

Low-energy electron-atom scattering in a magnetic field

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The threshold laws for electron-atom scattering processes in a magnetic field are shown not to contain singularities in general. Observed modulations of photodetachment cross sections are due to the presence of true resonances rather than divergence of phase space. These resonances may be associated with thresholds, or they may be analogous to the quasi-Landau resonances observed in photoionization.

I. INTRODUCTION

Theoretical work on low-energy electron-atom scattering in magnetic fields has been motivated by the anticipation of its importance in some problems of plasma physics and astrophysics,¹⁻⁶ and by the need to interpret existing experimental data.^{7,8} It has been asserted⁵⁻⁸ that various cross sections exhibit singular behavior, being proportional to the inverse of the escape velocity near excitation thresholds. I shall argue here that this singular behavior does not generally occur. In addition, I shall express an alternative view of the results of experiments on photodetachment of negative ions in a magnetic field. It differs quite considerably from the theory proposed⁸ by the original investigators, and is more akin to the prevailing interpretations^{9,10} of experiments^{11,12} on photoabsorption by neutral atoms in magnetic fields. Several distinct mechanisms may indeed be responsible for the observed modulations of photodetachment cross sections. Since their separate influences cannot easily be discerned in the currently available data, further experimental and theoretical work may be thought worthwhile.

II. FREE ELECTRON IN A MAGNETIC FIELD

This paper will primarily treat problems which can be described in terms of the scattering of an electron by an electrically neutral target atom, in the presence of a magnetic field. (Cases when the target atom has a net charge are of sufficient interest and importance to warrant a separate treatment.) In such cases, the electron-atom collision occurs in a limited interval of time, after which the electron and atom move without mutual interaction in the magnetic field. It is therefore appropriate to recall the properties of the motion of a free (nonrelativistic) electron in a magnetic field; these are well known and have been expounded with considerable elegance elsewhere.¹³

In atomic units, the Hamiltonian for an electron in a magnetic field \vec{B} is

$$H = \frac{1}{2}(\vec{p} + c^{-1}\vec{A})^2, \quad (1)$$

where the vector potential \vec{A} satisfies $\vec{\nabla} \times \vec{A} = \vec{B}$. For the present purpose it is most convenient to choose $\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B}$, so that Eq. (1) becomes

$$H = \frac{1}{2}\vec{p}^2 + (\omega/2)l_z + \frac{1}{2}(\omega/2)^2\rho^2, \quad (2)$$

where $\vec{B} = B\hat{z}$ defines the z axis of a conventional cylindrical polar-coordinate system ρ, ϕ, z ; ω is the cyclotron frequency ($\omega = eB/mc$ in Gaussian units, in atomic units $\omega = 4.25 \times 10^{-7} B/\text{kG}$); and l_z is the z component of the angular momentum of the electron. This choice of gauge is motivated by the fact that the most detailed experimental data on these processes have been obtained by producing the free electron by photoejection from an atom; in such cases only a few values of l_z are relevant because of optical selection rules.

The eigenfunctions ψ of the Hamiltonian in Eq. (2) may be chosen to have definite values of $l_z = m$, in which case they are separable in cylindrical polar coordinates

$$\psi_{nm}(\epsilon, \vec{r}) = f(\epsilon, z)\chi_{nm}(\rho, \phi), \quad (3)$$

$$H\psi_{nm}(\epsilon, \vec{r}) = \{\epsilon + \omega[n + \frac{1}{2} + (m + |m|)/2]\}\psi_{nm}.$$

The "Landau orbitals" χ_{nm} are defined in Eq. (A8) of the Appendix, and $f(\epsilon, z)$ is a solution of

$$\left[\frac{d^2}{dz^2} + 2\epsilon \right] f(\epsilon, z) = 0. \quad (4)$$

The Landau orbitals χ_{nm} are just wave functions of a two-dimensional harmonic oscillator ($n \geq 0$ is the radial quantum number); and the $f(\epsilon, z)$ describe free motion along the z direction, with kinetic energy ϵ . The correspondence with classical electrodynamics is fairly obvious: a charged particle moves with constant velocity along the magnetic field, and executes simple harmonic motion (a circular orbit) in the plane perpendicular to the field.

Equation (4) does not completely specify $f(\epsilon, z)$. Since the Hamiltonian of Eq. (2) is invariant under reflection in the plane $z=0$, one may require f to be either even or odd in z :

$$f^+(\epsilon, z) = (\pi k)^{-1/2} \cos(kz), \quad (5a)$$

$$f^-(\epsilon, z) = (\pi k)^{-1/2} \sin(kz), \quad (5b)$$

where $k = (2\epsilon)^{1/2}$. This choice of continuum functions again anticipates the imposition of optical selection rules. The polarization of an absorbed photon will dictate the inversion symmetry of the final-state wave function of the electron. The coefficient $(\pi k)^{-1/2}$ ensures¹⁴ that the f 's

are normalized on the energy scale, e.g.,

$$\int_{-\infty}^{\infty} dz [f^+(\epsilon, z)]^* f^+(\epsilon', z) = \delta(\epsilon - \epsilon'). \quad (6)$$

This normalization of the continuum incorporates the density of states per unit energy $\rho(\epsilon)$ into the amplitude of the wave function, and so eliminates the need to include $\rho(\epsilon)$ explicitly in expressions for transition probabilities. An alternative continuum normalization, which has been frequently used in this problem,⁵⁻⁸ is obtained by confining the z motion of the electron to the range $-L/2 \leq z \leq L/2$. The wave function is then normalized to unit probability in this interval, e.g.,

$$f_L^+(\epsilon, z) = (2/L)^{1/2} \cos(kz), \quad (7)$$

and the density of states is

$$\rho_L(\epsilon) = L / (2\pi k). \quad (8)$$

The spin of the electron has not been written explicitly in this section. In a uniform magnetic field the electron-spin projection s_z is a constant of the motion, so that the existence of spin can be indicated simply by a uniform shift of all the energies in Eq. (3) by the amount gBs_z .

III. EFFECTS OF INTERACTION

Equations (3)–(5) provide the basis for describing the effects of interaction between the electron and a target atom, on subsequent motion of the electron in the magnetic field. When electron and atom are sufficiently far apart, their joint wave function χ can be expressed as a sum of products of electron and target wave functions. The word “channel” denotes a specific state of the target and values of n, m, s_z of the electron; these are discrete quantum numbers, associated with quantities which are susceptible to measurement at infinite electron-atom separation. The motion of the electron along the z direction, on the other hand, is characterized by the continuous energy ϵ . In the complete absence of interactions the channel index i would be a constant of the motion. For systems treated in this paper it is assumed that the mixing of channels, though it may be arbitrarily strong, is due to electron-atom interactions of finite range.

The practical consequences of this assumption are developed in the Appendix, by an R -matrix description of the equations of motion. With the atom sited at $z=0$ and localized in the region $-z_0 \leq z \leq z_0$, the total wave function in the region $|z| \geq z_0$ is expanded in all channels i ,

$$\chi = \sum_i X_i \chi_{n_i m_i}(\rho, \phi) f_i(\epsilon_i, z), \quad (9)$$

where the X_i denote products of target states and the spin states of the scattering electron, as in Eqs. (A7) and (A11) of the Appendix. Each f_i is a solution to an equation identical to that of Eq. (4) in the region $|z| > z_0$, with $\epsilon \equiv \epsilon_i$ determined by energy conservation [e.g., Eq. (A16)]. Closed channels are those for which $\epsilon = -\frac{1}{2}\kappa^2 < 0$; at large $|z|$ the closed-channel components of Eq. (9) must vanish as $f_i \sim e^{-\kappa_i z}$.

All effects of the electron-target interaction can then be expressed in terms of a set of boundary conditions at $z = z_0$ for the open-channel ($\epsilon_i > 0$) wave functions f_i only. These take the form

$$f_i(\epsilon_i, z) \Big|_{z=z_0} = \sum_j R_{ij}(E) \frac{\partial}{\partial z} f_j(\epsilon_j, z) \Big|_{z=z_0}, \quad (10)$$

the sum being over open channels only, as in Eq. (A20). The derivation of Eq. (10), including an explicit expression for the matrix R_{ij} , is given in the Appendix. Since Eq. (10) is quite general, there is little that can be said *a priori* about the behavior of the R matrix in any particular case; it should be remarked, however, that R depends principally upon the wave function of the electron-atom system in the region $|z| < z_0$.

Within each channel one has the possibility of states which are either even or odd under the inversion $z \rightarrow -z$. Imposition of parity conservation on the system will select one class of these which needs to be considered. Equation (10) is therefore to be supplemented by the condition $f_i(-z) = \pm f_i(z)$, the sign as appropriate. The R -matrix elements for even and odd states will in general differ; however, the effect of the boundary condition (10) on even- and odd-channel wave functions is qualitatively the same, since both are sinusoidal functions. For free motion in three dimensions, on the other hand, parity is correlated with orbital angular momentum: Channels with different inversion symmetry are subject to centrifugal potentials of unequal magnitude, and their behaviors at small distance or low energy will differ.

The contrast between one- and three-dimensional scattering is seen clearly when only a single channel is open. Its even- and odd-parity wave functions $f^\pm(z)$ can then be written in symmetric form

$$f^\pm(\epsilon, z) = \begin{cases} (\pi k)^{-1/2} \sin(kz + \delta_\pm), & z > z_0 \\ (\pi k)^{-1/2} \sin(\mp kz \pm \delta_\pm), & z < -z_0 \end{cases} \quad (11a)$$

$$(11b)$$

The phase shifts δ_\pm are then determined by application of the condition (10) to Eq. (11a) alone,

$$\tan(kz_0 + \delta_\pm) = kR_\pm(E), \quad (12)$$

where R_\pm are the R -matrix elements for even and odd states in the open channel. Equation (12) implies that as $k \rightarrow 0$,

$$\delta_\pm \rightarrow k[R_\pm(E_0) - z_0] = -ka_\pm \quad (13)$$

with $E_0 = E(k=0)$, and a_\pm are scattering lengths defined by this equation. In particular, if a_+ is finite (i.e., the even-parity wave function does not have an antinode at $z = z_0$), then at low energy the even-parity function of Eq. (11a) is shifted in phase by $\pi/2$ from the free solution of Eq. (5a). Such behavior does not occur for motion in more than one dimension, and is related to the ability of any attractive one-dimensional potential to hold a bound state.¹⁵ Therefore, in the absence of zero-energy resonances ($a < \infty$), the low-energy behavior of energy normalized wave function is

$$f(\epsilon, z) \rightarrow (k/\pi)^{1/2} (z - a) \quad (14)$$

for $z > z_0$, irrespective of parity. Resonances at zero energy can in fact occur, as a result of some particular feature of the electron-atom interaction, just as they can occur in field-free electron-atom scattering. However, they should be expected to appear in exceptional circumstances, rather

than as a matter of course. The threshold law for any scattering process in a magnetic field should therefore be formulated in terms of the usual low-energy behavior of final-state wave functions.

IV. PHOTODETACHMENT IN A MAGNETIC FIELD

Blumberg *et al.*⁸ have explained the results of their impressive photodetachment experiments using a channel description similar to that employed here. They have examined photodetachment of the sulfur negative ion S^- held in an ion trap in magnetic fields of the order of 10 kG. This process is appropriately treated by application of the Fermi golden rule to an electric dipole transition. The initial state $|i\rangle$ is one of the Zeeman levels (i.e., definite M_j) of the $3p^{5/2}P_{3/2}$ state of S^- . The final state $|f\rangle$ consists of an electron escaping from a neutral S atom, which experimental procedure requires to be in one of the Zeeman levels of the $3p^{4/3}P_2$ state; therefore, the asymptotic form of $|f\rangle$ is given by Eq. (9) with each X_i being a product of one of the Zeeman levels of S $3p^{4/3}P_2$ with the outgoing spin state of the electron. The rate of photodetachment Γ_{if} is then proportional to the square of the electric dipole matrix element $\langle i | \vec{r} | f \rangle$.

To evaluate this matrix element Blumberg *et al.* take the asymptotic form [Eq. (9)] of $|f\rangle$ to be valid at all z , so that the rate of transition to a final state with Landau quantum numbers n, m is

$$\Gamma_{if} \sim |\langle i | \vec{r} | f \rangle|^2 = W \left| \int d\vec{r} \psi_{3p}^*(\vec{r}) r f(\epsilon, z) \chi_{nm}(p, \phi) \right|^2, \quad (15)$$

where W is a product of core overlap and angular momentum recoupling factors. The only energy dependence in Eq. (15) enters via the function $f(\epsilon, z)$. Selection rules imply that f is even in z . Blumberg *et al.* take f from Eq. (5a), which is the appropriately normalized even function for a free electron in a magnetic field. With this choice, $f \sim k^{-1/2}$ in the limit $\epsilon \rightarrow 0$; therefore, the photodetachment cross section appears to have singular behavior $\Gamma_{if} \sim k^{-1}$, at each Landau threshold. Blumberg *et al.* attribute the observed modulations of the photodetachment cross section to the existence of such singularities. Singularities are not directly observed, of course. The experimental data show a cross section which is averaged over the (unknown) velocity and state distribution of the S^- ions in the trap, as a result of which the singularities would be "washed out." The observed data can be fit quite well by adjusting the population-distribution parameters in the theoretical expressions derived from the arguments summarized in this paragraph.

However, the arguments of Sec. III indicate that there are generally no singularities in the photodetachment cross section. This is obvious in the case where only one channel is open. Examination of Eqs. (11)–(14) shows that in the neighborhood of the atom the appropriately normalized continuum function becomes proportional to $k^{1/2}$, rather than $k^{-1/2}$, near threshold. The true threshold law is therefore

$$\Gamma_{if} \sim k \quad (k \rightarrow 0). \quad (16)$$

When more than one channel is open, e.g., when the photon energy is sufficient to permit the escaping electron

to occupy a number of Landau levels, the same behavior is obtained. The multichannel case requires somewhat more careful formulation of the final-state wave function. If, for instance, one is interested in the yield of electrons in a particular Landau orbital n_i, m_i escaping along the $+z$ axis, then the final state must correspond to incoming waves in all channels and an outgoing wave in channel i in the $+z$ direction only. These partial cross sections must be summed to obtain the net photodetachment rate. It turns out that, subject to the qualification expressed by Eq. (18) below, the total cross section is continuous as the energy increases across the i th Landau threshold, and the cross section for escape in the i th Landau orbital starts off proportional to k_i . This can be seen in an eigenchannel formulation of the problem. If i channels are open, one can find i solutions of each parity for which the channel functions f_i take the form

$$f_j^{\alpha\pm}(\epsilon, z) = \begin{cases} A_{\alpha j}^{\pm} k_j^{-1/2} \sin(k_j z + \delta_{\alpha}^{\pm}), & z > z_0 \\ A_{\alpha j}^{\pm} k_j^{-1/2} \sin(\mp k_j z + \delta_{\alpha}^{\pm}), & z < -z_0 \end{cases} \quad (17)$$

The $\delta_{\alpha}^{\pm}, A_{\alpha j}^{\pm}$ ($\alpha = 1, \dots, i$) are, respectively, the eigenphase shifts and eigenchannel vectors; they are determined by substituting Eq. (17) in Eq. (10). As each new channel opens a new eigenphase appears. If at the energy of the i th threshold the determinant

$$|\delta_r \sin(k_s z_0) - k_r^{1/2} R_r k_s^{1/2} \cos(k_s z_0)| \neq 0 \quad (18)$$

($r, s = 1, \dots, i-1$), then the i th eigenphase $\delta_i \sim k_i$ near threshold, and with $A_{ii} = 1$ the lower channel eigenvector components $A_{ij} \sim k_i^{1/2}$, $j = 1, \dots, i-1$. Similarly $A_{\alpha i} \sim k_i^{1/2}$ for $\alpha < i$. Therefore the wave function in the i th channel behaves as in Eq. (14), and the threshold law for each partial cross section is the same as for the one-channel case, Eq. (16). Exceptions are permitted when Eq. (18) is not satisfied, but this is a condition for a threshold resonance analogous to the existence of an antinode at z_0 in the one-channel case.

It is therefore apparent that the formulation of Blumberg *et al.* does not provide a correct threshold law, since their description is valid only in the special (and hypothetical) case of vanishing electron-target interaction. It must be noted, however, that their treatment does on the whole provide a satisfactory fit to the experimental data. This may be due in part to the use of adjustable parameters, such as initial-state population and ion temperature; but any theoretical analysis of those experiments must employ such parameters, and there is no indication that the adjusted values used by Blumberg *et al.* are greatly at variance with those which might be obtained by independent measurement. In addition, Blumberg *et al.* present an argument showing that their k^{-1} threshold law reduces to the familiar Wigner threshold law (for an s wave in this case, $\Gamma \sim k$) in the limit of zero magnetic field.

This latter point will be addressed first, since its resolution will help set the stage for more detailed considerations. As a simplified model problem, suppose the electron-atom interaction to be represented by a simple spherical-box potential $V(r) = -V_0$ for r less than some r_0 . The wave function can then be expanded in the form of Eq. (9) throughout all space (the θ_i being simply Landau orbitals), and the equations of motion then take the form of Eq. (A15) of the Appendix

$$\left\{ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + V_{ii}(z) - \epsilon_i \right\} f_i = \sum_j V_{ij}(z) f_j(z) \quad (19)$$

with

$$V_{ij}(z) = \delta_{m_i m_j} \int_0^\infty d\rho \rho V((\rho^2 + z^2)^{1/2}) \times \chi_{n_i m_i}(\rho) \chi_{n_j m_j}(\rho), \quad (20)$$

where $\chi_{nm}(\rho)$ is the normalized radial part of Eq. (A8). The effective upper limit of radial integration in Eq. (20) is $\rho = (r_0^2 - z^2)^{1/2}$; $V_{ij}(z) = 0$ for $z > r_0$. The root-mean-square radius $\bar{\rho}$ of an electron in a Landau orbital nm is $\bar{\rho} = [2(2n + |m| + 1)/\omega]^{1/2}$ in atomic units. Since $\omega \sim B$, $\bar{\rho}$ will become arbitrarily large as $B \rightarrow 0$. Therefore, the χ_{nm} in Eq. (20) may be replaced by their values at $\rho = 0$; for $m = 0$ it is seen from Eqs. (A8) and (A9) that $\chi_{n0}(\rho = 0) = \omega^{1/2}$. Thus, for $m = 0$,

$$V_{ij}(z) = -V_0 \omega (r_0^2 - z^2)/2, \quad |z| < r_0 \quad (21)$$

in the limit $\omega \rightarrow 0$. The effective potentials of Eq. (19) become arbitrarily small as the field vanishes. Recall that in one dimension, any attractive potential holds a bound state; as the potential goes to zero, so does the energy of the bound state. If channel coupling is ignored for the moment, it is seen that there is a bound state attached to each Landau threshold; in the zero-field limit it becomes a zero-energy resonance. Therefore, in the zero-field limit the threshold law becomes k^{-1} [it is more accurate to say that the range of validity of Eq. (16) goes to zero, and the cross section becomes dominated by threshold resonances]; Blumberg *et al.* then show⁸ that the simultaneous coalescence of thresholds leads to reproduction of the Wigner law in zero field.

Accessible laboratory fields yield values for ω in the 10^{-5} -a.u. range: For a typical field strength employed in the photodetachment experiments, 10.7 kG, $\omega = 4.56 \times 10^{-6}$. With reasonable guesses for the strength and radius of an effective electron-sulfur potential $V(\vec{r})$, this could lead to resonances very near their associated thresholds. Such states would have very diffuse wave functions, of mean radius $\bar{\rho}$ in the plane perpendicular to the field but with much greater extent along the field direction. Note, however, that the interaction $V_{ij}(z)$ between channels given by Eq. (21) is just as strong as the "central" potential $V_{ii}(z)$; and both are comparable to the energy spacing ω between successive Landau thresholds. A resonant state of this type will be degenerate in energy with free states in channels associated with lower Landau levels. Therefore, it is not clear what role such states will play in the photodetachment spectrum.

In experiments on atomic photoabsorption in a magnetic field as well, substantial modulations of the cross section are observed^{11,12} above the ionization limit. These are attributed^{9,10} to an entirely different type of resonant state than that which has just been described. In photoabsorption the ejected electron experiences a long-range Coulomb attraction. In the naive view this would result in a Rydberg series converging to each Landau threshold, with the total photoabsorption cross section being continuous across the threshold, and partial cross sections starting from finite values at their respective thresholds. The most prominent features in the spectrum are, however, not asso-

ciated with the Landau thresholds at all; the modulations are spaced in energy by an amount which decreases from $3\omega/2$ at the ionization threshold to ω at high energy.

The explanation of this phenomenon which has come to be accepted is that these modulations are associated with "quasi-Landau" resonances, which are states in which the electron remains fairly localized in the plane $z = 0$ which contains the residual ion. At large electron-ion distances the motion of the electron is governed by the combined Coulomb potential and diamagnetic potential of Eq. (2)

$$V(\vec{r}) = -1/r + \frac{1}{8} \omega^2 r^2 \sin^2 \theta. \quad (22)$$

The direction $z = 0$ ($\theta = \pi/2$) corresponds to the most repulsive part of the potential surface (22) at fixed r . The quasi-Landau resonances are therefore described as states which are confined to the ridge of this potential surface. Details of the mechanism responsible for this confinement are by no means entirely understood, although evidence that it may be of fundamental importance has been accumulating.¹⁶

The quasi-Landau resonances decay by, so to speak, falling off the ridge; the electron escapes along the direction $\theta = 0$, into those Landau orbits which its energy may allow. There has been no determination of the branching ratios for decay of a quasi-Landau resonance into alternative Landau final states. For typical laboratory fields, however, the wave function of the first quasi-Landau level above the ionization limit has ~ 40 radial nodes in the plane $z = 0$. The lowest Landau orbital at $z = \infty$, on the other hand, has no radial nodes. One cannot therefore expect a unique correspondence to exist between a quasi-Landau resonance and a dissociation limit of the system. The quasi-Landau levels are formed as a result of competition between two forces—Coulomb and magnetic—of comparable strengths but incompatible symmetries; they have little relationship to states which are governed by one of those forces alone.

It seems reasonable to inquire whether resonances of the quasi-Landau type exist in the case of photodetachment. The distinction between quasi-Landau states and the threshold resonances described previously is similar to that between Feshbach and compound nucleus resonances. A threshold resonance is loosely "attached" to a particular Landau level; a quasi-Landau state is instead a transient mixture of a large number of Landau orbitals. A mechanism for the formation of this latter type of state is suggested by Eq. (21), in which interchannel coupling is independent of channel number. I am unable to state firmly whether quasi-Landau resonances will show prominently in photodetachment spectra, but some preliminary investigation of their expected characteristics is not too difficult.

The quasi-Landau resonances in photoionization are localized in a region where the Coulomb and magnetic interactions are of comparable strength. In photodetachment the long-range Coulomb interaction is not present; higher electric multipole potentials constitute the dominant electron-atom interaction at large separation r . The electron-atom interaction at small r is, for laboratory fields, much stronger than the magnetic interaction; but over the energy range of interest (say, 100 cyclotron frequency units) it can be adequately represented by a scattering length. It will be shown that if these combined finite-

range forces result in quasi-Landau resonances of the same type that occur in photoionization, the energy e_n of the n th such resonance (for given m) is

$$e_n = \omega \left[n - \mu + \frac{|m| + m + 1}{2} \right], \quad (23)$$

where μ varies slowly with n . An estimate will then be given of the value of μ for the case of S^- in a magnetic field of 10.7 kG.

For $\mu=0$, Eq. (23) reduces to the energies of the Landau orbitals, as in Eq. (3). It is reminiscent of the formula which gives the energies of atomic Rydberg states by replacement in the hydrogenic formula of the integer principal quantum number n by $n^* = n - \mu$, where μ is the quantum defect. It is perhaps easiest to justify Eq. (23) by development of this formal correspondence. If, as in photoionization, we treat the quasi-Landau levels as confined to the plane $z=0$, then their wave functions ξ_n satisfy the two-dimensional Schrödinger equation

$$\left[-\frac{1}{2} \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{m^2}{\rho^2} \right) + \frac{1}{2} \omega^2 \rho^2 + V(\rho) \right] \xi_n = \left[e_n - \frac{m}{2} \omega \right] \xi_n, \quad (24)$$

where $V(\rho)$ is the finite-range electron-atom interaction. Over a limited energy range the effect of $V(\rho)$ can be represented by requiring that

$$\left. \frac{\rho}{\xi_n} \frac{\partial}{\partial \rho} \xi_n \right|_{\rho=\rho_0} = b \quad (25)$$

and solving Eq. (24) with $V(\rho)=0$ in the region $\rho \geq \rho_0$, subject to Eq. (25). Setting $V=0$ and $y = \omega \rho^2$, Eq. (24) becomes

$$\left[-\frac{1}{2} \left(\frac{1}{y} \frac{\partial}{\partial y} y \frac{\partial}{\partial y} - \frac{(m/2)^2}{y^2} \right) - \frac{\xi}{y} + \frac{1}{8} \right] \xi_n = 0, \quad (26)$$

where $\xi = e_n/2\omega - m/4$, and Eq. (25) becomes

$$\left. \frac{y}{\xi_n} \frac{\partial}{\partial y} \xi_n \right|_{y=\omega \rho_0^2} = b/2. \quad (27)$$

For even m , Eq. (26) is recognizable as the Schrödinger equation for a two-dimensional hydrogen atom with nuclear charge ξ and energy $E = -\frac{1}{8}$, subject to the short-range boundary condition (27). Without this condition E would be one of the energies of the two-dimensional hydrogen spectrum

$$E = -\frac{1}{2} \frac{\xi^2}{\left[n + \frac{|m| + 1}{2} \right]^2}, \quad (28)$$

where n is an integer, the radial quantum number. The effect of the condition (27) on the hydrogenic spectrum is to cause n to be replaced by $n^* = n - \mu$. Therefore,

$$-\frac{1}{8} = -\frac{1}{2} \frac{\xi^2}{\left[n^* + \frac{|m| + 1}{2} \right]^2}, \quad (29)$$

so that

$$e_n = \omega \left[2\xi + \frac{m}{2} \right] = \omega \left[n^* + \frac{|m| + m + 1}{2} \right]. \quad (30)$$

In this model, then, the quasi-Landau spectrum is displaced from the Landau thresholds by a constant energy $\omega\mu$. I have attempted to estimate the magnitude of μ for the $m=0$ states of S^- in a 10.7 kG field by the following means. I employ Eq. (24) with $V(\rho) = -\alpha/2\rho^4$ for $\rho > 10a_0$, where α is the dipole polarizability of neutral sulfur, taken to be 10.42 a.u.¹⁷ Since $\omega = 4.56 \times 10^{-6}$ for this field strength, the polarization and magnetic potentials become equal in magnitude at $\rho \sim 125a_0$, and the cyclotron radius $\bar{\rho} = (2/\omega)^{1/2} = 660a_0$. The electron-sulfur interaction in the region $\rho < 10a_0$ is represented by Eq. (25) with $b=0.91$. This value for b was obtained by using the doublet scattering length given by Rau and Fano¹⁸ to determine the slope of the field-free zero-energy wave function at infinity, and then propagating the logarithmic derivative $\xi^{-1} \partial \xi / \partial \rho$ inwards to $\rho=10$ by using the known solutions for a wave function of zero energy in a polarization potential. The resulting equations equivalent to (24) and (25) were then integrated numerically, and the effective oscillator quantum numbers were found to be (for the first four states with $m=0$)

n	n^*
0	0.093
1	1.101
2	2.106
3	3.109

The "quantum defect" μ is thus of the order -0.1 and varies slowly with n as expected.

This elementary calculation is intended to illustrate the order of magnitude of the quasi-Landau shift rather than to provide a firm prediction of its value. The electric quadrupole interaction and the presence of nondegenerate m sublevels of the residual sulfur atom, have not been accounted for. There are no physical grounds for restricting the range of values of μ ; and since the electron-sulfur interaction does not appear to be exceptional in any way, it may be expected that, in general, the quasi-Landau shift will amount to an appreciable fraction of the cyclotron frequency. In this sense quasi-Landau states should be experimentally distinguishable from threshold resonances. Since the experiments of Blumberg *et al.* do not determine the absolute values of threshold energies, it is not possible to make this distinction in their data. In addition, the mix of possible initial and final states, which obtains when an open-shell target atom is employed, results in considerable averaging of effects. Experiments on alkali-metal negative ions may be better able to examine this question. Alkali-metal polarizabilities are 10–20 times that of sulfur, so that competition between magnetic and atomic potentials occurs over a greater volume; and the multiplicity of initial and final states is reduced.

V. OTHER SCATTERING PROCESSES

The considerations of Secs. III and IV have implications for scattering processes in which a continuum electron is present in both initial and final states. Because of the one-dimensional nature of the continuum, it is more convenient to formulate such processes in terms of transmission and reflection matrices rather than scattering amplitudes. A process in which a unit flux of electrons in channel i enters the reaction zone from the $-z$ direction, is described by

$$f_j(\epsilon_j, z) = \begin{cases} \delta_{ji} k_j^{-1/2} e^{ik_j z} + R_{ij} k_j^{-1/2} e^{ik_j z}, & z \rightarrow -\infty \\ T_{ij} k_j^{-1/2} e^{ik_j z}, & z \rightarrow +\infty \end{cases} \quad (31)$$

using the notation of Eq. (9). The squared moduli of the R_{ij} and T_{ij} in Eq. (31) give the outgoing flux in the j th channel in backward and forward directions, respectively. Onda and Schmitt *et al.*³ have calculated these matrix elements by direct numerical solution of coupled differential equations of the type (A15); other published work^{2,4,5} which deals with the determination of R and T has, however, relied on Born-type approximations.

If applied to low-energy finite-range potential scattering in three dimensions, the Born approximation yields results which are quantitatively wrong, but in one sense qualitatively correct: it gives the proper energy dependence of phase shifts $\delta_l \sim k^{2l+1}$. In one dimension, however, the Born approximation is qualitatively wrong. This seems to have been pointed out first by Ventura,² in the context of electron-ion scattering in a magnetic field. It is a fact which has perhaps not received adequate attention in later work, so I think it appropriate to emphasize it here.

The contrast between Eq. (5a) and Eqs. (11a) and (13) indicates the degree of error which can be introduced by substitution of the free-particle wave function for the actual wave function at low energy. In the single-channel case, use of Eq. (5a) in a Born approximation yields a T -matrix element which goes to a constant value as $k \rightarrow 0$; this gives a k^{-1} singularity in the cross section.⁵ Equations (11a), (11b), and (13), however, give $T \sim k$ at threshold, in the absence of a resonance. In the multichannel case, eigenchannel analysis gives a similar result. If Eq. (18) holds, then near the threshold of the i th channel

$$\begin{aligned} T_{ji} &= T_{ij} \sim k_i^{1/2} \quad (j < i) \\ R_{ji} &= R_{ij} \sim k_i^{1/2} \quad (j < i) \\ T_{ii} &\sim k_i; \quad R_{ii} \rightarrow -1. \end{aligned} \quad (32)$$

(The equalities $T_{ij} = T_{ji}$ and $R_{ij} = R_{ji}$ hold if the Hamiltonian is invariant under $z \rightarrow -z$; equality of the square moduli holds generally.) For finite-range interactions, then, scattering cross sections do not generally show singularities at Landau thresholds.

When a long-range Coulomb field is present, Eq. (10) provides a suitable boundary condition for the channel functions f_i . In the absence of interchannel coupling in the region $|z| > z_0$, the f_i become solutions to the one-dimensional Coulomb equation in that region. With each

Landau threshold there are then associated two Rydberg series (of even- and odd-parity states), the members of which are broadened by interaction with the continua of lower Landau thresholds. The threshold laws for various scattering processes should be identical to their three-dimensional counterparts, e.g., partial Landau excitation cross sections should start at a finite value at threshold.

However, a detailed description of Coulomb scattering in a magnetic field requires an account of the specific variation of Eq. (10) with respect to energy. In the only resolved experimental data on this process now available—atomic photoabsorption spectra—the most notable feature is the series of quasi-Landau resonances. The properties of electron motion in the asymptotic region appear to have only indirect relevance for the understanding of these phenomena.

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APPENDIX

This appendix provides the formulas underlying Eq. (10), which are derived along the same lines as conventional R -matrix treatments¹⁹ of electron-atom scattering. Atomic units are used throughout.

Consider the system of an electron and a target atom (containing N electrons) confined to a region Γ : $|z| < z_0$, where z is the coordinate in the magnetic field direction and the atomic nucleus lies in the plane $z=0$. The width $2z_0$ of this region is chosen to be sufficiently large that the target electrons have negligible probability of reaching its boundary; so that, in other words, for $|z| \geq z_0$, only the motion of a single electron need be considered. Let z_{N+1} denote the z coordinate of that electron, and Φ a wave function of the combined electron-target system. Under the restriction just mentioned, which precludes the treatment of ionizing collisions, the imposition of the boundary condition

$$\left. \frac{d}{dz_{N+1}} \Phi \right|_{z_{N+1} = \pm z_0} = 0 \quad (A1)$$

on Φ suffices to produce a set of solutions Φ_i to the equation of motion

$$H\Phi_i = E_i\Phi_i, \quad (A2)$$

which is complete in the region Γ . In Eq. (A2), H is the Hamiltonian operator for the $N+1$ electron system in Γ , defined in the usual way, and E_i is the energy of the i th eigenstate. The solutions Φ_i are normalized in the following sense:

$$\langle \Phi_i | \Phi_i \rangle = \int_{\Gamma} \cdots \int_{\Gamma} d\vec{r}_1 \cdots d\vec{r}_{N+1} \Phi_i^* \Phi_i = 1, \quad (A3)$$

the range of integration of each electron coordinate \vec{r}_i being Γ . By construction, it is supposed that for $i = 1, \dots, N$ the integral is practically the same as if taken over all space. Equations (A1)–(A3) thus yield the orthogonality condition $\langle \Phi_i | \Phi_j \rangle = \delta_{ij}$, since

$$\begin{aligned}
\langle \Phi_i | H \Phi_j \rangle - \langle H \Phi_i | \Phi_j \rangle &= (E_j - E_i) \langle \Phi_i | \Phi_j \rangle = \int_{\Gamma} \cdots \int_{\Gamma} d\vec{r}_1 \cdots d\vec{r}_{N+1} (\Phi_i^* H \Phi_j - \Phi_j^* H \Phi_i) \\
&= \int_{\Gamma} \cdots \int_{\Gamma} d\vec{r}_1 \cdots d\vec{r}_N \int_{-\infty}^{\infty} dx_{N+1} \int_{-\infty}^{\infty} dy_{N+1} \int_{z_0}^{z_0} dz_{N+1} \left[-\frac{1}{2} \right] \left[\Phi_i^* \frac{\partial^2}{\partial z_{N+1}^2} \Phi_j - \Phi_j^* \frac{\partial^2}{\partial z_{N+1}^2} \Phi_i \right] \\
&= \frac{1}{2} \int \cdots \int d\vec{r}_1 \cdots d\vec{r}_N dx_{N+1} dy_{N+1} \left[\Phi_j^* \frac{\partial}{\partial z_{N+1}} \Phi_i - \Phi_i^* \frac{\partial}{\partial z_{N+1}} \Phi_j \right] \Bigg|_{z_{N+1}=-z_0}^{z_{N+1}=z_0} = 0.
\end{aligned} \tag{A4}$$

Therefore, any wave function ψ which corresponds to a single electron being present in the region outside Γ , may be represented within Γ by an expansion in the Φ_i :

$$\psi = \sum_i \alpha_i \Phi_i \tag{A5}$$

(in Γ). The coefficients α_i are then determined from

$$\begin{aligned}
(E - E_i) \alpha_i &= \langle \Phi_i | H \psi \rangle - \langle H \Phi_i | \psi \rangle \\
&= \int_{\Gamma} \cdots \int_{\Gamma} d\vec{r}_1 \cdots d\vec{r}_N dx_{N+1} dy_{N+1} \int_{-z_0}^{z_0} dz_{N+1} \frac{1}{2} \left[\psi^* \frac{\partial^2}{\partial z_{N+1}^2} \Phi_i - \Phi_i^* \frac{\partial^2}{\partial z_{N+1}^2} \psi \right] \\
&= -\frac{1}{2} \int_{\Gamma} \cdots \int_{\Gamma} d\vec{r}_1 \cdots dy_{N+1} \left[\Phi_i^* \frac{\partial}{\partial z_{N+1}} \psi \right] \Bigg|_{-z_0}^{z_0}.
\end{aligned} \tag{A6}$$

E is the total energy of the system in the state ψ .

On the surfaces $|z| = z_0$ of Γ the Φ_i themselves may be expanded in products of target wave functions X_j and Landau orbitals χ_{nm} . The X_j are eigenfunctions of the Hamiltonian of the N -electron atom and can also include the spin of the $N+1$ electron

$$X_j \equiv X_j(\vec{r}_1, \dots, \vec{r}_N; \vec{\sigma}_1, \dots, \vec{\sigma}_{N+1}) \tag{A7}$$

is understood to be fully antisymmetric under interchanges $(\vec{r}_i, \vec{\sigma}_i) \leftrightarrow (\vec{r}_j, \vec{\sigma}_j)$ for $i, j = 1, \dots, N$. For brevity the variables of X_j will not be written explicitly, and all overlap integrals, etc., involving X_j are to be interpreted in the conventional manner. The χ_{nm} are the wave functions for electron motion in the plane perpendicular to the magnetic field, written in the polar coordinates ρ, ϕ of that plane

$$\begin{aligned}
\chi_{nm}(\rho, \phi) &= \frac{e^{im\phi}}{\sqrt{2\pi}} \left[\frac{\omega(n!)}{(n+|m|)!} \right]^{1/2} e^{-(\omega\rho^2/4)} \\
&\times \left[\frac{\omega}{2} \rho^2 \right]^{|m|/2} L_n^{|m|}(\omega\rho^2/2),
\end{aligned} \tag{A8}$$

where

$$L_n^m(x) = \begin{bmatrix} n+m \\ n \end{bmatrix} {}_1F_1(-n, m+1, x). \tag{A9}$$

Thus, for $z_{N+1} = \pm z_0$

$$\Phi_i = \sum_{j,n,m} X_j a_{ijnm}(z_{N+1} = \pm z_0) \chi_{nm}(\rho_{N+1}, \phi_{N+1}), \tag{A10}$$

where the sum over target states j is restricted to those whose wave functions X_j are negligible for $|\vec{r}_i| \geq z_0$. This justifies the expression (A10) for the fully antisym-

metric function Φ_i , since additional terms deriving from interchanges of \vec{r}_{N+1} and \vec{r}_i will be exponentially small.

The wave function ψ may be expanded outside Γ as well,

$$\psi = \sum_{j,n,m} X_j \chi_{nm}(\rho_{N+1}, \phi_{N+1}) f_{jnm}(z_{N+1}). \tag{A11}$$

Since the full Hamiltonian of the system is invariant under inversion in the plane $z=0$, i.e., $z_i \rightarrow -z_i$, $i=1, \dots, N+1$, ψ may be taken to be even or odd under that inversion. The X_j also possess definite inversion symmetry, and therefore so do the f_{jnm} . The coefficients a_{ijnm} of Eq. (A10) must thus have the same inversion symmetry as the f_{jnm} , which is opposite to the inversion symmetry of the derivatives $\partial f_{jnm} / \partial z_{N+1}$. Therefore, Eq. (A6) can be further developed as

$$(E - E_i) \alpha_i = - \sum_{j,n,m} a_{ijnm}^* \frac{\partial}{\partial z} f_{jnm}(z) \Bigg|_{z=z_0}. \tag{A12}$$

By inserting this result in Eq. (A5), and equating the coefficients of the product $X_j \chi_{nm}$ on either side, it is seen that

$$f_{jnm}(z_0) = \sum_{i,k,n',m'} \frac{a_{ijnm} a_{ikn'm'}^*}{(E_i - E)} \frac{\partial}{\partial z} f_{kn'm'}(z) \Bigg|_{z=z_0}. \tag{A13}$$

Thus a boundary condition for the z motion in each channel jnm can be computed solely from the solutions of Eqs. (A1) and (A2) in Γ (which give the a_{ijnm}) and the total energy E . It will be convenient to designate by a single index j the three-channel quantum numbers j, n, m , so that Eq. (A13) may be read in the matrix form

$$f_j(z_0) = \sum_k R_{jk}(E) \frac{\partial}{\partial z} f_k(z) \Bigg|_{z=z_0}. \tag{A14}$$

The interaction between the electron outside Γ and the residual target atom is presumed to be described by a potential $V \equiv V(\vec{r}_{N+1}; \vec{r}_1, \dots, \vec{r}_N)$. The Schrödinger equation for the channel functions $f_i(z)$ for $z > z_0$ is then

$$\left[-\frac{1}{2} \frac{\partial^2}{\partial z^2} + V_{ii}(z) - \epsilon_i \right] f_i(z) = \sum_j V_{ij}(z) f_j, \quad (\text{A15})$$

where

$$\epsilon_i = \frac{1}{2} k_i^2 = E - \epsilon_i - \frac{\omega}{2} [2n_i + 1 + (m_i + |m_i|)/2] \quad (\text{A16})$$

and

$$V_{ij}(z) = \langle X_i \chi_{n_i m_i} | V | X_j \chi_{n_j m_j} \rangle \quad (\text{A17})$$

and ϵ_i is the energy of the residual target state X_i plus the paramagnetic energy of the spin of the scattering electron $g\vec{S}_{N+1} \cdot \vec{B}$. For most practical purposes V will consist of electric multipole and polarization potentials $V \sim r^{-\mu}$. In such cases the $V_{ij}(z)$ may be evaluated in terms of exponential integrals and error functions. The diagonal terms $V_{ii}(z)$ represent the average, over a probability distribution in the plane $z = \text{constant}$, of a potential which is strongest at $\rho = 0$; therefore the numerical value of $V_{ii}(z)$ must be less in magnitude than that obtained by substituting z for r in V .

Equation (A14) determines the solution of the system of equations (A15) for $z > z_0$, up to boundary conditions which are imposed at infinity (the solution for $z < -z_0$ can be obtained by invoking the inversion symmetry of the f_i). The conservation of the projection of the total angular momentum on the magnetic field axis will simplify this system of equations, for instance, by permitting

separate treatment of channels associated with different values of m . All simplifications which may be made on the basis of symmetry arguments nevertheless still result in infinite systems of equations, whereas for any given energy E only a finite number of channels are open (i.e., have $k_i^2 > 0$). Elimination of the closed channels (those with $k_i^2 = -\kappa_i^2 < 0$) is, in general, a laborious procedure which must be carried out iteratively. However, when the electron-target interaction vanishes in $|z| \geq z_0$, this elimination is fairly straightforward. The basic idea is that since the closed-channel wave functions must die off exponentially, $f_c \sim e^{-\kappa_c z}$, there is a fixed relationship in each closed-channel c between the value of f_c and $\partial f_c / \partial z$ at the boundary z_0 . This takes the form of an additional constraint upon the linear relations (A14), which can be eliminated in the usual way to reduce (A14) to an equation involving open-channel wave functions only.

Specifically, let $\vec{f}_o, \vec{f}_c, \vec{f}'_o, \vec{f}'_c$, denote the sets of open- and closed-channel wave functions and their z derivatives, respectively, and let (A14) be cast in the form

$$\begin{aligned} \vec{f}'_o &= R^{oo} \vec{f}'_o + R^{oc} \vec{f}'_c \Big|_{z=z_0}, \\ \vec{f}'_c &= R^{co} \vec{f}'_o + R^{cc} \vec{f}'_c \Big|_{z=z_0}. \end{aligned} \quad (\text{A18})$$

For a closed channel i , $f_i(z) = F_i e^{-\kappa_i z}$ ($z > z_0$), which may be written in matrix form as

$$\vec{f}'_c = -\kappa \vec{f}_c, \quad (\text{A19})$$

κ being diagonal. Routine manipulation of Eqs. (A18) and (A19) then yields

$$\begin{aligned} \vec{f}'_o &= \bar{R} \vec{f}'_o, \\ \bar{R} &= R^{oo} - \kappa R^{oc} (1 + \kappa R^{cc})^{-1} R^{co}. \end{aligned} \quad (\text{A20})$$

- ¹L. M. Tannenwald, Phys. Rev. **113**, 1396 (1959); R. Goldman, *ibid.* **133**, A647 (1964).
- ²J. Ventura, Phys. Rev. A **8**, 3021 (1973).
- ³K. Onda, J. Phys. Soc. Jpn. **45**, 216 (1978); W. Schmitt, H. Herold, H. Ruder, and G. Wunner, Astron. Astrophys. **94**, 194 (1981).
- ⁴H. S. Brandi, B. Koiller, H. G. P. Lius de Barros, and L. C. M. Miranda, Phys. Rev. A **18**, 1415 (1978).
- ⁵G. Ferrante, S. Nuzzo, M. Zarccone, and S. Bivona, J. Phys. B **13**, 731 (1980).
- ⁶S. M. Kara and M. R. C. McDowell, J. Phys. B **14**, 1719 (1981).
- ⁷W. A. M. Blumberg, R. M. Jopson, and D. J. Larson, Phys. Rev. Lett. **40**, 1320 (1978).
- ⁸W. A. M. Blumberg, W. M. Itano, and D. J. Larson, Phys. Rev. A **19**, 139 (1979).
- ⁹A. R. Edmonds, J. Phys. (Paris) Colloq. **31**, C4-71 (1970); A. F. Starace, J. Phys. B **6**, 585 (1973).
- ¹⁰U. Fano, J. Phys. B **13**, L519 (1980); C. W. Clark and K. T. Taylor, Nature **292**, 437 (1981).
- ¹¹K. T. Lu, F. S. Tomkins, and W. R. S. Garton, Proc. R. Soc. London, Ser. A **364**, 421 (1978); W. R. S. Garton, F. S. Tomkins, and H. M. Crosswhite, *ibid.* **373**, 189 (1980), and references therein.

- ¹²J.-C. Gay, D. Delande, and F. Biraben, J. Phys. B **13**, L729 (1980); D. Delande and J.-C. Gay, Phys. Lett. **82A**, 393 (1981); 399 (1981).
- ¹³L. Landau, Z. Phys. **64**, 629 (1930); M. H. Johnson and B. A. Lippmann Phys. Rev. **76**, 828 (1949).
- ¹⁴Note that this differs by a factor of $2^{-1/2}$ from the normalization coefficient of three-dimensional radial wave functions, due to doubling of the range of radial integration.
- ¹⁵An attractive potential in two dimensions will also always hold a bound state; see, e.g., L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non Relativistic Theory*, 3rd ed. (Pergamon, London, 1977), p. 163. I thank Ravi Rau for bringing this to my attention. The energy of the bound state is exponentially small in the well depth; the phase shift $\delta \sim 1/\ln E$ as $E \rightarrow 0$.
- ¹⁶A. R. P. Rau, J. Phys. (Paris) Colloq. **43**, C2-211 (1982); U. Fano, in Atomic Physics 8 (Plenum, New York, in press).
- ¹⁷T. M. Miller and B. Bederson, Adv. At. Mol. Phys. **13**, 1 (1977).
- ¹⁸A. R. P. Rau and U. Fano, Phys. Rev. A **4**, 1751 (1971).
- ¹⁹P. G. Burke and W. D. Robb, Adv. At. Mol. Phys. **11**, 144 (1975); and references therein.