Resonance enhancement of relativistic effects for the scattering of very slow electrons by heavy atoms

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Polarization of scattered electrons is enhanced up to 1 near p- and d-wave resonances or weakly bound negative-ion energy levels ($|E| \lesssim 0.1$ eV, $v^2/c^2 \lesssim 10^{-6}$). We consider as example Ra and Ba. We also note that the cross section for Ra is very large ($> 10^{11}$ b at electron energy $\sim 10^{-2}$ eV).

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Usually one can roughly estimate the value of relativistic corrections as a ratio v^2/c^2, where v is the velocity of the electron, and c is the velocity of light. However, sometimes the magnitude of the effect can be essentially larger. An example is the "Fano effect" in photoionization [1]. This enhancement is also possible in resonance electron scattering (see, e.g., Ref. [2] and references therein). The relativistic effect in this case is the polarization of scattered electrons [correlation $\mathbf{s}(\mathbf{n}\times\mathbf{n}')$, where $\mathbf{s}$ is the electron spin, $\mathbf{n}$ and $\mathbf{n}'$ are the initial and final directions of the electron momentum]. For example, in electron-neon scattering polarization near the resonance exceeds 10% (see, e.g., Refs. [3] and [2]). Feschbach resonance occurs here due to negative-ion formation in the excited state of neon. The electron in this case has enough energy (16 eV) to excite the atom to the quasistationary state.

There is another possibility for very slow electrons. The effect can arise due to potential scattering (shape) resonance or due to a negative-ion energy level close to the continuous spectrum. In heavy atoms spin-orbit interaction is strong, and the splitting between the components of the spin-orbit doublet can be larger than the resonance width. In this case the value of the electron polarization can reach unity.

The purpose of this work is to present an interesting example of such a situation. In Ref. [4] we calculated the energy levels and fine-structure intervals of negative ions using many-body perturbation theory and the correlation potential method. We found that the $7P_{1/2}$ level in the Ra^- negative ion lies in the discrete spectrum ($E=-0.0109$ Ry; calculations in Ref. [5] give $E=-0.0055$ Ry) and the $7P_{3/2}$ level lies practically on the border between the discrete and continuous spectra ($E=0.0013$ Ry with accuracy ~ 0.001 Ry). In our present work we have found that for electron-radium scattering, electron polarization can exceed 90% in the energy interval $0.01\ \text{Ry} \lesssim E \lesssim 0.02$ Ry near the scattering angle $\theta = 90°-100°$.

Note that the energy region of large polarization is essentially higher and wider than the energy of the $P_{3/2}$ resonance. Actually, the scale here is determined by the distance between the $P_{1/2}$ and $P_{3/2}$ levels. We have considered also polarization effects in electron-barium scattering. Large polarization here appears only in the narrow region near d-wave resonance since the distance between $d_{3/2}$ and $d_{5/2}$ levels is twice as small as the d-resonance width. This resonance with $E=0.016$ Ry was predicted in Ref. [6].

The amplitude of electron scattering on a spinless atom can be written as follows (see, e.g., Ref. [7]):

$$\begin{aligned} \hat{f} &= A + 2B\boldsymbol{\nu}\cdot\hat{\mathbf{s}} , \\ A &= \frac{1}{2ik}\sum_{l=0}^{\infty}[(l+1)(e^{2i\delta_l^+}-1) \\ &\qquad + l(e^{2i\delta_l^-}-1)]P_l(\cos\theta) , \\ B &= \frac{1}{2k}\sum_{l=1}^{\infty}(e^{2i\delta_l^+}-e^{2i\delta_l^-})P_l^1(\cos\theta) . \end{aligned} \tag{1}$$

Here $\boldsymbol{\nu}=(\mathbf{n}\times\mathbf{n}')/|\mathbf{n}\times\mathbf{n}'|$ is the unit vector normal to the scattering plane, $\hat{s}$ is the electron spin operator, δ^+ is a phase corresponding to $j=l+\frac{1}{2}$, and δ^- corresponds to $j=l-\frac{1}{2}$. For the zero spin-orbit interaction, $\delta^+=\delta^-$ and $B=0$, i.e., the value of B determines the discussed relativistic effects.

The cross section for polarized electron scattering is (see, e.g., Ref. [7])

$$\frac{d\sigma}{d\Omega} = |A|^2 + |B|^2 + 2\,\mathrm{Re}(AB^*)\boldsymbol{\nu}\cdot\mathbf{P} , \tag{2}$$

where $\mathbf{P}=2\langle\mathbf{s}\rangle$ is an initial polarization of the electron

beam. For an unpolarized initial state ($P=0$) there is polarization of scattered electrons (see Ref. [7]):

$$\mathbf{P}'=\frac{2\,\mathrm{Re}(AB^*)}{|A|^2+|B|^2}\boldsymbol{\nu}\ . \tag{3}$$

It follows from Eqs. (1)–(3) that polarization effects are large near the resonance with fixed j, where a difference between δ_+ and δ_- is large ($\sim\pi/2$). However, it is easy to verify that in the one-wave approximation (e.g., for only one resonance term in A and B) there are no polarization effects [$B\sim iA$, $\mathrm{Re}(AB^*)=0$]. In practice, it does not suppress the effect substantially. Thus, for very small energy the s wave dominates. Near p resonance, the p wave dominates. Therefore, in the case of low-energy p resonance, there always must be a point where s-wave and p-wave amplitudes are comparable. Their interference produces the discussed effects.

It is easy to carry out a simple estimate of the effect in this case. For very small electron energy the nonresonance part of the amplitude A is equal to (see, e.g., Ref. [8]):

$$A_n=-\lambda-\frac{\pi\alpha}{2}k\sin(\theta/2)\ . \tag{4}$$

Here λ is the scattering length and α is the atomic polarizability (in Ra, $\lambda=-9.4$, $\alpha=250$; we use atomic units). The second term arises due to the long-range polarization potential:

$$V(r)\to-\frac{\alpha}{r^4}\ . \tag{5}$$

The contribution of $P_{3/2}$ resonance is

$$\begin{aligned}
A_p&=-\frac{1}{k}\frac{\Gamma(\kappa)}{E-E_p+i\Gamma(k)/2}\cos\theta\ ,\\
B_p&=\frac{1}{2i\kappa}\frac{\Gamma(\kappa)}{E-E_p+i\Gamma(k)/2}\sin\theta\ ,\\
\Gamma(k)&=\Gamma(k_p)\cdot(k/k_p)^3\ ,\\
A&\approx A_n+A_p\ ,\quad B\approx B_p\ .
\end{aligned} \tag{6}$$

Here we have taken into account that the nonresonance phase in the p wave is small. In atomic units $\kappa=\sqrt{E}$, E_p is the energy of $P_{3/2}$ resonance.

The maximum effect is at $A=\pm B$ [see Eq. (3)]. There are two energy points (before and after resonance) where $|B|=|A_n|$ (it is possible to choose A_p in an optimal way by varying the angle θ, in particular, for $\theta=\pi/2$, $A_p=0$). However, there is a question about the relative phase of A and B. In the resonance, $\arg(B)\approx\arg(A_n)\approx 0$. Far from resonance there is no phase equality and it could suppress the effect. However, in the region above p resonance the phase of B changes very slowly due to a rapid increase of Γ with energy [see Eq. (6)]. Therefore in the large energy interval ($E\gtrsim E_p$), at the angle $\theta\sim\pi/2$ the polarization P' reaches a value close to unity.

Note that the same formulas describe the effect for $E_p<0$ (bound level close to continuum). The parameter Γ in this case is defined only for $E>0>E_p$ ($\Gamma\sim k^3$). It depends analytically on potential parameters at fixed E.

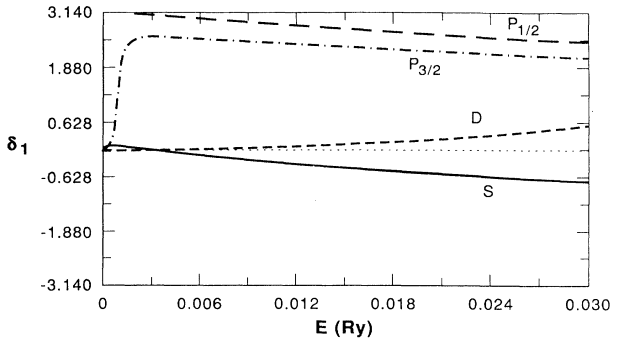

FIG. 1. Dependence of s, $p_{1/2}$, $p_{3/2}$, and d phases on energy for Ra.

Therefore, in the Ra case for $E\sim 0.01$ Ry polarization does not change essentially if the level E_p crosses the boundary of the continuous spectrum under variation of potential parameters (remember that $|E_p|\sim 0.001$ Ry).

For comparison, it is also useful to estimate this effect in the nonresonance regions. For small k, $\delta_1\ll\delta_0\ll 1$. In this case we have the simple formulas (first order in δ_1) and second in order δ_0)

$$P'\approx 2\,\mathrm{Re}(-i\kappa B)\approx 2(\delta_1^+-\delta_1^-)\sin\theta\ . \tag{7}$$

Far from resonances $\delta_1^+-\delta_1^-\sim Z^2\alpha^2\delta_1$. [It is easy to verify this estimate using the perturbation theory formula for δ or using a two-resonance approximation, see Eq. (6), and a fine-structure estimate $E_+-E_-\sim Z^2\alpha^2 E$, $\delta_1\sim k^3R^3$, where R is atomic size ($R\sim a_B$, a_B is the Bohr radius).] Therefore, far from resonances at $v\ll v_{\mathrm{at}}$ ($v_{\mathrm{at}}\sim\alpha c$ is the velocity of external atomic electrons)

$$P'\sim Z^2\alpha^2k^3R^3\sim Z^2\left[\frac{v}{c}\right]^2\cdot\left[\frac{v}{v_{\mathrm{at}}}\right]\ . \tag{8}$$

Note that there is a large enhancement factor Z^2 here which can be explained by the singularity of spin-orbit interaction ($H_{ls}\sim 1/r^3$). The main contribution to the matrix element of H_{ls} is given by small distances $r\sim a_B/Z$. In this region $v^2/c^2\sim Z^2\alpha^2$, i.e., relativistic effects are

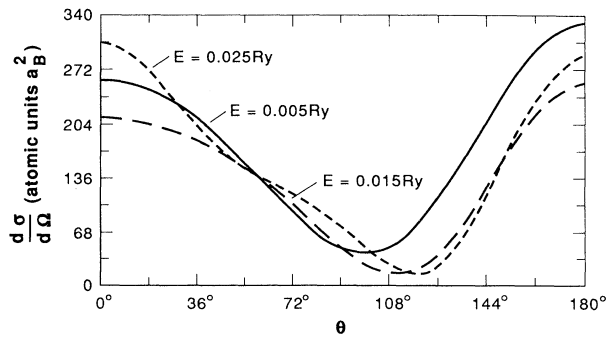

FIG. 2. Differential cross section in atomic units (a_B^2) for Ra (at electron energy 0.005, 0.015, and 0.025 Ry).

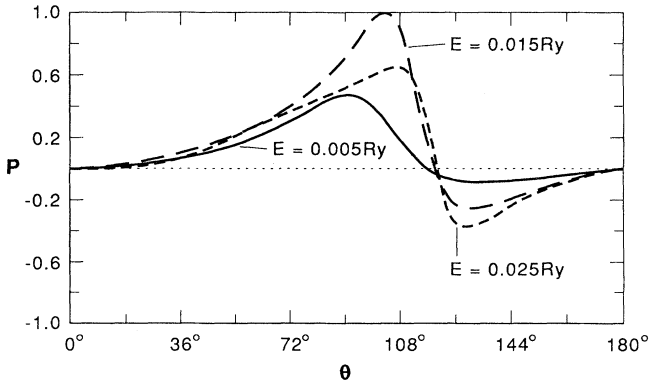

FIG. 3. Polarization of scattered electrons (at $E=0.005$, 0.015, and 0.025 Ry) for Ra.

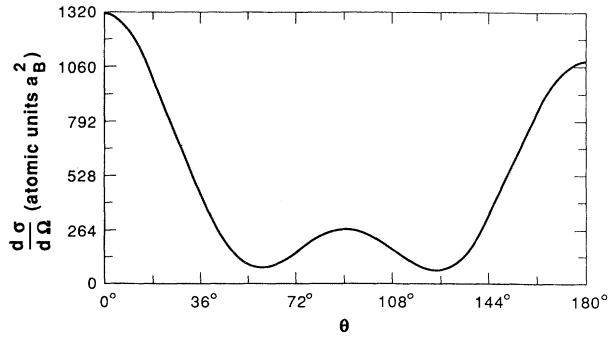

FIG. 5. Differential cross section in atomic units for Ba in the d resonance (energy between $d_{3/2}$ and $d_{5/2}$).

enhanced by Z^2 times. Nevertheless, far from resonance P' is not larger than a few percent at $E \lesssim 1$ eV.

Formulas (1)–(6) could be used only for qualitative consideration of the effect [the low-energy approximation (4) is not good enough due to the closeness of the Ramsauer minimum, and resonance approximation (6) is not good far from resonance]. Therefore, we have carried out accurate numerical calculations of s-, p-, and d-wave phases [other phases can be estimated using formula (4), see Ref. [8]; they are very small]. This calculation was carried out by the Hartree-Fock method taking into account correlation (polarization) effects. In our calculation of the bound level $7P_{1/2}$ and resonance $7P_{3/2}$ of the Ra negative ion,[4] the nonlocal correlation potential [integration operator $\int \Sigma(r_2,r_1)dr_2$] was found using many-body perturbation theory in residual electron-electron interaction (see, e.g., Ref. [9]). The positions of the negative-ion levels are very sensitive to the accuracy of the calculation. But if we know the positions of the levels we do not need extremely high accuracy because the amplitudes near the resonance are described reasonably well by general formulas. Therefore, in the present work we use a simple local fit of the correlation potential that reproduces correctly the positions of the levels:

$$V(r)=-\frac{\alpha}{r^4+a^4}\ . \tag{9}$$

Parameter α in potentials for the p wave and s wave has been found from the asymptotic form of the calculated nonlocal correlation potential (for Ra, $\alpha=206$). Parameter $a=7.1$ was fitted to reproduce correctly the $P_{1/2}$ and $P_{3/2}$ levels ($E_{1/2}=-0.0109$ Ry, $E_{3/2}\approx 0.001$ Ry).

Calculations [6] that predicted low-lying d resonance in barium ($E_d=0.0162$ Ry) have been communicated to us by Gribakin. He supposed that a similar resonance should be present in radium too. Our calculation confirms this supposition. We have found that at the energy $E_d=0.044$ Ry there is resonance with the width $\Gamma(E_d)=0.03$ Ry [for the d wave we chose the following parameters of potential (9): $\alpha=260$ and $a=7.1$]. We also calculated the fine structure of the Ba d resonance: $E_{d_{5/2}}-E_{d_{3/2}}\approx 0.001\,15$ Ry. According to our calculations, the width of this resonance $\Gamma(E_d)\approx 0.0025$ Ry is in agreement with that in Ref. [6].

Calculated phases, differential cross sections, and polarizations P' are presented in Figs. 1–6. In radium, maximal electron polarization is about unity in the region above the $P_{3/2}$ resonance at 0.01 Ry $\lesssim E \lesssim 0.02$ Ry.

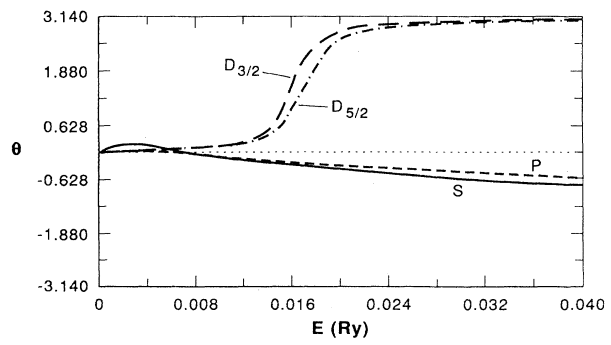

FIG. 4. Dependence of s, p, $d_{3/2}$, and $d_{5/2}$ phases on energy for Ba.

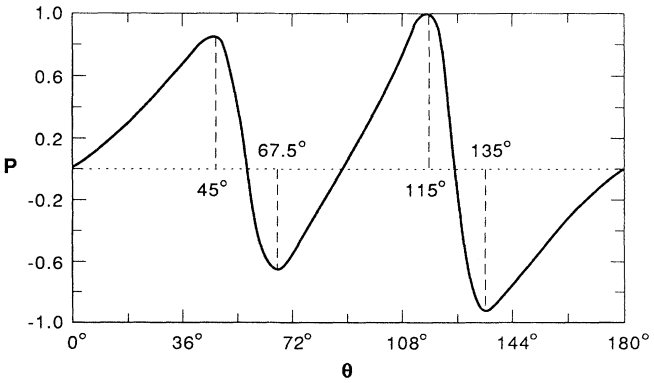

FIG. 6. Polarization of scattered electrons near d resonance for Ba (energy between $d_{3/2}$ and $d_{5/2}$).

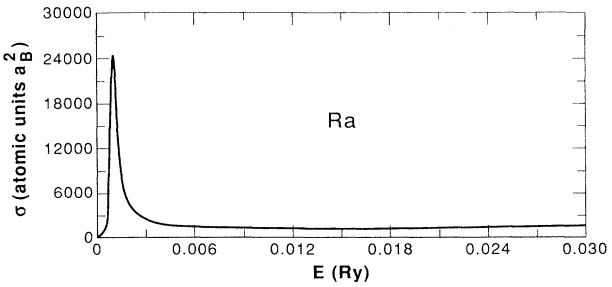

FIG. 7. Total cross section for Ra as a function of energy.

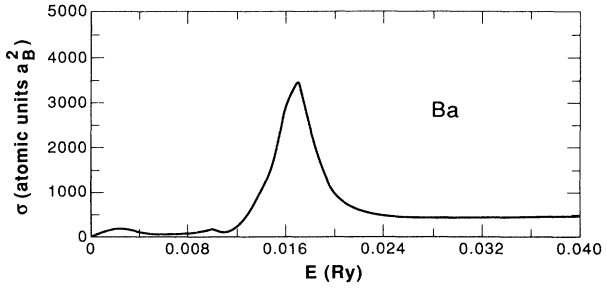

FIG. 8. Total cross section for Ba as a function of energy.

Note that due to the slow energy dependence in this region there is no substantial suppression of the effect if the experimental energy resolution is not worse that 0.01 Ry. In barium, polarization is large only near the d-wave resonance (it does not change essentially within the width of the resonance).

Both Ra and Ba cross sections have Ramsauer minima [zero of s wave amplitude—see Eq. (4)]. The energy dependence of phases clearly shows $P_{3/2}$ resonance in Ra and $d_{3/2}$, $d_{5/2}$ resonances in Ba. The phase in Ra is fitted by the width $\Gamma(E)=(E/0.001\ \mathrm{Ry})^{3/2}0.5\times10^{-3}$ Ry. The angular maximum of polarization in Ra is close to the point where the spin-independent resonance amplitude is zero since it stands in the denominator of formula (4) for P' [for Ra, $A_p=0$ at $\theta=\pi/2$—see Eq. (6)]. This point is close to the minimum of the differential cross section. For Ba, the angular dependence of the polarization is more complicated since here both spin-dependent and spin-independent resonance amplitudes have zeros inside the interval $0<\theta<\pi$.

It is interesting that in radium the electron cross section is very large at small energies ($\sigma>10^{11}$ b at $E\sim10^{-2}$ eV) due to low-lying $P_{3/2}$ resonance. Graphs of total cross sections as a function of energy for Ra and Ba are presented in Figs. 7 and 8.

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