Broadening of spectral lines of ionized atoms in a constant magnetic field

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The dependence of the shape of the resonance absorption spectrum of ionized atoms on the angle between the wave vector **q** and the field **H** is investigated. The conditions are found under which a spectral line resolution smaller than the Doppler width $|\mathbf{q}|v(|\mathbf{q}|v \gg \Omega$, where v and Ω are respectively the thermal velocity and the cyclotron frequency of the ion, can be obtained even when the thermal motion is strong.

1. The Doppler broadening of a spectral line in a gas is usually much larger than the radiative width Γ_{21}. This means that in a transition of frequency $\omega_{21} = (E_2 - E_1)/\hbar$, where E_1 and E_2 are the energy levels of the atom, we have

$$\Gamma_{21} \ll \omega_{21}(v/c) = |\mathbf{q}|v, \tag{1}$$

where $v = (2T/M)^{1/2}$ is the thermal velocity of the atom at the temperature T, and q is the wave vector. The resolution of the natural width is possible in this case only by using special research methods (nonlinear-spectroscopy methods, cooling the gas, beam spectroscopy, and others[1,2]).

The situation can change radically for ionized atoms in the presence of a constant magnetic field **H**. Indeed, owing to the periodicity of the charged-particle motion the absorption (emission) spectrum comprises in the vicinity of the transition frequency ω_{21} a sum over the harmonics of the cyclotron frequency $\Omega = zeH/Mc \ll \omega_{21}$ (z and M are the charge and mass of the ion). In a coordinate frame moving along **H** together with the ion, the frequencies radiated in this case are

$$\omega_s = \omega_{21} + s\Omega. \tag{2}$$

To each frequency corresponds a Lorentz profile with natural width Γ_{21}. In the laboratory frame these frequencies are shifted by one and the same amount $q_\parallel v_\parallel$ ($v_\parallel$ and $q_\parallel$ are the longitudinal components of the ion velocity and of the wave vector). Since the partial contribution of the sth harmonic is determined by the factor[3] $J_s^2(q_\perp v_\perp/\Omega)$ ($v_\perp$ and $q_\perp$ are the transverse components of the ion velocity and the wave vector, and $J_s(x)$ is a Bessel function), the spectrum in a gas with equilibrium distribution of the ions is obviously of the form

$$\sum_{s=-\infty}^{\infty} \int_{-\infty}^{\infty} dv_\parallel \int_0^{\infty} dv_\perp^2 \exp\left[-\frac{v_\parallel^2 + v_\perp^2}{2v^2}\right] J_s^2\left(\frac{q_\perp v_\perp}{\Omega}\right) \times \frac{1}{\pi} \frac{\Gamma_{21}}{(\omega - \omega_{21} - s\Omega - q_\parallel v_\parallel)^2 + \Gamma_{21}^2}. \tag{3}$$

Here $v = (2T/M)^{1/2}$ is the thermal velocity of the ion. It is easy to verify that Eq. (3) depends strongly on the angle between **q** and **H**. Indeed, in strictly transverse wave propagation we have $q_\parallel = 0$ and the spectrum (3) is (just as in the case of one ion) a sum of Lorentz profiles. At $\Gamma_{21} \ll \Omega$ these profiles do not overlap, i.e., (3) differs from zero only in the vicinity of the frequencies (2) [the maximum resolvable number of harmonics is $|s|_{\max} \lesssim q_\perp v/\Omega \equiv |\mathbf{q}|v/\Omega$)]. In the other limiting case ($q_\perp = 0$) the spectrum (3) is obviously independent of the presence of the field **H** and is determined under the condition (1) by the usual Doppler profile (with characteristic width $|\mathbf{q}|v$).

2. We shall investigate the resonant-absorption spectrum in greater detail on the basis of quantum-mechanical perturbation theory (in which case the recoil effect can be accounted for most simply). We express the Hamiltonian of an ionized atom in a magnetic field in the form

$$\hat{H} = \hat{H}_\nu + \frac{1}{2M}\left[\left(\hat{p}_x - \frac{zeH}{c}y\right)^2 + \hat{p}_y^2 + \hat{p}_\parallel^2\right]. \tag{4}$$

The Hamiltonian $\hat{H}_\nu$ is connected here with the internal degrees of freedom and determines the atom's energy levels E_ν and its eigenfunctions $|\nu\rangle$. The remainder of the Hamiltonian (4) describes the mass-center motion. Its wave functions $|n, p_x, p_\parallel\rangle$ and its eigenvalues $E_{np_\parallel} = \hbar\Omega(n + 1/2) + p_\parallel^2/2M$ are known in this case[4] ($\Omega = zeH/Mc$, $n = 0, 1, 2, \ldots$, $p_\parallel$ is the ion momentum along **H**). We do not need the actual values of E_ν and $|\nu\rangle$, and assume only that the atom levels E_1 and E_2 correspond to an allowed transition of frequency $\omega_{21} = (E_2 - E_1)/\hbar \gg \Omega$.

Let a wave

$$\mathbf{E}(\mathbf{r}t) = \mathbf{E}\exp(i\mathbf{q}\mathbf{r} - i\omega t) + \text{c.c.} \tag{5}$$

whose frequency is close to the transition frequency ω_{21} ($|\omega - \omega_{21}| \ll \omega_{21}$) and having a wave vector **q** be incident on the atom.

The probability of resonant absorption in a transition of the atom from the state $|i\rangle = |1\rangle|n, p_x, p_\parallel\rangle$ to all states $|f\rangle = |2\rangle|n', p_x', p_\parallel'\rangle$ is equal to

$$W = \frac{2\pi}{\hbar}|\mathbf{d}_{21}\mathbf{E}|^2 \sum_{n', p_x', p_\parallel'} |\langle n', p_x', p_\parallel'|e^{i\mathbf{q}\mathbf{r}}|n, p_x, p_\parallel\rangle|^2 \times \delta\left[\frac{p_\parallel'^2}{2M} - \frac{p_\parallel^2}{2M} + \hbar\Omega(n'-n) + \hbar(\omega_{21} - \omega)\right]. \tag{6}$$

Here $\mathbf{d}_{21} = \langle 2|\mathbf{d}|1\rangle$ is the matrix element of the dipole moment of the atom over all the states $|\nu\rangle$.

Using the results of Ref. 5, we can represent (6) in the form

$$W(\omega, E_{np_\parallel}) = W_{21} \sum_{n'=0}^{\infty} \Lambda_{n'n}(g_\perp^2)\,\delta(g_\parallel^2 + 2\varkappa_\parallel g_\parallel + n' - n - \Delta), \tag{7}$$

where

$$\mathbf{g} = \frac{\hbar\mathbf{q}}{(2M\hbar\Omega)^{1/2}}, \quad \varkappa_\parallel = \frac{p_\parallel}{(2M\hbar\Omega)^{1/2}}, \quad \Delta = \frac{\omega - \omega_{21}}{\Omega},$$

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$$W_{21}=\frac{2\pi}{\Omega}\left|\frac{\mathbf{d}_{21}\mathbf{E}}{\hbar}\right|^2, \tag{8}$$

$$\Lambda_{n'n}(g_\perp^2)=\int_0^\infty dx e^{-x}L_{n'}(x)L_n(x)J_0(2g_\perp x^{1/2}).$$

Here $L_n(x)$ are Laguerre polynomials and $J_0(y)$ is a Bessel function.

We recognize now that the atom energy levels E_ν have finite widths Γ_ν ($\nu=1,2$) governed by the radiative damping. In accord with the results of Ref. 6 we obtain in lieu of (7)

$$W(\omega,E_{np_\parallel})=W_{21}\sum_{n'=0}^\infty\Lambda_{n'n}(g_\perp^2)\frac{1}{\pi}\frac{\gamma}{(g_\parallel^2+2\varkappa_\parallel g_\parallel+n'-n-\Delta)^2+\gamma^2}, \tag{9}$$

where $\gamma=\Gamma_{21}/\Omega\equiv(\Gamma_1+\Gamma_2)/2\Omega$. Using in (9) the representation

$$\frac{1}{\pi}\frac{\gamma}{x^2+\gamma^2}=\frac{1}{2\pi}\int_0^\infty dt\exp(-\gamma t+ixt)+\text{c.c.}$$

and formula 8.975(1) of Ref. 7 for the summation of Laguerre polynomials, we obtain

$$W(\omega,E_{np_\parallel})=\frac{W_{21}}{2\pi}\int_0^\infty dt\ \exp[-\gamma t+it(g_\parallel^2+2\varkappa_\parallel g_\parallel-\Delta)]$$
$$\times\exp[-g_\perp^2(1-e^{it})]L_n[4g_\perp^2\sin^2(t/2)]+\text{c.c.} \tag{10}$$

Averaging (10) over the equilibrium distribution of the ions with temperature T:

$$f(n,\varkappa_\parallel)=(\tau/\pi)^{1/2}\exp(-\varkappa_\parallel^2\tau)(1-e^{-\tau})e^{-n\tau},$$

where $\tau=\hbar\Omega/T$, we have

$$W(\omega)=\frac{W_{21}}{2\pi}\int_0^\infty dt\exp\left[-\gamma t+it(g_\parallel^2-\Delta)-\frac{1}{4}\delta_\parallel^2t^2\right]$$
$$\times\exp\left[-g_\perp^2\frac{\text{ch}(\tau/2)-\cos(t-i\tau/2)}{\text{sh}(\tau/2)}\right]+\text{c.c.} \tag{11}$$

Here $\delta_\parallel=2g_\parallel/\tau^{1/2}\equiv q_\parallel v/\Omega$ is the longitudinal component of the Doppler frequency. Equation (11) is valid for arbitrary values of τ; in the calculations that follow, however, we confine ourselves to the case $\tau\ll1$.

3. We show first and foremost that Eq. (11) goes over as $\Omega\to0$ to the usual resonant-absorption profile[8] known from the theory of broadening at $\mathbf{H}=0$. Indeed, as $\Omega\to0$ the parameters γ and $\delta_\parallel$ greatly exceed unity, i.e., the main contribution to the interval with respect to t is made by the region $t\lesssim\min(\gamma^{-1},\delta_\parallel^{-1})\ll1$. Confining ourselves at $\tau\ll1$ to expansion of the expression

$$\frac{\text{ch}(\tau/2)-\cos(t-i\tau/2)}{\text{sh}(\tau/2)}\approx-it+\frac{t^2}{\tau},$$

we write

$$W(\omega)=\frac{W_{21}}{2\pi}\int_0^\infty dt\exp\left[-\gamma t+it(g^2-\Delta)-\frac{1}{4}\delta^2t^2\right]+\text{c.c.} \tag{12}$$

Here

$$g^2=g_\parallel^2+g_\perp^2\equiv\hbar q^2/2M\Omega$$

is the total recoil theory and

$$\delta=2g/\tau^{1/2}\equiv qv/\Omega$$

is the Doppler frequency. (Since $\Omega=zeH/Mc$, the resultant Eq. (12) is naturally valid also for neutral atoms ($z=0$) even if $\mathbf{H}\neq0$.) The case (1) corresponds then to the Doppler profile

$$W_D(\omega)=\frac{W_{21}\Omega}{\pi^{1/2}|\mathbf{q}|v}\exp\left[-\left(\frac{\omega-\omega_{21}-\hbar q^2/2M}{|\mathbf{q}|v}\right)^2\right]. \tag{13}$$

For arbitrary values of γ and $\delta_\parallel$ in the integral (11), the entire integration region is important. Using the known expansion[7]

$$e^{y\cos y}=\sum_{s=-\infty}^\infty e^{isy}I_s(y),$$

we represent (11) in the form

$$W(\omega)=W_{21}\sum_{s=-\infty}^\infty Z_s(g_\parallel^2)R_s(g_\perp^2), \tag{14}$$

where

$$Z_s(g_\parallel^2)=\frac{1}{2\pi}\int_0^\infty dt\exp\left[-\gamma t+it(g_\parallel^2+s-\Delta)-\frac{1}{4}\delta_\parallel^2t^2\right]+\text{c.c.}, \tag{15}$$

$$R_s(g_\perp^2)=e^{s\tau/2}I_s\left[\frac{g_\perp^2}{\text{sh}(\tau/2)}\right]\exp\left(-g_\perp^2\,\text{cth}\frac{\tau}{2}\right). \tag{16}$$

If $\tau\ll1$ and

$$\delta_\perp=2g_\perp/\tau^{1/2}\equiv q_\perp v/\Omega\gg1$$

expression (16) becomes much simpler if we use the asymptotic equation

$$I_s(x)\approx\frac{1}{(2\pi x)^{1/2}}\exp\left(x-\frac{s^2}{2x}\right),$$

which is valid for all $|s|<x$.[7,9] Assuming in addition that $\delta_\perp^2\gg\max(\delta_\perp,\delta_\parallel,\gamma)$ we obtain ultimately

$$W(\omega)\approx W_{21}\sum_{s=-\infty}^\infty Z_s(g_\parallel^2)\frac{1}{(\pi\delta_\perp^2)^{1/2}}\exp\left[-\left(\frac{s-g_\perp^2}{\delta_\perp}\right)^2\right]. \tag{17}$$

At $\delta_\perp>\max(\delta_\parallel,\gamma)$ the spectrum (17) contains generally speaking at the frequencies

$$\omega_s=\omega_{21}+s\Omega+g_\parallel^2\Omega \tag{18}$$

resonant peaks whose envelope is characterized by a Doppler profile of width $\Omega\delta_\perp\equiv q_\perp v$ (i.e., the maximum resolvable number of harmonics is $|s|\lesssim\delta_\perp$). The integral (15), which determines the shapes of the resonances, has been tabulated (see, e.g., Refs. 2 and 7); we confine ourselves, however, to its limiting values

$$Z_s(g_\parallel^2)\approx\frac{1}{\pi}\frac{\gamma}{(\Delta-s-g_\parallel^2)^2+\gamma^2},\quad\gamma\gg\delta_\parallel \tag{19}$$

and

$$Z_s(g_\parallel^2)\approx\frac{1}{(\pi\delta_\parallel^2)^{1/2}}\exp\left[-\left(\frac{\Delta-s-g_\parallel^2}{\delta_\parallel}\right)^2\right],\quad\delta_\parallel\gg\gamma. \tag{20}$$

The representation (20) is known to be valid only near the line center at

$$|\Delta-s-g_{\parallel}^2|\ll\delta_{\parallel}[\ln(2\pi^{1/2}\delta_{\parallel}/\gamma)]^{1/2};$$

at larger detunings the distribution (20) is replaced by a Lorentz wing.[2] To investigate the conditions for the resolution of the resonances (18) in the spectrum (17) it is not important to specify the actual line shape, since it suffices only to consider the behavior of (15) at

$$|\Delta-s-g_{\parallel}^2|\lesssim\delta_{\parallel}<\delta_{\parallel}[\ln(2\pi^{1/2}\delta_{\parallel}/\gamma)]^{1/2}.$$

From (17) and (10) we get thus

$$W(\omega)=W_{21}\sum_{s=-\infty}^{\infty}\frac{1}{(\pi\delta_\perp^2)^{1/2}}\exp\left[-\left(\frac{s-g_\perp^2}{\delta_\perp}\right)^2\right]\frac{1}{(\pi\delta_{\parallel}^2)^{1/2}}\times\exp\left[-\left(\frac{\Delta-s-g_{\parallel}^2}{\delta_{\parallel}}\right)^2\right]. \quad (21)$$

The harmonics (18), obviously, become distinguishable here starting with $\delta_{\parallel}<\pi^{-1/2}$. At $\delta_{\parallel}\ll 1\ll\delta_\perp\approx\delta$ the modulation of the spectrum becomes particularly noticeable; Eq. (21) can now be represented in the form

$$W(\omega)\approx W_D(\omega)\sum_{s=-\infty}^{\infty}\frac{1}{(\pi\delta_{\parallel}^2)^{1/2}}\exp\left[-\left(\frac{\Delta-s-g_{\parallel}^2}{\delta_{\parallel}}\right)^2\right] \quad (22)$$

(we have used here the notation (13)) i.e., substantial absorption takes place only near the frequencies (18), and within the limits of the characteristic width we have $\Omega\delta_{\parallel}\equiv q_{\parallel}v\ll\Omega$ (we recall that Ω is the distance between neighboring resonances). At $\delta_{\parallel}\gg 1$ (i.e., $q_{\parallel}v\gg\Omega$) the spectrum (21) is characterized by a large number of terms. The summation over s can then be replaced by an integral. Simple integration leads to Eq. (13) which corresponds to absorption when the influence of the magnetic field is negligible.

In the other limiting caes, $\delta_{\parallel}\ll\gamma\ll\delta_\perp\ll\delta$, it follows from (17) and (19) that

$$W(\omega)\approx W_D(\omega)\sum_{s=-\infty}^{\infty}\frac{1}{\pi}\frac{\gamma}{\gamma^2+(\Delta-s-g_{\parallel}^2)^2}. \quad (23)$$

The sum

$$Z(x)=\sum_{s=-\infty}^{\infty}\frac{1}{\pi}\frac{\gamma}{\gamma^2+(x-s)^2},\quad x=\Delta-g_{\parallel}^2 \quad (24)$$

is easily calculated (see Ref. 10), and then

$$Z(x)=\mathrm{sh}\,2\pi\gamma/[\mathrm{ch}\,2\pi\gamma-\cos 2\pi x].$$

In particular, at $\gamma\gg 1$ ($\Gamma_{21}\gg\Omega$) we have

$$Z(x)\approx 1+2e^{-2\pi\gamma}\cos 2\pi x\approx 1,$$

i.e., the absorption spectrum (23) is characterized in accord with (13) by the usual Doppler profile.

By examining the ratio

$$\frac{Z_{max}}{Z_{min}}=\frac{Z(\omega_s)}{Z(\omega_s+{}^1/_2\Omega)}=\frac{\mathrm{ch}\,2\pi\gamma+1}{\mathrm{ch}\,2\pi\gamma-1},$$

we easily verify that the modulation of the spectrum (23) becomes noticeable already at $\gamma<\pi^{-1}$. At $\gamma\ll 1$ the modulation is of the order of $(\pi\gamma)^{-2}\gg 1$, i.e., the absorption is exclusively resonant at the frequencies (18). The profile of each sth resonance is Lorentzian (with a characteristic width $\Omega\gamma\equiv\Gamma_{21}\ll\Omega$).

4. Thus, in a gas of ionized atoms located in a constant magnetic field **H** the shape of the resonant-absorption spectrum ($|\omega-\omega_{21}|\ll\omega_{21}$) depends substantially on the parameter $\delta\equiv|\mathbf{q}|v/\Omega$ (i.e., given the value $\delta\equiv|\mathbf{q}|v/\Omega$ it depends on the angle ϑ between the wave vector **q** and **H**). Therefore even in the case of strong thermal motion of the ions, $|\mathbf{q}|v>\Omega\gg\Gamma_{21}$ [see (1)] it is possible in principle to resolve the natural width of the transition. The deviation of the angle ϑ from the normal to **H** should satisfy in this case the condition

$$|\mathbf{q}|v|\vartheta-\pi/2|<\Gamma_{21}<\Omega. \quad (25)$$

Since the radiative width increases rapidly with increasing frequency ω_{21} of the transition[6]

$$\Gamma_{21}\sim\omega_{21}\frac{e^2}{\hbar c}\left(\frac{\omega_{21}a}{c}\right)^2\sim\omega_{21}\left(\frac{e^2}{\hbar c}\right)^3$$

(a is the characteristic dimension of the atom), the most important in (25) is the restriction imposed by the magnetic field ($H>10^{13}(e^2/\hbar c)^5(m/M)\sim 10^5$ G). At $v\sim(e^2/\hbar)(m/M)^{1/2}$ and $H\sim 10^5$–10^6 G the inequality (25) holds for all transitions with $\Gamma_{21}<10^9$–10^{10} sec^{-1}, if

$$|\vartheta-\pi/2|<(M/m)^{1/2}(e^2/\hbar c)^2\sim 10^{-3}. \quad (26)$$

(The contribution of the collisions to the broadening of the resonance (18) can be neglected[8] if the particle density $n\lesssim 10^{15}\ll(e^2/\hbar c)^3a^{-3}\sim 10^{18}$ cm^{-3}.)

The modulation of the spectrum (17) is preserved, however, also under the less stringent condition of quasiperiodic (relative to the direction of **H**) propagation of the wave:

$$\left(\frac{M}{m}\right)^{1/2}\left(\frac{e^2}{\hbar c}\right)^2<\left|\vartheta-\frac{\pi}{2}\right|<\left(\frac{\hbar c}{e^2}\right)^3\left(\frac{m}{M}\right)^{1/2}\frac{H}{10^{13}}\sim 10^{-3}\text{–}10^{-2}. \quad (27)$$

Starting with angles $|\vartheta-\pi/2|>10^{-3}$–$10^{-2}$, the spectrum (17) is transformed into the usual Doppler profile (13). So strong a dependence of the shape of the spectrum (17) an the angle ϑ can be used in principle to determine the direction of the vector **H** (at least of its mean value over the path over the ray).

We note in conclusion that Eqs. (17) and (15), neglecting the recoil effect $[g_\perp^2\ll\delta_\perp, g_{\parallel}^2\ll\min(\delta_{\parallel},\gamma)]$ are in full agreement with the qualitative analysis of the spectrum in Sec. 1. A formal transition to the classical case can be obtained also directly from Eq. (10). It suffices to put here

$$g_{\parallel}^2=\frac{\hbar q_{\parallel}^2}{2M\Omega}\to 0,\quad g_{\parallel}^2=\frac{\hbar q_\perp^2}{2M\Omega}\to 0$$

and use the limiting relation

$$L_n(x)\approx J_0[2(nx)^{1/2}],$$

which is valid at $n\gg 1$ and $nx=$ const. Using in addition the expansion[7]

$$J_0\left(2y\sin\frac{t}{2}\right)=\sum_{s=-\infty}^{\infty}J_s^2(y)e^{ist}, \quad (28)$$

we obtain

$$W(\omega, v_{\parallel}, v_{\perp}) \approx W_{21}\Omega \sum_{s=-\infty}^{\infty} J_s^2\left(\frac{q_\perp v_\perp}{\Omega}\right)\frac{1}{\pi}\frac{\Gamma_{21}}{(\omega-\omega_{21}-s\Omega-q_\parallel v_\parallel)^2+\Gamma_{21}^2}. \quad (29)$$

Here $q_\perp v_\perp/\Omega \equiv 2g_\perp\sqrt{n}^{1/2}$, and $v_\perp \equiv (2\hbar\Omega n/M)^{1/2}$ is the classical transverse velocity. Averaging of (29) over the Maxwellian distribution of the ions leads to (3).

We note that the recoil effect can certainly be neglected if the quasi-transverse propagation conditions (26) and (27) are satisfied. A characteristic feature is that at $v\sim(e^2/\hbar)(m/M)^{1/2}$ and $H\sim 10^5$–10^6 G the cyclotron frequency of the electrons is $\Omega_e = eH/mc \gtrsim q_\perp v \approx |\mathbf{q}|v$. Therefore each of the components of the Zeeman splitting of the frequency ω_{21} can be resolved in the spectra (22) and (23) at practically all $|s| < |s|\max \lesssim q_\perp v/\Omega$.

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