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¹High-resolution experiments using metastable-atom beams are fairly common—see *Electronic and Atomic Collisions*, edited by J. S. Risley and R. Geballe (Univ. of Washington Press, Seattle, Wash., 1975), pp. 433–445. Optically excited Na has been used as a target for electron scattering.

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Derivation of Dispersion Relations for Atomic Scattering Processes*

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We point out that it now appears very likely that because of the properties of the exchange amplitude the customary forward dispersion relations do not hold for electron-atom elastic scattering.

In this note we wish to point out that recent experimental progress makes it seem very likely that the customary forward dispersion relations do not hold for electron-atom elastic scattering.

Let us begin by assuming that we are dealing with nonrelativistic elastic scattering of electrons by noble gases where the scattering amplitude can be written as

$$f(E, \theta) = f^d(E, \theta) - g(E, \theta), \quad (1)$$

f^d being the direct amplitude and g being the exchange amplitude. [We shall also use the first

Born approximation to f^d and g , which we shall denote respectively by f_{B1}^d and g_{B1} ; all quantities will be expressed in atomic units (a.u.).] If we restrict our attention to forward scattering and assume that, as in potential scattering, $f(E, 0)$ [denoted henceforth as $f(E)$] is analytic in the complex E plane cut along the positive real axis, then we may write

$$2\pi i f(E) = \oint_C \frac{f(E')}{E' - E} dE'. \quad (2)$$

Here C is the well-known contour in the cut plane

consisting of straight-line segments C_+ and C_- along the upper and lower edges of the cut, respectively, and a large circle "at infinity" (C_∞) joining these two segments, while E is any point within the contour. In writing Eq. (2), we are assuming that $f(E)$ has no poles on the negative real axis.

In order to obtain a dispersion relation for $f(E)$, it is necessary that $f(E) \rightarrow 0$ as $E \rightarrow \infty$ along any ray in the E plane. This is not the case for $f(E)$ as given by Eq. (1); it is widely believed that as $E \rightarrow \infty$, $f(E) \rightarrow \text{const}$, the constant being simply the quantity $f_{B_1}^d(0)$, since $f_{B_1}^d(E)$ is independent of energy. The validity of the above statement has never been rigorously demonstrated except in potential scattering, but much experimental^{1,2} and theoretical³ work in recent years tends to support it rather strongly.

As a result of the above considerations, it is sensible to consider a new analytic function

$$\bar{f}(E) = f(E) - f_{B_1}^d(0). \quad (3)$$

As stated above, $\bar{f}(E) \rightarrow 0$ as $E \rightarrow \infty$, so we may write

$$\begin{aligned} 2\pi i \bar{f}(E) &= \oint_C \frac{\bar{f}(E')}{E' - E} dE' \\ &= \int_{C_\infty} \frac{\bar{f}(E')}{E' - E} dE' + \int_{C_+} \frac{\bar{f}(E')}{E' - E} dE' \\ &\quad + \int_{C_-} \frac{\bar{f}(E')}{E' - E} dE'. \end{aligned} \quad (4)$$

The integral along C_∞ vanishes since $\bar{f}(E') \rightarrow 0$ as $E' \rightarrow \infty$. The other two integrals along the upper and lower edges of the cut may be combined in the usual way to give

$$2\pi i \bar{f}(E) = \int_0^\infty \frac{\bar{f}(E' + i\epsilon) - \bar{f}(E' - i\epsilon)}{E' - E} dE', \quad (5)$$

where the integral is now along the real axis. Since $f_{B_1}^d(0)$ is just a constant, this may also be written as

$$f(E) = f_{B_1}^d(0) + \frac{1}{2\pi i} \int_0^\infty \frac{f(E' + i\epsilon) - f(E' - i\epsilon)}{E' - E} dE'. \quad (6)$$

But the discontinuity across the cut is just $2i \times \text{Im}f(E')$, so we have finally

$$f(E) = f_{B_1}^d(0) + \frac{1}{\pi} \int_0^\infty \frac{\text{Im}f(E')}{E' - E} dE'. \quad (7)$$

The point E can now be brought down onto the pos-

itive real axis in the familiar manner, giving

$$\text{Re}f(E) = f_{B_1}^d(0) + \frac{1}{\pi} \text{P} \int_0^\infty \frac{\text{Im}f(E')}{E' - E} dE'. \quad (8)$$

We now make an observation of considerable practical importance. One might think that in Eq. (3) there are a great many functions which we could subtract besides $f_{B_1}^d(0)$. We would seem to need only a function which tends to $f_{B_1}^d(0)$ as E tends to infinity. However, this function must also be analytic everywhere in the cut E plane if Eq. (4) is to hold. In the past, many authors⁴⁻⁹ have subtracted the function $f_{B_1}^d(E) - g_{B_1}(E) \equiv f_{B_1}^d(0) - g_{B_1}(E)$. However, although $g_{B_1}(E) \rightarrow 0$ as $E \rightarrow \infty$, as is well known, g_{B_1} is not analytic throughout the cut E plane. Indeed for the case of electron scattering by atomic hydrogen, one can evaluate $g_{B_1}(E)$ exactly; it is found to have a pole of order three at $E = -0.5$ a.u. Thus, $f_{B_1}^d(0) - g_{B_1}(E)$ is not an appropriate subtraction function. We may remark that, given the singularity of $g_{B_1}(E)$, it is clear that if the Born series for the exchange amplitude converges the convergence will have to be very special if $g(E)$ is to have the desired analyticity properties discussed above. In particular, higher-order terms in the series must cancel the singularities occurring in lowest order. We note that in potential scattering the analyticity properties of the full amplitude hold in each order of perturbation theory.

Let us now turn to the question of whether or not the dispersion relation of Eq. (8) is satisfied in practice. We first focus our attention on the zero energy case, where $\text{Re}f(0) = -A$, with A the scattering length. Since by unitarity

$$\text{Im}f(E) = (2E)^{1/2} \sigma_{\text{tot}}(E)/4\pi, \quad (9)$$

where σ_{tot} is the total (complete) scattering cross section, we may write Eq. (8) as

$$-A = f_{B_1}^d(0) + (2\pi)^{-2} \int_0^\infty \sigma_{\text{tot}}(k) dk, \quad (10)$$

where we have made the change of variables $E' = k^2/2$. In the case of electron scattering by noble gases, this equation can easily be checked. For helium¹⁰ and neon,¹¹ A is known to be positive. Also, $f_{B_1}^d(0)$ is positive for any electron-atom scattering system. Since σ_{tot} is by definition positive, the right-hand side of Eq. (10) is always positive, while for the electron-helium and electron-neon systems the left-hand side ($-A$) is negative. Thus, Eq. (10) fails for these cases, and presumably also for all other electron-atom systems.

According to our above analysis, the reason

for this failure can *only* be in the assumption that $f(E) \equiv f^d(E) - g(E)$ is analytic throughout the cut E plane. Thus, either $f^d(E)$ or $g(E)$ or both must fail to be analytic in the cut plane. Given the similarity between $f^d(E)$ and the potential-scattering amplitude, it is tempting to look in the direction of $g(E)$ for the difficulties. The nonanalyticity of $g_{B1}(E)$ lends some support to this possibility, but it is clearly not overwhelming.

If $f^d(E)$ does have the desired analyticity properties, one would expect to find Eq. (10) satisfied for positron-atom scattering where $g(E) \equiv 0$.

Bransden and Hutt,⁹ using data from recent experiments, conclude that Eq. (10) is satisfied for positron-helium scattering to an accuracy of better than 10%. Given that positron-helium experiments are still in their infancy, this is a reasonable level of agreement, although of course much more work needs to be done.

In recent years, much effort has been expended in an attempt to verify that dispersion relations are valid in atomic physics.⁶⁻⁹ All such attempts use a subtraction function of the form $f_{B1}^d(0) - g_{B1}(E)$, thereby obtaining the dispersion relation

$$\text{Re}f(E) = f_{B1}^d(0) - g_{B1}(E) + \frac{1}{\pi} P \int_0^\infty \frac{\text{Im}f(E')}{E' - E} dE' \quad (11)$$

instead of Eq. (8). At zero energy this becomes, by analogy with Eq. (10),

$$-A = f_{B1}^d(0) - g_{B1}(0) + (2\pi^2)^{-1} \int_0^\infty \sigma_{\text{tot}}(k) dk. \quad (12)$$

At the present time the best available experimental and theoretical results for electron-helium scattering indicate that Eq. (12) is not satisfied, as pointed out elsewhere by one of us.¹² The value of the left-hand side is given from experimental work by $-A = -1.15$ with a maximum error¹³ of about ± 0.04 . Using the well-known result¹⁴ $f_{B1}^d(0) = 0.79$ and the recent value¹⁵ $g_{B1}(0) = 3.92 \pm 0.05$, one need only calculate the integral over σ_{tot} in order to complete the evaluation of the right-hand side of Eq. (12). Making use of theoretical values¹⁶ between 0 and 17 eV, empirical cross sections¹⁷ up to 3000 eV, and Born cross sections above, one finds¹² the value 2.57 ± 0.16 for the third term on the right-hand side of Eq. (12). On the other hand, if the total cross sections of Andrick and Bitsch¹⁸ are used below 20 eV, then this term has the value 2.66 ± 0.16 . Combining these results with the values for $f_{B1}^d(0)$

and $g_{B1}(0)$ quoted above, we obtain for the right-hand side of Eq. (12) the result -0.56 ± 0.17 (by using low-energy theoretical values¹⁶) or -0.47 ± 0.17 (by using the values of Andrick and Bitsch¹⁸) in clear disagreement with the left-hand side which has the value -1.15 ± 0.04 .

The disagreement found between the two sides of Eq. (12) is obviously by no means as large as that found between the two sides of Eq. (10), but nevertheless it appears to be conclusive. Apart from pure coincidence, the most likely explanation would appear to be that the bulk of the non-analytic part of $f(E)$ is contained in $g_{B1}(E)$, so that in subtracting $f_{B1}^d(0) - g_{B1}(E)$ one obtains a modified amplitude which is "nearly" analytic.¹⁹

Finally, we consider briefly the intermediate- and high-energy regime of the dispersion relations of Eqs. (8) and (11). Here recent theoretical work³ agrees fairly well with calculations⁹ based on either of these equations. However, the effect of exchange on $\text{Re}f$ in the intermediate- and high-energy region is rather small, so the agreement that is found is *primarily* a test of dispersion relations for the direct amplitude, and within the direct amplitude one is in fact looking predominantly at the second Born term.

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Feshbach and Shape Resonances in the $e\text{-H } ^1P$ System

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Using a Born-Oppenheimer-type expansion for the two-electron wave functions in hyperspherical coordinates, three potential curves are obtained for H^- 1P states converging to the $n=2$ state of the hydrogen atom. It is shown that the Feshbach resonances are associated with one curve and the shape resonance with another. The connections with the "+" and "-" classification of helium doubly excited states and with the asymptotic dipole-field representation of H^- are discussed.

Various elaborate methods have been employed to obtain accurate positions and decay widths of resonances in electron-hydrogen-atom collisions.¹ The most careful and thorough study of this system is the close-coupling calculations by Burke and co-workers.² Besides the numerous Feshbach resonances below the $n=2$ threshold of H, they predicted the existence of a narrow shape resonance of 1P symmetry, with energy only 18 meV above the $n=2$ threshold. This shape resonance greatly influences the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation cross sections in electron-hydrogen scattering² and also the photodetachment cross section of H^- near the $n=2$ threshold.³

As is well known, a shape resonance can be produced from potential scattering if the potential possesses a barrier at large distances R from the force center and is attractive enough at small R . In electron-hydrogen scattering, the existence of potential barriers at large R in certain channels has been known for many years.⁴ Because of the complicated interactions at small R , however, it has not been possible to get an estimate of the strengths of the potential wells, if any, at small R , so as to connect the two regions. In this note, we will show that, by using hyperspherical coordinates, it is possible to approximate the electron-hydrogen scattering by one-di-

mensional (1D) potential scattering. In particular, for 1P states, three potential curves associated with the $n=2$ state of H are obtained, one being completely repulsive at all R , one having the property that it can produce a shape resonance, and one having the ability to support an infinite number of Feshbach resonances.

In a recent paper⁵ (to be called I), I have used hyperspherical coordinates to study the properties of doubly excited states of helium. In this coordinate system, the distances of the two electrons from the nucleus r_1 and r_2 are replaced by a hyperradius $R = (r_1^2 + r_2^2)^{1/2}$ and a hyperangle $\alpha = \arctan(r_2/r_1)$. The angle α , together with the usual polar coordinates (θ_1, φ_1) and (θ_2, φ_2) of the two electrons represented collectively as $\Omega \equiv \{\alpha, \theta_1, \varphi_1, \theta_2, \varphi_2\}$, identify the orientation of the electron pair on a 5D spherical surface, whereas the coordinate R measures the size of the system. An interchange of the positions of electrons 1 and 2 amounts to changing α into $\frac{1}{2}\pi - \alpha$ and interchanging (θ_1, φ_1) and (θ_2, φ_2) , with R fixed.

Using atomic units and expanding the two-electron wave function $\psi(R, \Omega)$ as

$$\psi = R^{-5/2} \sum_{\mu} F_{\mu}(R) \Phi_{\mu}(R; \Omega), \quad (1)$$

where R is treated as a parameter in $\Phi_{\mu}(R; \Omega)$, we can reduce the Schrödinger equation for the