f_l' and these decrease only slowly with l. If $M_{AB} \sim m_e$, as, for example, when the projectile is a positronium atom, the f_l' satisfy the unitarity bound $|f_l'| < 1$, as long as $p < a^{-1}$. However, if $M_{AB} \gg m_e$, e.g., if the projectile is an ordinary atom, this bound is grossly violated, unless p is extremely small. Therefore our second Born approximation formulas can certainly not be applied, in the doubly degenerate case, to the scattering of an ordinary atom or molecule by another, except perhaps at ridiculously low energies. Furthermore, for $l=0$ and 1 the full partial wave amplitudes f_l get large contributions from higher Born approximations, from short-distance effects such as those contained in K'' [Eq. (15)], and from other excited states in the second Born approximation. Because of these, the values of f_0 and f_1 cannot be approximated by f_0' and f_1' in any case.

We can, however, use (23) to estimate f_l' for $l > 1$ for positronium, e.g., for positronium in the 2^3S state scattering from a polar molecule in its ground state, for which it may be the dominant contribution to f_l. To see this we present, in Table I, the order of magnitude of various contributions to f_l: the long-range part f_l' coming from degenerate states, the short-range part f_l'' coming from all states, and a part $f_l'^{nd}$ coming from intermediate states in which only one of the two colliding systems retains its initial energy.

From Table I we see that for $pa < 1$ and $l \geq 2$ the quantity f_l' begins to dominate f_l''. We also note that for $pa < 1$ the contribution $f_l'^{nd}$ is much smaller than f_l'; if both systems are excited to nondegenerate states the contribution is still smaller. If ground-state positronium is scattered from a molecule, only $f_l'^{nd}$ is present in higher partial waves.[7,8]

An accurate measurement of the elastic differential cross section for $2\,^3S$-state positronium on a polar molecule may be able to reveal these novel effects of degeneracy in long-range interactions.

ACKNOWLEDGMENTS

We thank C.-K. Au for a useful discussion of this topic. This work was supported in part by the Department of Energy and in part by the National Science Foundation.

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