Oscillations in photodetachment cross sections for negative ions in magnetic fields

Oakley H. Crawford
Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6123
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Theory is developed for photodetachment of an electron from a potential well in a magnetic field. The cross section has a maximum as a function of photon energy just above each Landau-level threshold. If the final-state interaction is effectively negative, there is in addition a Feshbach resonance below each of these thresholds, except the first. However, none of these maxima occurs if the final-state wave function is antisymmetric with respect to reflection in a plane perpendicular to the magnetic field direction. The oscillations observed experimentally are attributed to the maxima located above the thresholds, not the Feshbach resonances.

I. INTRODUCTION

Photodetachment of electrons from negative ions in magnetic fields has attracted considerable interest recently, because of experiments[1-6] showing oscillations in the near-threshold cross sections. This effect was first observed by Blumberg, Jopson, and Larson.[1] Performing high-resolution photodetachment spectroscopy on sulfur negative ions in an ion trap, they discovered oscillations in the cross section versus laser frequency, with a period proportional to the magnetic field strength. Blumberg and co-workers[1,2] attributed these features to detachment into a series of Landau levels[7] of the free electron in the magnetic field.

Analogous oscillations in photodetachment of electrons from D^- centers in semiconductors have been observed[8-10] as well, and are similarly understood to be due to Landau levels of quasifree electrons in the magnetic field.[11] Furthermore, several interesting transport phenomena arising from the discrete nature of these levels have been discovered in solids.[11,12]

A free electron in a magnetic field has an infinite set of quantized energy levels (Landau levels) for motion perpendicular to the field (while motion parallel to the field is unquantized).[7] The spacing between these levels is $\hbar\omega_H$, where $\omega_H = 2\pi\nu_H = eH/Mc$, ν_H being the cyclotron frequency, H the magnetic field, e and M the charge (absolute value) and mass of the electron, and c the velocity of light. As a consequence, there is an infinite set of thresholds, separated by energy $\hbar\omega_H$, for detachment of an electron in a magnetic field (ignoring any fine structure of the ion and atom for the moment). At each threshold, the density of states of the free electron is singular.

When the final-state interaction, i.e., between the detached electron and the atom, is ignored, the energy dependence of the cross section is determined by the density of states of the free (or quasifree) electron. Theory derived on this basis (developed for the solid[13] and for the gas[1,2] independently) predicts that the cross section σ_ν for detachment into the Landau state ν is infinite at the threshold (angular) frequency ω_ν, and decreases as $(\omega-\omega_\nu)^{-1/2}$ for laser frequency $\omega > \omega_\nu$. The total photodetachment cross section, obtained by summing the σ_ν, thus consists of a series of infinite spikes. However, the result of convolution to account for broadening (e.g., due to imperfections in the crystal, or Doppler and motional Stark effects in the gas) is finite. Such a convolution, using as free parameters the overall scale of the cross sections, the origin of the frequency scale, and the ion temperature, has been shown by Blumberg and co-workers[2] to give a good fit to their data.[1]

Subsequent work on the theory has incorporated the final-state interaction,[3,14-18] i.e., between the electron and the atom, which had previously been ignored. It has been proven[15,17] that the cross section remains finite near threshold, given this interaction. A detailed expression for the cross section has been presented by Gurvich and Zil'bermints[17] for the case where the initial state (bound by a small-radius potential) has zero component of orbital angular momentum in the direction of the field **H**, and the electric field of the light is perpendicular to **H**. The various theories cited above differ as to the mechanism of the cross-section oscillations, as well as to their form and their precise location.

In the following sections expressions are derived for the cross sections for photodetachment in a magnetic field of electrons initially bound by short-range potentials. Arbitrary initial angular momentum and polarization of light are considered. The results are illustrated by calculations, comparisons are made with zero-field cross sections, and the mechanism is discussed.

II. THEORY

We consider an electron interacting with a spherically symmetric potential V in a uniform magnetic field of strength H. It is convenient to work in cylindrical polar coordinates ρ, z, ϕ, with the z axis in the direction of the magnetic field. The vector potential is given by

$$A_\phi = \tfrac{1}{2}H\rho, \quad A_z = A_\rho = 0 \ .$$

Then the Hamiltonian is given by[7]

$$\mathcal{H}=-\frac{\hbar^2}{2M}\nabla^2+V+\tfrac{1}{2}\mathcal{L}_z\omega_H+\tfrac{1}{8}\hbar\omega_H\left[\frac{\rho}{a_H}\right]^2 , \quad (1)$$

where $\mathcal{L}_z$ is the operator for the z component of orbital angular momentum, ω_H and a_H are the (angular) cyclotron frequency and the cyclotron radius,

$$a_H=\left[\frac{\hbar}{M\omega_H}\right]^{1/2}=\left[\frac{\hbar c}{eH}\right]^{1/2} ,$$

and $-e$ and M are the charge and mass of the electron. The electron's spin is ignored. Its component in the direction of **H** does not change, so it does not affect photodetachment in this model.

In the absence of a potential, the Hamiltonian has the following complete set of eigenfunctions $\psi_{\nu k_\nu}$ having definite orbital angular momentum about the z axis and even or odd symmetry with respect to reflection through the $z=0$ plane:

$$\psi_{\nu k_\nu}=\frac{1}{2(2\pi)^{1/2}}R_{mn}(\rho)e^{im\phi}(e^{ik_\nu z}+\sigma_{xy}e^{-ik_\nu z}) , \quad (2)$$

where[7]

$$R_{mn}(\rho)=\frac{1}{a_H\,|m|!}\left[\frac{(|m|+n)!}{2^{|m|}n!}\right]^{1/2}\left[\frac{\rho}{a_H}\right]^{|m|} \times \exp\left[-\frac{\rho^2}{4a_H^2}\right]{}_1F_1(-n;|m|+1;\rho^2/2a_H^2) , \quad (3)$$

where ${}_1F_1$ is the confluent hypergeometric function, and where ν stands for the quantum numbers $\nu=\{m,n,\sigma_{xy}\}$. The latter take values $m=0,\pm1,\pm2,\ldots$; $n=0,1,2,\ldots$; and $\sigma_{xy}=\pm1$. The energy spectrum in each channel is a continuum, with lower bound E_ν given by

$$E_\nu=E_{mn}=(\tfrac{1}{2}m+n+\tfrac{1}{2}|m|+\tfrac{1}{2})\hbar\omega_H , \quad (4)$$

and k_ν and the energy E are related by

$$k_\nu=k_{mn}=\left[\frac{2M}{\hbar^2}(E-E_\nu)\right]^{1/2} . \quad (5)$$

The normalization of these wave functions is

$$\langle\psi_{\nu'k'}|\psi_{\nu k}\rangle=\delta(k'-k)\delta^{\nu}_{\nu'} . \quad (6)$$

In the problem of interest, the electron is initially bound by a potential $V(r)$. We assume that both the potential and the amplitudes of the bound-state wave functions have negligible amplitudes outside of some radius $r_0, r_0/a_H \ll 1$. This should be valid for potentials and one-electron wave functions that model the binding of an electron in a negative ion, for magnetic field strengths of a few T or less. ($a_H=2\times10^{-6}$ cm when $H=1$ T.) Thus, the last term in $\mathcal{H}$, Eq. (1), may be neglected for the initial bound state, which therefore has definite values of both the orbital angular momentum and its z component. We also assume that $k_\nu r_0 \ll 1$ and $|\beta_m| \ll 1$. This latter quantity is defined by Eq. (27).

The continuum wave function $\Psi_{\nu k_\nu}$ of interest for photodetachment into the ν channel is the one having an outgoing component in only that channel. It is the solution of the Lippmann-Schwinger integral equation

$$\Psi_{\nu k_\nu}=\psi_{\nu k_\nu}+G_H V\Psi_{\nu k_\nu} , \quad (7)$$

where G_H is the outgoing Green's function integral operator

$$G_H\equiv G_H^-(E)=[E-i\epsilon-(\mathcal{H}-V)]^{-1} . \quad (8)$$

The solution of Eq. (7) has the same δ-function normalization (6) as $\psi_{\nu k_\nu}$. To simplify the notation, we will drop the subscript k_ν from wave functions, except where it adds clarity.

We solve Eq. (7) to lowest order in the small quantities r_0/a_H and $k_\nu r_0$ by a generalization of the method used by Gurvich and Zil'bermints.[17] We begin with the following ansatz for Ψ_ν in the region $r<r_0$:

$$\Psi_\nu\approx M_\nu\Phi_\nu(\mathbf{r}),\quad r<r_0 \quad (9)$$

where M_ν is a constant (i.e., independent of $\mathbf{r}$) to be determined, and Φ_ν is a scattering wave function derived by dropping the $\frac{1}{8}\hbar\omega_H(\rho/a_H)^2$ term from the Hamiltonian, Eq. (1). Specifically, Φ_ν is the solution of the equation

$$\Phi_\nu=\phi_\nu+G_0V\Phi_\nu , \quad (10)$$

where G_0 is the free-particle outgoing Green's function

$$G_0\equiv G_0^-(E)=(E-i\epsilon-\mathcal{H}_0)^{-1} , \quad (11a)$$

with

$$\mathcal{H}_0=\mathcal{H}-V-\tfrac{1}{8}\hbar\omega_H\left[\frac{\rho}{a_H}\right]^2=-\frac{\hbar^2}{2M}\nabla^2+\tfrac{1}{2}\mathcal{L}_z\omega_H , \quad (11b)$$

and

$$(\mathcal{H}_0-E)\phi_\nu=0 . \quad (11c)$$

ϕ_ν is the free-particle[19] continuum wave function, well behaved at the origin. It has definite angular quantum numbers l and m, where l takes the lowest value for which ϕ_ν and ψ_ν have the same symmetry in the neighborhood of the origin,[20] i.e.,

$$l=\begin{cases}|m| , & \sigma_{xy}=+1 \quad (12a)\\ |m|+1, & \sigma_{xy}=-1 . \quad (12b)\end{cases}$$

The normalization of ϕ_ν is chosen such that ϕ_ν approaches ψ_ν at small r in the following sense:

$$(lm|\phi_\nu\rangle\sim(lm|\psi_\nu\rangle \quad as\ r\to0 , \quad (13)$$

where the $(lm|\ \rangle$ notation implies a scalar product of the normalized spherical harmonic $|lm)=Y_{lm}$ with the ket $|\ \rangle$, in which integration is performed over solid angle, the result being a function of a radial variable r. Thus,

$$\phi_\nu = B_\nu k_m^{-l}\left[\frac{2}{\pi}\right]^{1/2} j_l(k_m r) Y_{lm}(\theta,\phi)\ , \tag{14}$$

where

$$k_m = \left[\frac{2M}{\hbar^2}(E-\tfrac{1}{2}m\hbar\omega_H)\right]^{1/2}\ , \tag{15}$$

and where

$$B_\nu = \left[-\frac{m}{|m|}\right]^m a_H^{-l-1}\left[\begin{bmatrix}|m|+n\\ n\end{bmatrix}(2l+1)!!\right]^{1/2} \times\begin{cases}1, & \sigma_{xy}=+1\\ ik_\nu a_H, & \sigma_{xy}=-1\ .\end{cases} \tag{16}$$

To solve for M_ν, substitute (9) into the Lippmann-Schwinger equation (7) for Ψ_ν. Then eliminate Φ_ν from the left-hand side of the resulting equation by the use of (10), and rearrange to give

$$[\phi_\nu-(G_H-G_0)V\Phi_\nu]M_\nu=\psi_\nu,\quad r<r_0\ .$$

Taking the scalar product of $|lm)$ with both sides of this equation and solving gives

$$M_\nu=\left[1-\frac{(lm\,|(G_H-G_0)V\Phi_\nu\rangle}{(lm\,|\phi_\nu\rangle}\right]^{-1}\ . \tag{17}$$

The right-hand side of the above equation is to be evaluated in $r<r_0$, in which region it is independent of r, to lowest order in r_0/a_H and $k_\nu r_0$.

Next, we derive an approximation for G_H-G_0, valid to lowest order in r_0/a_H and $k_\nu r_0$. Representing G_H^-, Eq. (8), in a basis of Landau wave functions[7] gives the following expression for the kernel of the Green's function:

$$\begin{aligned}G_H(E,\mathbf{r},\mathbf{r}') &= \frac{M}{2\pi^2\hbar^2}\sum_m e^{im(\phi-\phi')}\sum_n R_{mn}(\rho)R_{mn}(\rho')\int_{-\infty}^{\infty}dk\frac{e^{ik(z-z')}}{k_\nu^2-i\epsilon-k^2}\\ &= i\frac{M}{\hbar^2}\sum_m(2\pi)^{-1}e^{im(\phi-\phi')}\sum_n R_{mn}(\rho)R_{mn}(\rho')\frac{\exp(-ik_\nu^*|z-z'|)}{k_\nu^*}\ .\end{aligned} \tag{18}$$

To simplify the notation, we use the same symbol for the Green's function and its kernel throughout. We need only the mm matrix element of G_H, which is obtained by dropping a factor $(2\pi)^{-1}\exp[im(\phi-\phi')]$ from the summand in the above expression. Thus,

$$(G_H)_{mm}=i\frac{M}{\hbar^2}\sum_n R_{mn}(\rho)R_{mn}(\rho')\frac{\exp(-ik_\nu^*|z-z'|)}{k_\nu^*}\ , \tag{19}$$

where k_ν, defined by Eq. (5), is taken to lie on the positive imaginary axis when $E<E_\nu$. Next, separate the right-hand side of (19) into two terms, $(G_1)_{mm}$ containing the sum over the open channels and the first closed channel (for given m), and $(G_2)_{mm}$ containing the sum over the rest of the closed channels.

In $(G_2)_{mm}$, replace R by the following, which is obtained from a series expansion[21] for the confluent hypergeometric function:

$$\begin{aligned}R_{mn}(\rho) &= \frac{C_{mn}}{a_H}\sum_{j=0}^{\infty}A_j\left[\frac{\rho}{2a_H}\right]^j(2n+|m|+1)^{-j/2}\\ &\quad\times J_{|m|+j}((2n+|m|+1)^{1/2}\rho/a_H)\ ,\end{aligned}$$

$$A_0=1,\quad A_1=0,\quad A_2=\tfrac{1}{2}(|m|+1)\ ,$$

$$(j+1)A_{j+1}=(j+|m|)A_{j-1}-(2n+|m|+1)A_{j-2}\ ,$$

where

$$C_{mn}=\left[\frac{(n+|m|)!}{n!(n+\frac{1}{2}|m|+\frac{1}{2})^{|m|}}\right]^{1/2}\ .$$

One finds that a large number of closed channels contribute to $(G_2)_{mm}$, and that the summand does not change rapidly with n. Therefore, one can replace the sum by an integration. Defining a new variable,

$$p=\frac{(2n+|m|+1)^{1/2}}{a_H}\ ,$$

the sum over n is approximated by $\frac{1}{2}a_H^2$ times an integral with respect to p^2. Next, replace C_{mm} by unity. This is exact when $|m|=0,1$, and the error is only of the order $(m/n)^2$ otherwise, which is negligible, as most of the integral comes from large n. Finally, one can show that the lower limit of the integral can be replaced by zero, with negligible error. The result is that $(G_2)_{mm}$ is approximated by

$$i\frac{M}{\hbar^2}\int_0^{\infty}p\,dpJ_{|m|}(p\rho)J_{|m|}(p\rho')\frac{\exp(-ik_\nu^*|z-z'|)}{k_\nu^*}\ , \tag{20}$$

where k_ν is a function of p [see Eqs. (4) and (5)]. Now, the above expression is precisely[22,23] the m,m component, $(G_0)_{mm}$, of the Green's function defined by Eq. (11). Therefore, we have

$$(G_H)_{mm}-(G_0)_{mm}\approx i\frac{M}{\hbar^2}\sum_{n=0}^{N_m}R_{mn}(\rho)R_{mn}(\rho')\frac{\exp(-ik_\nu^*|z-z'|)}{k_\nu^*}\ ,\quad r<r_0,\ r'<r_0 \tag{21}$$

where N_m is the value of the Landau radial quantum number of the first closed channel for given m and E.

The above result is now used to evaluate Eq. (17) for M_ν. In the case $\sigma_{xy}=-1$, the exponential in G_H-G_0, Eq. (21), may be replaced by $-ik_\nu^*|z-z'|$. (The leading term, unity, does not contribute to M_ν.) It can then be shown that the second term on the right-hand side of Eq. (17) is $\ll 1$. Therefore, to lowest order in r_0/a_H and $k_\nu r_0$, $M_\nu=1$ when $\sigma_{xy}=-1$.

In the case $\sigma_{xy}=+1$, the exponential in G_H-G_0 may be replaced by unity. Then, when $R_{mn}(\rho')$ is replaced by its small-ρ form, Eq. (17) contains the following integral:

$$\int d^3r'\, Y_{lm}^*(\theta',\phi')r'^l V(r')\Phi_\nu(r') \ . \tag{22}$$

Now, from the definition of Φ_ν it follows that

$$\Phi_\nu \sim \{\sin(k_m r - l\pi/2) + f_l^* k_m \exp[-i(k_m r - l\pi/2)]\} \times \left[\frac{2}{\pi}\right]^{1/2} \frac{B_\nu}{k_m^{l+1} r} Y_{lm}(\theta,\phi) \quad \text{as } r\to\infty \ , \tag{23}$$

where f_l is the scattering amplitude of the l partial wave,

$$f_l(k_m)=\frac{\exp(2i\eta_l)-1}{2ik_m} \ , \tag{24}$$

where η_l is the phase shift at wave number k_m. Substitution of Eq. (23) into the Lippmann-Schwinger equation (10) (with G_0 expanded in a spherical-wave basis[23]) gives the relation

$$f_l(k_m)=-\left[\frac{\pi}{2}\right]^{1/2}\frac{2Mk_m^{2l}}{\hbar^2(2l+1)!!B_\nu} \times \int d^3r'\, Y_{lm}^*(\theta',\phi')r'^l V(r')\Phi_\nu(\mathbf{r}') \ . \tag{25}$$

Therefore, the integral (22) is given by

$$-\left[\frac{2}{\pi}\right]^{1/2}\frac{\hbar^2(2l+1)!!B_\nu}{2Mk_m^{2l}} f_l^*(k_m) \ .$$

The resulting expression for M_ν is

$$M_\nu=\begin{cases}\left[1-i2^{1/2}\beta_m^* \sum_{n'=0}^{N_m}\begin{pmatrix}|m|\,n' \\ n'\end{pmatrix}(k_{mn'}a_H)^{-1}\right]^{*-1}, & \sigma_{xy}=+1 \quad (26a)\\ 1, \quad \sigma_{xy}=-1 & \quad (26b)\end{cases}$$

where

$$\beta_m=\frac{(2|m|+1)!!}{2^{1/2}a_H^{2|m|+1}}\frac{f_{|m|}(k_m)}{k_m^{2|m|}} \ . \tag{27}$$

Note that M_ν varies with m, σ_{xy}, and E, but is independent of n. The ratio $f_{|m|}(k_m)/k_m^{2|m|}$ may be replaced by its $k_m=0$ limit, $-\alpha_{|m|}$, when $\alpha_{|m|}$, the $|m|$-wave scattering length, exists.

Note that β_m is a function of k_m. Gurvich and Zil'bermints[17] give a result corresponding to (26) and (27) for $\sigma_{xy}=1$, but having $-\alpha_{|m|}$ in place of $f_{|m|}k_m^{-2|m|}$. When $\alpha_{|m|}$ exists, the two results are, of course, equivalent. On the other hand, there can in principle be cases where the potential decays too slowly at large r for the scattering length to exist, but is small enough in $r>r_0$ (for some r_0 small relative to a_H) for the above results (26) and (27) to be valid. Note that Eq. (27) is not required to be evaluated at $k_m=0$, since the minimum value reached by k_m, i.e., at the $(m,0,1)$ threshold, is $(|m|+1)^{1/2}/a_H$.

The cross section for detachment into state νk_ν from initial state μ by absorption of a photon of polarization ϵ is given by

$$\sigma_{\nu k_\nu}=\frac{4\pi^2 M\omega}{\hbar^2 c k_\nu}|\langle \nu k_\nu|\mathbf{D}\cdot\epsilon|\mu\rangle|^2 \ , \tag{28}$$

where ω and c are the angular frequency of the radiation, and its speed, respectively, $\mathbf{D}$ is the dipole operator, and $|\nu k_\nu\rangle$ is the final-state wave function having an outgoing component in only the ν channel, i.e., $\Psi_{\nu k_\nu}$.

In the absence of a magnetic field, the cross section $\sigma_{lmk_m}^{(0)}$ for photodetachment into the l,m channel is given by

$$\sigma_{lmk_m}^{(0)}=\frac{4\pi^2 M\omega}{\hbar^2 c k_m}|\langle lmk_m|\mathbf{D}\cdot\epsilon|\mu\rangle|^2 \ , \tag{29}$$

where the wave function $|lmk_m\rangle$ has an outgoing component in only the l,m channel, and is normalized to $\delta_l^{l'}\delta_m^{m'}\delta(k_m-k_m')$.

Now, the two different kinds of final-state wave functions are proportional to each other in $r<r_0$ in the following sense:

$$(lm|\nu k_\nu\rangle = M_\nu B_\nu k_m^{-l-1}(lm|lmk_m\rangle, \quad r<r_0 \ , \tag{30}$$

in which the factor M_ν comes from Eq. (9), and the other factors come from the ratio of $(lm|\Phi_{\nu k_\nu}\rangle$ to $(lm|lmk_m\rangle$. The matrix elements in the above two cross-section formulas are related in the same way. Therefore, the matrix elements can be eliminated, giving the following expression for the relation between photodetachment cross sections with and without a magnetic field:

$$\sigma_{\nu k_\nu}=\frac{|M_\nu B_\nu|^2}{k_\nu}\frac{\sigma_{lmk_m}^{(0)}}{k_m^{2l+1}} \ , \tag{31}$$

where, for given $\nu=\{m,n,\sigma_{xy}\}$, l is chosen according to Eq. (12). Using the Wigner threshold law for the field-free cross section,

$$\sigma^{(0)}_{lmk_m} = \zeta_{lm} k_m^{2l+1} , \tag{32}$$

we get the final result,

$$\sigma_{\nu k_\nu} = \zeta_{lm} \, | B_\nu M_\nu |^2 k_\nu^{-1} , \tag{33}$$

with B_ν and M_ν calculable from Eqs. (16) and (26), respectively. Features of this expression will be explored below.

A. Cross sections for $\sigma_{xy} = +1$ final states

For the case $\sigma_{xy} = +1$, B_ν is independent of energy, so the cross section, Eq. (33), goes as $|M_\nu|^2 k_\nu^{-1}$. Since $k_\nu = [2(\omega - \omega_{mn})/\omega_H]^{1/2}/a_H$, the frequency dependence of the cross section is given by

$$\sigma_\nu \sim (\omega - \omega_{mn})^{-1/2} |M_\nu|^2 , \tag{34}$$

with

$$\begin{aligned} M_\nu &= \left[1 - i\beta_m^* \sum_{n'=0}^{N_m} \begin{bmatrix} |m| + n' \\ n' \end{bmatrix} \left[\frac{\omega - \omega_{mn'}}{\omega_H} \right]^{-1/2} \right]^{*-1} \\ &= \left[1 - \beta_m \begin{bmatrix} |m| + N_m \\ N_m \end{bmatrix} \left[\frac{\omega_{mN_m} - \omega}{\omega_H} \right]^{-1/2} \right. \\ &\quad \left. + i\beta_m \sum_{n'=0}^{N_m - 1} \begin{bmatrix} |m| + n' \\ n' \end{bmatrix} \left[\frac{\omega - \omega_{mn'}}{\omega_H} \right]^{-1/2} \right]^{-1} . \end{aligned} \tag{35}$$

Note that the final-state interaction influences the cross section through only the factor β_m, which appears only in M_ν. If the final-state interaction is ignored, putting $\beta_m = 0$, then, from the above equations, $M_\nu = 1$, and the cross section σ_ν is proportional to $(\omega - \omega_\nu)^{-1/2}$, for $\omega > \omega_\nu$. This is consistent with earlier work.[1,13] However, it is clear from Eq. (35) that when $\beta_m \neq 0$ the behavior of σ_ν is modified when ω is close to any threshold.

At energies close to the $(m,n,1)$ threshold, the terms in Eq. (35) that contain $\beta_m((\omega - \omega_{mn'})/\omega_H)^{-1/2}$, $n' \neq n$, are of order β_m, which is negligible compared with unity by assumption. Therefore, the $n' \neq n$ terms may be neglected in this case, giving

$$\sigma_\nu \sim \frac{(\omega - \omega_{mn})^{1/2}}{\begin{bmatrix} |m| + n \\ n \end{bmatrix}^2 \beta_m^2 \omega_H + \omega - \omega_{mn}} . \tag{36}$$

Thus, the cross section for detachment into channel $\{m,n,1\}$ rises from its threshold (at $\omega = \omega_{mn}$) with an $(\omega - \omega_{mn})^{1/2}$ dependence, goes through a maximum, and then over to an $(\omega - \omega_{mn})^{-1/2}$ behavior, with increasing frequency. The maximum occurs at a frequency

$$\omega_{mn} + \begin{bmatrix} |m| + n \\ n \end{bmatrix}^2 \beta_m^2 \omega_H , \tag{37}$$

which is very close to the threshold ($|\beta_m| \ll 1$). As the calculations below will illustrate, the cross section is very large at the maximum, compared with normal zero-field values.

For frequencies just above an $n' > n$ threshold, σ_ν has the $|M_\nu|^2$ frequency dependence, with

$$|M_\nu|^2 = \frac{\omega - \omega_{mn'}}{\begin{bmatrix} |m| + n' \\ n' \end{bmatrix}^2 \beta_m^2 \omega_H + \omega - \omega_{mn'}} . \tag{38}$$

Thus, σ_ν is zero at every threshold, i.e., at every $\omega_{mn'}$, but only at its own threshold ω_{mn} does it have the large peak above threshold. Note that the above expression is independent of the sign of β_m.

Next, consider the behavior of the system at frequencies close to, but *below* a threshold frequency ω_{mN_m}. Suppose $\beta_m > 0$, which is the case when the interaction in the final state is effectively attractive. In this neighborhood, according to Eq. (35), there is a value E_r of the energy

$$E_r = E_{mN_m} - \begin{bmatrix} |m| + N_m \\ N_m \end{bmatrix}^2 \beta_m^2 \hbar\omega_H , \tag{39}$$

for which the real part of $M_\nu^{-1} = M_{mn1}^{-1}$ vanishes, independent of n, while the imaginary part is a sum over $n' < N_m$. For energies close to E_r, the energy dependence of σ_ν is that of $|M_\nu|^2$, Eq. (35), which takes the Breit-Wigner form

$$|M_\nu|^2 = \frac{\left[\frac{1}{2} \begin{bmatrix} |m| + N_m \\ N_m \end{bmatrix} \beta_m^2 \hbar\omega_H \right]^2}{(E - E_r)^2 + (\frac{1}{2}\gamma)^2} , \tag{40}$$

where the width γ is given by

$$\gamma = 4\beta^3 \hbar\omega_H \begin{bmatrix} |m| + N_m \\ N_m \end{bmatrix} \times \sum_{n'=0}^{N_m - 1} \begin{bmatrix} |m| + n' \\ n' \end{bmatrix} (N_m - n')^{-1/2} . \tag{41}$$

Note that γ is much smaller than the energy separation $E_{mN_m} - E_r$, between closed channel and resonance, which, in turn, is $\ll \hbar\omega_H$.

Consider now the bound the quasibound states that occur only in the presence of the magnetic field when β_m is positive. If the Hamiltonian is truncated by removing the open channels, and the definition (9) of M_ν is extended analytically to the first closed channel, $\nu = \{m, N_m, +1\}$ (and this could be any channel of this symmetry, depending on the total energy), then $M_{mN_m 1}$ is given by Eq. (35), but without the imaginary part, and is singular at the energy E_r given by (39). This, together with Eq. (9), implies that a bound state of the same symmetry $\{m, +1\}$ occurs at this energy. In the full Hilbert space (including the open channels), this state is quasibound for $N_m > 0$, since it can decay into open channels, but it is a true bound state for $N_m = 0$. The binding energy of the state located just below the threshold of the $\{m,n,1\}$ channel is thus given by

$$\begin{bmatrix} |m| + n \\ n \end{bmatrix}^2 \beta_m^2 \hbar\omega_H . \tag{42}$$

Comparison with (37) shows that the peak and the resonance (or bound state) associated with any $\{m,n,1\}$ threshold have their maxima symmetrically located about the threshold energy.

In summary, for any m, the cross section σ_{mn1} is zero at each $\{m,n',1\}$ threshold, has a maximum just above its own threshold, and (if $\beta_m > 0$) has an additional maximum below each $\{m,n',1\}$ $(n' > n)$ threshold. The large peak in σ just above its threshold has a similar origin as, and the same form as, the low-energy peak in s-wave elastic scattering from a potential that supports a low-energy bound or virtual state.[24] In the case of a magnetic field, where the free motion is confined to one dimension, a zero-energy bound state occurs in the absence of a potential. The effect of the final-state interaction upon the photodetachment cross section σ_ν close to its own threshold is (as previously discussed[14]) to decrease the cross section close to threshold, thereby moving the peak up in energy by an amount equal to the binding or virtual binding energy. The peak below each threshold (when $\beta_m > 0$) is a Feshbach resonance, which decays into all open channels of the same symmetry.

The above formulas for M_ν and for the binding energies have been given previously by Gurvich and Zil'bermints.[17] A different value,

$$\frac{1}{2}\left|\frac{M}{2\pi\hbar^2 a_H}\int V\,d\tau\right|^2 \hbar\omega_H \;, \tag{43}$$

where the integral extends over all space, has been derived[3,24] for the binding energy of the state associated with the $\{0,0,1\}$ channel. The latter result is valid only for sufficiently small V.[24] More precisely, (43) is equivalent to (42) if and only if α_0 exists and is given by the Born approximation, which is accurate for $|\alpha_0| \ll 1$. On the other hand, it can be shown (starting from the single-channel treatment[3]) that (43) is the value of the binding energy that follows from the close-coupling Hamiltonian (where only one or a few channels are included) when α_0 exists and $|\beta_0| \ll 1$. Accordingly, when $|\alpha_0|$ does not exist or is not small, the close-coupling treatment is subject to error near threshold.

B. Cross sections for $\sigma_{xy} = -1$ final states

For $\sigma_{xy} = -1$ states, the factor $|M_\nu B_\nu|^2 k_\nu^{-1}$ in Eq. (33) is proportional to k_ν, so the cross section σ_ν goes simply as $(\omega - \omega_\nu)^{1/2}$. Here we have assumed, as in the discussion of the $\sigma_{xy} = +1$ case, that the zero-field photodetachment cross section $\sigma_{lm}^{(0)}$ goes as k_m^{2l+1}. In the present case $l = |m| + 1$.[20] The large peaks found in the $\sigma_{xy} = +1$ case do not appear, nor does the final-state interaction affect the cross section in this case. This is because a magnetic field does not give rise to bound or virtual states of the $\sigma_{xy} = -1$ symmetry.

III. CALCULATIONS

The total cross section σ for photodetachment in a magnetic field for given initial-state angular momentum quantum numbers l_i, m_i, and given polarization index (or quantum number for photon angular momentum component in the **H** direction) q, is given by

$$\sigma = \sum_{n=0}^{N_m - 1} \sigma_{\nu k_\nu} \;, \tag{44}$$

where $\nu = \{m, n, \sigma_{xy}\}$ with $m = m_i + q$ and $\sigma_{xy} = (-1)^{(l_i + m_i + q + 1)}$. In this section calculations of σ will be presented and compared with the field-free photodetachment cross section $\sigma_{lm}^{(0)}$ from the same initial state. In $\sigma^{(0)}$ one uses $l = l_i - 1$ (but if $l_i - 1 < |m|$, then $l = l_i + 1$).

The calculations of σ are simple, requiring only the sum over open channels of $\xi_{lm} |B_\nu M_\nu|^2 k_\nu^{-1}$ [Eqs. (44) and (33)], using Eq. (16) for B_ν and Eq. (26) or (35) for M_ν, when values of the parameters ξ_{lm} and $\alpha_{|m|}$ [or $\beta_m(k_m)$] are available.

Figure 1 shows σ (solid curve) and $\sigma^{(0)}$ (dashed curve) for detachment from a p_0 state $(l_i, m_i) = (1,0)$ by a $q = 0$ photon. The origin of the frequency scale is the zero-field photodetachment threshold. The strength of the magnetic field is 1.07 T, wherein the cyclotron frequency $\nu_H = \omega_H / 2\pi$ is 30 GHz, $\hbar\omega_H = 4.56 \times 10^{-6} e^2/a_0$, and $a_H = 468 a_0$, where a_0 is the Bohr radius. We have assumed the s-wave scattering length α_0 to be $-1\ a_0$, so $\beta_0 = 1.51 \times 10^{-3}$. We have taken the zero-field cross section to be equal to $a_0^3 k_0$. The figure covers a frequency range of $3\nu_H$ (or an energy interval of $3\hbar\omega_H$), and includes the thresholds of the $n = 0$, 1, and 2 channels $(m = 0, \sigma_{xy} = +1)$. The behavior of the cross sections very near the various thresholds is not resolved in this figure, which therefore has the appearance of a sum of partial cross sections that go as $(\omega - \omega_{mn})^{-1/2}$, as predicted by Blumberg *et al.*[1,2] Note that the cross section oscillates about the zero-field cross section. If the former is averaged over a rectangular frequency distribution of width ν_H, centered at, say ν_c, the result is (to lowest order in the small quantities) equal to the zero-field cross section at frequency ν_c. Plots of σ for detachment from $p_{\pm 1}$ states with $q = -m_i$ are the same as the σ shown in Fig. 1 except that they are shifted in frequency by $-m_i \nu_H / 2$.

Figure 2 shows a portion of the σ calculation discussed above, on a greatly expanded frequency scale, whose ori-

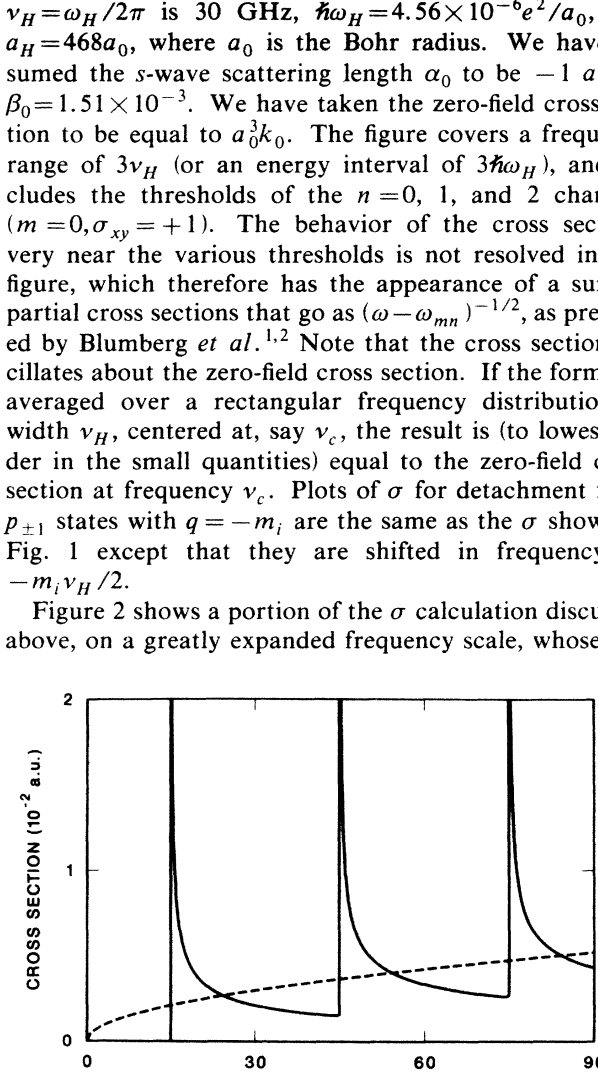

FIG. 1. Total cross section for photodetachment from a p state $(l_i, m_i = 1,0)$ by a photon having polarization index $q = 0$ vs light frequency, in a 1.07-T field (solid curve) and in zero field (dashed curve). The origin of the relative frequency scale is the zero-field detachment threshold. The atomic unit of cross section is $a_0^2 = 2.80 \times 10^{-17}$ cm^2.

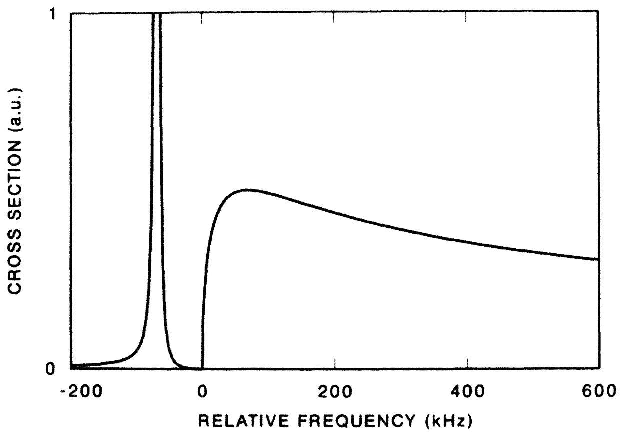

FIG. 2. Total cross section for photodetachment from a p state $(l_i,m_i=1,0)$ by a photon with polarization index $q=0$ vs light frequency, in a 1.07-T field. The origin of the relative frequency scale is the threshold for detachment into the $(m,n)=(0,1)$ Landau level. This plot shows the structure of the 45-GHz feature of Fig. 1 on a greatly expanded frequency scale.

gin is the threshold of the $n=1$ channel. The sharper peak is the resonance, while the broader feature beginning at the threshold is the peak in the $n=1$ channel. Note that the scale of the ordinate has been contracted by a factor of 50 to accommodate this peak. Similar features appear at each threshold, except at the $n=0$ one, where the resonance does not appear.

The behavior of a $\sigma_{xy}=-1$ cross section is illustrated in Fig. 3, which gives the total cross section σ (solid curve) for photodetachment from an s state in a 1.07-T field, by photons having polarization index $q=-1$. The parameter ξ_{10} is assumed to be $871a_0$, which happens to

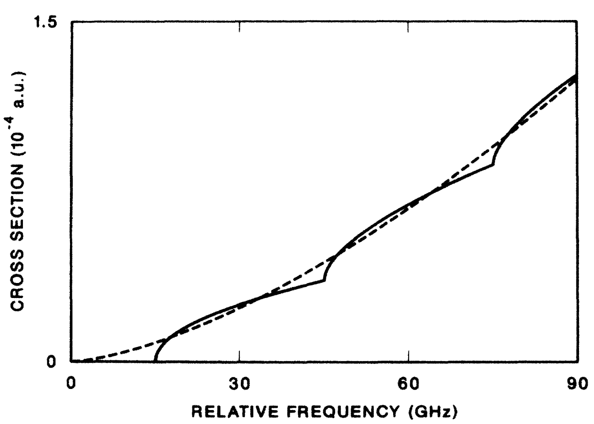

FIG. 3. Total cross section for photodetachment from an s state by a photon having polarization index $q=-1$ vs light frequency, in a 1.07-T field (solid curve) and in zero field (dashed curve). The origin of the relative frequency scale is the zero-field detachment threshold. The atomic unit of cross section is $a_0^2=2.80\times10^{-17}$ cm^2. The absence of maxima in the solid curve is associated with odd reflection symmetry $(\sigma_{xy}=-1)$ of the final-state wave function.

be the correct value[25] for H^-. The dashed curve in the figure is the zero-field photodetachment cross section $\sigma_{10k_0}^{(0)}$ for the same frequency and polarization.

As in Fig. 1, the abscissa is the light frequency, relative to the threshold frequency at zero field, i.e., $(\hbar\omega-A)/h$, where A is the electron affinity. The figure shows that the detachment cross section σ has an abrupt change in slope at each threshold, where the slope is in fact infinite, due to the k_ν dependence. One also sees that σ does not deviate much from the field-free cross section, and that the two are very close, when averaged over a frequency range ν_H.

Detachment from an s state with light having polarization index $q=\pm1$ (i.e., by polarized light propagating along the direction of $\mathbf{H}$) gives $\sigma_{xy}=+1$ final states. In this case, σ (which has been plotted previously[17,18]) has features similar to those shown in Fig. 1, but [assuming comparable magnitudes of $V(r)$] the peaks lie much closer to the thresholds than when $m=0$. When $q=-1$, σ oscillates about $\sigma_{10}^{(0)}$.

IV. DISCUSSION

Simple formulas are derived for cross sections for photodetachment of electrons from a potential well in a magnetic field. Arbitrary values of the initial angular momentum and the photon polarization index are treated. The potential in the exit channels is assumed to be small in $r>r_0$ (for some r_0 small relative to a_H), but it is not required that the $|m|$-wave scattering length $\alpha_{|m|}$ exist. When the final-state interaction is effectively attractive, the total photodetachment cross section σ displays a pair of maxima symmetrically displaced about each threshold. The lower-frequency one (missing from the first threshold) is a Feshbach resonance. The other maximum is contributed by the cross section of the newly opened channel, and occurs regardless of whether the final-state potential is attractive, repulsive, or zero. This peak, which is due to the existence of a near-threshold bound state or virtual state in that channel, has a close analogue in the feature sometimes called a low-energy resonance or zero-energy resonance in s-wave elastic scattering. The cross section σ oscillates about the zero-field cross section $\sigma^{(0)}$, and the average of σ over a rectangular distribution of full width ν_H approximates $\sigma^{(0)}$ (except for a frequency shift, depending on initial and final quantum numbers m_i and m).

The oscillations observed experimentally are due to the maxima that are located just above thresholds, not to the Feshbach resonances. The Feshbach resonances, although having the larger cross sections, are narrow and contribute negligibly to σ when the latter is convoluted to account for a realistic experimental resolution. The remainder of this section is devoted to comparisons with previous theory and with experiment.

The close-coupling method has been the one most used in discussing the wave functions of the continuum states that are populated in photodetachment in a magnetic field. The wave function is written as a sum over functions $u_n(z)R_{mn}(\rho)(2\pi)^{-1/2}\exp(im\phi)$, $n=0,1,2,\ldots$, for a given m, and the Schrödinger equation is reduced to a set of coupled equations for the unknown functions $u_n(z)$,

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dz^2}+V_{nn}(z)-E_{mn}\right]u_n(z)$$
$$=-\sum_{n'\neq n} V_{nn'}(z)u_{n'}(z),\quad n=0,1,2,\ldots \tag{45}$$

with

$$V_{nn'}(z)=\int_0^{\infty} d\rho\,\rho V((\rho^2+z^2)^{1/2})R_{mn}(\rho)R_{mn'}(\rho)\ . \tag{46}$$

These equations have been studied by Clark[15] using a square-well potential of depth V_0 and radius r_0, where

$$V_{nn'}(z)=-V_0\frac{r_0^2-z^2}{2a_0^2},\quad |z|<r_0 \tag{47}$$

for any pair of levels, as long as n and n' are much less than $(r_0/a_H)^{-2}$. Thus, there are a great number of channels coupled together. Of these, a large group have all of their $V_{nn'}$ (whether off diagonal or diagonal) approximately equaling each other and being of the same order of magnitude as the difference $\hbar\omega_H$ between channel energies. This presents a difficult problem. Clark infers that the cross-section maxima observed in photodetachment may be due either to Feshbach resonances or to "quasi-Landau" resonances analogous to what occur in photoionization in a magnetic field. If the latter, the maxima would be located above the thresholds by an appreciable amount, e.g., by about (Ref. 15) 0.1 $\hbar\omega_H$ in the case of S^-.

Larson and Stoneman[3] assume an attractive potential (that is too weak to bind an electron in the absence of a field), solve the one-dimensional Schrödinger equation [Eq. (45), neglecting $V_{nn'}$ for $n'\neq n$] for an $\{m,n,\sigma_{xy}\}=\{0,n,1\}$ channel, and calculate σ_v. In spite of the difficulties in principle cited above, the conclusions drawn from this single-channel treatment agree qualitatively in most respects with the present theory. The cross section is of the form shown in Eq. (36), exhibiting a maximum above threshold, but the displacement of the peak from threshold is different, corresponding to the different value of the binding energy [see Eq. (43)] of the bound state. The bound state is recognized[3] as being the origin of a Feshbach resonance in the $n'<n$ channels. It was pointed out in Sec. III that those results agree closely with ours only when the potential is small enough for the Born approximation for the (field-free) scattering length α_0 to be accurate. Comparison with the present theory shows that the effect of inclusion of the closed channels (beyond the first one) is to improve the description of the bound, quasibound, and virtual states. However, to affect this improvement within the conventional framework of close-coupling computation would be impractical because of the large number of closed channels that make comparable contributions.

This critique of the applicability of the close-coupling method is directed toward photodetachment from atoms in the gas, with magnetic field strengths less than 10^3 T, so that the cyclotron radius a_H and energy $\hbar\omega_H$ are, respectively, large relative to atomic dimensions and small relative to atomic binding energies. However, for much larger magnetic field strengths (or perhaps in a solid with small enough effective mass and large enough dielectric constant[26]), only a few channels need be considered, so close-coupling calculations are appropriate. Such calculations have been reported, for example, for scattering from a screened Coulomb potential in a 2×10^4-T field.[27]

The results presented here agree with those of Gurwich and Zil'bermints[17] where comparison is possible. Those workers assume the existence of the $|m|$-wave scattering length $\alpha_{|m|}$. Under that assumption, the $\sigma_{xy}=1$ continuum wave functions given here are the same as theirs, as is the energy dependence of the cross section for photodetachment from an s state by circularly polarized light propagating in the direction of the field.

Comparison with existing experiments[1,3,5] on S^- and Se^- requires extension of the theory to accommodate magnetic fine structure. Each Landau threshold is replaced by a set of thresholds due to the Zeeman effect on the ion and atom. (This Zeeman structure has been resolved[5] in the case of Se^-.) Let us assume that the cross sections predicted for Landau levels (in the absence of fine structure) are divided among the fine-structure states in such a way that the features associated with Landau-level thresholds are reproduced at the various fine-structure thresholds. (This is what is predicted[2] when the final-state interaction potential is ignored.) Then, the present theory implies that observation of effects of the final-state electron-atom interaction requires resolution (on an energy scale) on the order of $\beta_0^2\hbar\omega_H$ or less. Assuming that the scattering length α_0 is of the order of a_0, and the magnetic field is 1 T, $\beta_0^2=10^{-5}$. Since ν_H here is 30 GHz, the necessary resolution is 10^2 kHz. Since that resolution is not yet achievable, shifts of the maxima in σ from the thresholds should not be observed. Larson and Stoneman[3] conclude that their S^- data contain a strong indication of a shift upward from threshold, which is in conflict with the present theory as applied to systems containing fine structure. It would be interesting to see the results of measurements of yet higher resolution on this system. Krause[28] has reported on a beam apparatus under construction for high-resolution measurements of magnetic field effects in photodetachment.

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[20]In principle, Eq. (9) should contain a sum over l values, but the component having the smallest value of l allowed by symmetry is by far the dominant one in $r<r_0$ since $kr_0 \ll 1$. Note, however, that this restriction limits the treatment to situations where the $l=|m|$ or $|m|+1$ final state is allowed by dipole selection rules for the particular initial-state quantum numbers and photon polarization of interest. This should cover all situations of practical significance since the cross sections that are omitted are in each case very small compared with those that are treated for the same initial orbital angular momentum quantum number l_i.
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