Instituto de Física
Universidade de São Paulo

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Hussein, M.S

Departamento de Física Nuclear, Instituto de Física,
Universidade de São Paulo, São Paulo, Brazil

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THEORY OF COMPLEX SCATTERING LENGTHS

M.S. Hussein

Instituto de Física, Universidade de São Paulo,

C.P. 66318, São Paulo, 05315-970, Brazil

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Abstract

We derive a generalized Low equation for the T-matrix appropriate for complex atom-molecule interaction. The properties of this new equation at very low energies are studied and the complex scattering length and effective range are derived.

The recent realization of Bose-Einstein condensation (BEC) of ultracold atoms with the accompanying upsurge of theoretical activities have rekindled interest in low energy collisions of atoms and molecules. The subsequent proposals for the creation of ultracold molecular [1-5] and hybrid atomic-molecular BEC [6,7] intensified the above mentioned interest Of particular importance in the above recent developments is the idea of decay of the condensates. In a series of papers, Dalgarno and collaborators [8-12] have looked into the idea of using a complex scattering length to represent the low-energy atom-molecule scattering. Implicit in this is the multichannel nature of the collision process: an atom hits a vibrationally excited molecule at extremely low energies. The open inelastic channels are those where the molecule is excited into lower vibrational states. In this sense one has a depletion of the elastic channel. In Ref. [8], the quenching of H_2 molecules in collisions with H was considered. It was found that, the inelastic cross-sections and the corresponding depletion rate coefficients were very large for high vibrational levels of H_2.

In the above studies, the following form of low-energy S-wave scattering amplitude is used

$$f(k) = \frac{1}{g(k^2) - i\,k}\ , \tag{1}$$

where k is the wave number related to the center of mass energy of the colliding partners, E, by $\frac{\hbar k^2}{2\mu} = E$, with μ being the reduced mass of the system. The function $g(k^2)$ is even in k and is given by the effective range formula.

$$g(k^2) = -\frac{1}{a} + \frac{1}{2} r_o k^2\ , \tag{2}$$

where a is the scattering length and r_o the effective range, both directly related to the interaction. When applied to atom-molecule scattering at very low energies, with the molecules suffering inelastic transitions to lower vibrational states, the scattering length a is taken to be complex, $a = \alpha - i\beta$, with β related to the total inelastic cross-section.

The question we raise here is the validity of Eq. (1) with a and eventually $r_\circ$ taken as complex in the case of the elastic scattering with strong coupling to inelastic channels. Of course, an equivalent one-channel description of the elastic scattering can be formulated with the introduction of an appropriate complex optical potential as described by Feshbach [13]. It is therefore legitimate to inquire about the validity of Eq. (1), originally obtained for real potential, if a complex interaction is used [14]. The general structure of the low energy scattering amplitude is also of potentially fundamental importance to very low energy matter interferometry. This method for the obtention of f for molecule-molecule scattering has been quite successful at room temperatures [15,16]. Extension to very low temperatures of this method seems natural and would welcome studies of the type reported here.

For the above purpose, it is useful to summarize the elegant derivation of Eq. (1) given by Weinberg [17]. If we denote the interaction by V and the free Green's function by $G_o^{(+)}(E) = (E - H_o + i\varepsilon)^{-1}$, then the T-matrix given by the Lippmann-Schwinger equation $T^{(+)} = V + VG_o^{(+)}T^{(+)}$, can be written as $T^{(+)} = V + VG^{(+)}V$, with the full Green's function $G^{(+)} = (E + i\varepsilon - H_o - V)^{-1}$. Using the spectral expansion of $G^{(+)}$, with the complete set of bound and scattering states $\left\{|B\rangle, |\Psi^{(+)}\rangle\right\}$, we obtain the Low-equation

$$\left\langle \vec{k\prime} \left| T^{(+)}(E) \right| \vec{k} \right\rangle = \left\langle \vec{k\prime} \left| V \right| \vec{k} \right\rangle + \sum_B \frac{\left\langle \vec{k\prime} \left| V \right| B \right\rangle \left\langle B \left| V \right| \vec{k} \right\rangle}{E + E_B} + \int d\vec{k''} \frac{T^{(+)}_{\vec{k\prime}k''}(E_{k''}) \left(T^{(+)}_{\vec{k''}k}(E_{k''}) \right)^*}{E - E_{k''} + i\varepsilon} . \tag{3}$$

At very low energies relevant for BEC, we seek a solution $T_{\vec{k\prime}k}(E) \equiv T(E)$ and writing $\left\langle \vec{k\prime} \left| V \right| \vec{k} \right\rangle = \bar{V}$ we have

$$t^{(+)}(E) = \bar{V} + \sum_B \frac{|g_B|^2}{E + E_B} + \int d\vec{k''} \frac{\left| t^{(+)}(E_{k''}) \right|^2}{E - E_{k''} + i\varepsilon} . \tag{4}$$

Calculating now $t^{(+)}(E)^{-1} - t^{(-)}(E)^{-1}$, we find

$$t^{(+)}(E)^{-1} - t^{(-)}(E)^{-1} = \frac{t^{(-)}(E) - t^{(+)}(E)}{t^{(-)}(E)\ t^{(+)}(E)} . \tag{5}$$

Since $t^{(-)}(E) = T(E-i\varepsilon) = \left(T^{(+)}(E+i\varepsilon)\right)^*$, if V is real, we have $t^{(+)}(E)^{-1} - t^{(-)}(E)^{-1} = -2ik\ 2\pi\frac{2\mu}{\hbar^2}$ which is just the discontinuity across the positive energy cut in the complex energy plane. Besides the poles in t, (zeros in $(t)^{-1}$), the only other terms in $\left(t^{(+)}\right)^{-1}$ are entire functions of $W \equiv E+i\varepsilon$. Accordingly, with the identification $f = -\frac{1}{2\pi}\frac{2\mu}{\hbar^2}t$, Eq. (1) follows.

We turn next to a complex interaction $V \neq V^\dagger$. The completeness relation now reads $\sum_B |B\rangle\langle B| + \int d\vec{k}\!\!/ \left|\Psi^{(+)}_{\vec{k}\!\!/}\right\rangle\left\langle\tilde{\Psi}^{(+)}_{k\!\!/}\right|$ where $\left|\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\right\rangle$ is the dual scattering state which is a solution of the Schrödinger equation with V replaced by $V^\dagger$ [18,19]. Another form of the completeness relation may also be used, $\sum_B |B\rangle\langle B| + \int d\vec{k}\!\!/ \left|\tilde{\Psi}^{(-)}_{\vec{k}\!\!/}\right\rangle\left\langle\Psi^{(-)}_{k\!\!/}\right|$,with $\left|\Psi^{(-)}_{\vec{k}\!\!/}\right\rangle$ being the physical scattering state with incoming wave boundary condition $\left(V^\dagger, -i\varepsilon\right)$ and $\left|\tilde{\Psi}^{(-)}_{\vec{k}\!\!/}\right\rangle$ its corresponding dual state $(V, -i\varepsilon)$. Thus, the full Green's function now has the spectral form

$$G^{(+)}(E) = \sum_B \frac{|B\rangle\langle B|}{E+E_B} + \int d\vec{k}\!\!/ \frac{\left|\Psi^{(+)}_{\vec{k}}\right\rangle\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\right|}{E-E_{k\!\!/}+i\varepsilon}\ . \tag{6}$$

Accordingly, Eq. (3) now reads

$$\left\langle\vec{k}\!\!'\left|T\right|\vec{k}\right\rangle = \left\langle\vec{k}\!\!'\left|V\right|\vec{k}\right\rangle + \sum_B \frac{\left\langle\vec{k}\!\!'\left|V\right|B\right\rangle\left\langle B\left|V\right|\vec{k}\right\rangle}{E+E_B+i\varepsilon} + \int d\vec{k}\!\!/ \frac{\left\langle\vec{k}\!\!'\left|V\right|\Psi^{(+)}_{\vec{k}\!\!/}\right\rangle\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\left|V\right|\vec{k}\right\rangle}{E-E_{k\!\!/}+i\varepsilon}\ . \tag{7}$$

It is clear that the Low equation, Eq. (3), is not valid anymore. However, as we show below Eq. (1) is still valid, with the appropriate generalization of the real function $g(k^2)$ to a complex one [16]. To see this we analyze the matrix element $\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\left|V\right|\vec{k}\right\rangle$. From the $L-S$ equation for $\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\right|$,

$$\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\right| = \left\langle\vec{k}\!\!'\right| + \left\langle\vec{k}\!\!'\right| V\frac{1}{E_{k\!\!/}-H_\circ-V-i\varepsilon} \equiv \left\langle\vec{k}\!\!'\right|\left[1+VG^{(-)}(E_{k\!\!/})\right]\ . \tag{8}$$

Thus $\left\langle\tilde{\Psi}^{(+)}_{\vec{k}\!\!/}\left|V\right|\vec{k}\right\rangle = \left\langle\vec{k}\!\!'\left|\tilde{T}(E_{k\!\!/}-i\varepsilon)\right|\vec{k}\right\rangle$, where the unphysical T-matrix $\tilde{T}$ is given by

$$\tilde{T} = V + VG^{(-)}V \ . \tag{9}$$

Accordingly the T-matrix equation, Eq (7), may be written as

$$\left\langle \vec{k\prime} \left| T\left(E\right) \right| \vec{k} \right\rangle = \left\langle \vec{k} \left| V \right| \vec{k} \right\rangle + \sum_{B} \frac{\left\langle \vec{k\prime} \left| V \right| B \right\rangle \left\langle B \left| V \right| \vec{k} \right\rangle}{E + E_B + i\varepsilon}$$
$$+ \int d\vec{k\prime\prime} \frac{\left\langle \vec{k\prime} \left| T\left(E\prime\prime\right) \right| \vec{k\prime\prime} \right\rangle \left\langle \vec{k\prime\prime} \left| \tilde{T}\left(E\prime\prime\right) \right| \vec{k} \right\rangle}{E - E\prime\prime + i\varepsilon} \ . \tag{10}$$

A similar equation holds for $\left\langle \vec{k\prime} \left| \tilde{T}\left(E\right) \right| \vec{k} \right\rangle$with $i\varepsilon$ replaced by $-i\varepsilon$. It is interesting at this point to show the relation between the physical T-matrix element $\left\langle \vec{k\prime} \left| T\left(E\right) \right| \vec{k} \right\rangle$ and $\left\langle \vec{k\prime} \left| \tilde{T}\left(E\right) \right| \vec{k} \right\rangle$. This can be done easily following operator manipulations of [18], and using the relation $\left\langle \tilde{\Psi}^{(+)}_{\vec{k\prime\prime}} \right| = \left\langle \Psi^{(+)}_{\vec{k\prime\prime}} \right| + \left\langle \Psi^{(+)}_{\vec{k\prime\prime}} \right| \left(V - V^{\dagger}\right) G^{(-)}\left(E_{k\prime\prime}\right)$, Eq. (8),

$$\left\langle \vec{k\prime} \left| \tilde{T}\left(E\right) \right| \vec{k} \right\rangle = \left\langle \vec{k\prime} \left| T\left(E\right) \right| \vec{k} \right\rangle^{*} + \int d\vec{k\prime\prime} \left\langle \Psi^{(+)}_{\vec{k\prime}} \left| \left(V - V^{\dagger}\right) \right| \Psi^{(+)}_{\vec{k\prime\prime}} \right\rangle S^{-1}_{\vec{k\prime\prime}\vec{k}} \ , \tag{11}$$

where S^{-1} is the inverse S-matrix in the elastic channel, $S^{-1}_{\vec{k\prime\prime}\vec{k}} = \left\langle \tilde{\Psi}^{(+)}_{\vec{k\prime\prime}} \left| \tilde{\Psi}^{(-)}_{\vec{k}} \right\rangle \right.$, and the diagonal part of the matrix element $\left\langle \Psi^{(+)}_{\vec{k\prime}} \left| \left(V - V^{\dagger}\right) \right| \Psi^{(+)}_{\vec{k\prime\prime}} \right\rangle$is directly related to the total inelastic scattering cross-section, σ_{in}, viz [18]

$$\left\langle \Psi^{(+)}_{\vec{k}} \left| \left(V - V^{\dagger}\right) \right| \Psi^{(+)}_{\vec{k}} \right\rangle = -2i\frac{E}{k}\sigma_{in}\left(E\right) \ . \tag{12}$$

Eq. (11) explicitly exhibits the connection between $\tilde{T}$ and T through the absorptive part of the effective interaction.

Now we seek the low energy solution $\left\langle \vec{k\prime} \left| T \right| \vec{k} \right\rangle \equiv t_{+}\left(E\right)$ and $\left\langle \vec{k\prime} \left| \tilde{T} \right| \vec{k} \right\rangle \equiv t_{-}\left(E\right)$ and following the same steps as Weinberg's [17], we find immediately, from Eq. (10), with $f_{\pm} = -\frac{1}{2\pi}\frac{2\mu}{\hbar^2}t_{\pm}$,

$$f_+^{-1} = g_c\left(k^2\right) - ik \ ; \tag{13}$$

$$f_-^{-1} = g_c\left(k^2\right) + ik \ , \tag{14}$$

where $g_c\left(k^2\right)$ is the complex generalization of $g\left(k^2\right)$ of Eq. (1).

We turn now to the connection between $g_c\left(k^2\right)$ and the low-energy observables. This is most conveniently accomplished by employing the generalized optical theorem

$$\frac{4\pi}{k} \operatorname{Im} f_+ = \sigma_{el} + \sigma_{in} \ , \tag{15}$$

where σ_{el} is the total elastic scattering cross section $4\pi \left|f_+\right|^2$ and σ_{in} the total inelastic cross-section.

Using (12), we find

$$\frac{-\operatorname{Im}\ g_c\left(k^2\right)}{\left(\operatorname{Re}\ g_c\left(k^2\right)\right)^2 + \left(\operatorname{Im}\ g_c\left(k^2\right) - k\right)^2} = \frac{k}{4\pi}\sigma_{in} \ . \tag{16}$$

At $k = 0$, $g_c\left(0\right) = -\frac{1}{a}$, where a is the complex scattering length written as [8] $\alpha - i\beta$. Thus the imaginary part of a, β, is found to be

$$\beta = \frac{\left(k\ \sigma_{in}\right)_{k=0}}{4\pi} \ , \tag{17}$$

an expression also derived in Ref. [8]. Eq. (16) clearly implies that σ_{in} should go as k^{-1} as k is lowered, in accordance with Wigner's law.

We go a bit beyond Refs. [8-12] and derive a relation between β and the imaginary part of the effective potential. Since σ_{in} is given by (for S-wave scattering), Eq. (12)

$$\sigma_{in} = \frac{4\pi}{kE} \int_0^\infty |u(r)|^2 \, |\mathrm{Im}\, V\ (r)| \ dr \ , \tag{18}$$

where $u(r)$ is the S-wave elastic radial wave function, we find

$$\beta = \left[\frac{1}{E} \int_0^\infty |u(r)|^2 \, |\mathrm{Im}\, V\ (r)| \ dr \right]_{E \to 0} \ . \tag{19}$$

An equation for the complex effective range, r_o, can also be easily derived. Equation (19) is the principle result of this work. It summarizes the following:

1) The coupled-channels calculation aimed to describe the molecular quenching can be recast as an effective one-channel calculation with a complex interaction whose imaginary part account for flux loss.

2) The low-energy behaviour of the scattering amplitude with the complex interaction alluded to above can be conveniently parametrized in terms of complex scattering length and effective range.

The message this work conveys is the potential usefulness of constructing the effective complex (optical) interaction for the scattering of ro-vibrational molecules from atoms at low energies. The calculation of a and r_o from knowledge of this potential can be done in a direct and unambiguous way.

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REFERENCES

[1] R. Wynar, R. Preelond, D.J. Han, C. Ryh and D.J. Henzen, Science, 287, 1016 (2000).

[2] J.M. Doyle, B. Friedrich, J. Kim and D. Patterson, Phys. Rev. A52, R2515 (1995).

[3] Y.B. Band and P.S. Juliene, Phys. Rev. A51, R4317 (1995).

[4] B. Friedrich and D.R. Herschbach, Phys. Rev. Lett. 74, 4623 (1995).

[5] J.T. Bahns, W.C. Stwalley, P.L. Gould, J. Chem. Phys. 104, 9689 (1996).

[6] E. Timmermans, P. Tommasini, R. Côte, M.S. Hussein and A.K. Kerman, Phys. Rev. Lett. 83, 2691 (1999).

[7] E. Timmermans, P. Tommasini, M.S. Hussein and A.K. Kerman, Phys. Reports 315, 199 (1999).

[8] N. Balakrishnan, R.C. Forrey and A. Dalgarno, Chem. Phys. Lett. 280, 5 (1997).

[9] N. Balakrishnan, R.C. Forrey and A. Dalgarno, Phys. Rev. Lett. 80, 3224 (1998).

[10] R.C. Forrey, N. Balakrishnan, V. Kharchenko and a. Dalgarno, Phys. Rev. A58, R2645 (1998).

[11] R.C. Forrey, V. Kharchenko, N. Balakrishnan and A. Dalgarno, Phys. Rev. A59, 2146 (1999).

[12] R.C. Forrey, N. Balakrishnan, A. Dalgarno, M.R. Haggarty and E.J. Heller, Phys. Rev. Lett. 82, 2657 (1999).

[13] H. Feshbach, Ann. Phys. (NY) 15, 357 (1958); Ann. Phys. (NY) 19, 287 (1962).

[14] L.D. Landau and E. Lifchitz, Quantum Mechanics (1966).

[15] J. Schmiedmayer, M.S. Chapman, C.P. Ekstrom, T.D. Hammod, S.Wehinger and D.E. Pritchard, Phys. Rev. Lett. 74, 1043 (1995).

[16] M.S. Chapman, C.R. Ekstrom, T.D. Hammond, R. Rubenskin, J. Schmiedmayer, S. Hehinger and D.E. Pritchar, Phys. Rev. Lett. 74, 4783 (1995).

[17] S. Weinberg, Brandeis Summer Institute in Theoretical Physcis, S. Desser and K.W. Ford, Editors (Prentice Hall Inc.) (1965), vol. II, p. 291-403.

[18] M.S. Hussein, Ann. Phys. (NY) 175, 197 (1987); H. Feshbach, Ann. Phys. (NY) 164, 398 (1985).

[19] M.S. Hussein and E.J. Moniz, Phys. Rev. C29, 2054 (1984).