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Finite-temperature effects on the energy levels of hydrogenlike atoms

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It is shown that level-dependent finite-temperature effects on hydrogenlike atoms are of the order $\alpha^3(T/m)^2$.

Recently it has been shown[1,2] that finite-temperature effects on atomic energy levels are level independent up to the order α. The purpose of this Comment is to show that level-dependent temperature effects on hydrogenlike atoms are of the order $\alpha^3(T/m)^2$, and are indeed too small to be observable up to the temperature at which the atoms remain stable in their bound states.

The dominant thermal contribution to the atomic energy levels comes from the temperature-dependent parts of the electron self-energy $\Sigma(p)$ and the vertex function $\Gamma^\mu(p,p')$, which can be written as

$$\Sigma(p)=\Sigma_0(p)+\Sigma_\beta(p) \;, \qquad \Gamma^\mu(p,p')=\Gamma^\mu_0(p,p')+\Gamma^\mu_\beta(p,p') \;, \tag{1}$$

where the subscripts 0 and β denote the temperature-independent and the temperature-dependent parts, respectively. For the problem at hand, we need the low-temperature approximation for $\Sigma_\beta(p)$ and $\Gamma^\mu_\beta(p,p')$. At low temperature ($\beta m = m/T \gg 1$), the temperature-dependent part of the self-energy is given by[3,4]

$$\Sigma_\beta(p)=A\gamma\cdot p+B\gamma^0p^0 \;, \tag{2}$$

where

$$A=\frac{e^2}{36\beta^2}\frac{1}{{p_0}^2}\left(1+\frac{\mathbf{p}^2}{{p_0}^2}\right) \;,$$

and

$$B=\frac{e^2}{18\beta^2}\frac{1}{{p_0}^2} \;.$$

The temperature-dependent part of the vertex function at low temperature is given by[3,4]

$$\Gamma^\mu_\beta(p,p')=\frac{e^2}{36\beta^2}\frac{1}{p_0p_0'}\left(\frac{2m^2}{p_0p_0'}-1\right)\gamma^\mu+\frac{e^2}{18\beta^2}\frac{1}{p_0p_0'}\gamma^0\delta^{\mu 0} -\frac{i}{2m}\frac{e^2}{18\beta^2}\frac{m^2}{(p_0p_0')^2}\sigma^{\mu\nu}q_\nu \;, \tag{3}$$

where $q_\mu=p_\mu'-p_\mu$. For atomic systems the kinetic energy of electrons is much smaller than the rest mass, and A and B can be approximated to be

$$A=\frac{B}{2}=\frac{e^2}{36\beta^2m^2} \;, \tag{4}$$

and the vertex function is approximated to be

$$\Gamma^\mu_\beta=A\gamma^\mu+B\gamma^0\delta^{\mu0}-\frac{i}{2m}B\sigma^{\mu\nu}q_\nu \;. \tag{5}$$

At finite temperature the wave function of a free electron satisfies the modified Dirac equation

$$(\gamma\cdot p-m-\Sigma_\beta)\psi=0$$

or

$$[\gamma^0p^0(1-A-B)-\boldsymbol{\gamma}\cdot\mathbf{p}(1-A)-m]\psi=0 \;, \tag{6}$$

where m denotes the renormalized electron mass.[5] This suggests that one can compute the finite-temperature effects on atomic level shifts by solving the modified Dirac equation in the Coulomb potential,

$$[\boldsymbol{\alpha}\cdot(1-A)\mathbf{p}+\beta m-e\gamma^0\not{A}]\psi=E(1-A-B)\psi \;, \tag{7}$$

where $\boldsymbol{\alpha}=\gamma^0\boldsymbol{\gamma}$, $\beta=\gamma^0$, and the potential is given by

$$e\gamma^0\not{A}=\frac{Z\alpha}{r}(1+\gamma^0\Gamma^0_\beta) \;,$$

including the thermal effect.[6] One can easily show[6] that the contribution of the last term of Eq. (5) to the energy eigenvalues starts from the terms of order $(Z\alpha)^4$. Substituting (5) into (7), one obtains

$$\left[\boldsymbol{\alpha}\cdot(1-A)\mathbf{p}+\beta m-\frac{z\alpha}{r}(1+3A)\right]\psi=E(1-A-B)\psi \tag{8}$$

for the energy-eigenvalue equation for hydrogenlike atoms. Since A and B are constants, given by Eq. (4), one can easily solve Eq. (8) to obtain energy eigenvalues. If we set

$$m'=\frac{m}{1-A},\quad Z'=Z\frac{(1+3A)}{1-A},$$

and

$$E'=E\frac{1-A-B}{1-A} \;,$$

Eq. (8) becomes

$$\left[\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m'-\frac{Z'\alpha}{r}\right]\psi=E'\psi \;, \tag{9}$$

which has the same form as the eigenvalue equation for hydrogenlike atoms at zero temperature. Thus, we can read off the energy eigenvalue from the well-known result,[6]

$$E_{nj}=m_\beta\Big/\left[1+\frac{Z\alpha^2(1+3A)^2}{(1-A)^2}\frac{1}{(n-\delta_j)^2}\right]^{1/2} \;, \tag{10}$$

where $m_\beta=m/(1-A-B)$ is the temperature-dependent electron mass,[3,4] and

$$\delta_j=j+\tfrac{1}{2}-[(j+\tfrac{1}{2})^2-Z^2\alpha^2(1-A)^2(1+3A)^2]^{1/2} \;.$$

Expanding (10) in α, we obtain

$$E_{nj}=E_{nj}^0+3mA-\tfrac{11}{2}mA\frac{Z^2\alpha^2}{n^2}+O(\alpha^4)$$

$$=E_{nj}^0+\frac{\pi a}{3\beta^2 m}-\frac{11\pi\alpha}{18\beta^2 m}\frac{Z^2\alpha^2}{n^2}+O(\alpha^4)\ , \tag{11}$$

where E_{nj}^0 is the energy eigenvalue at zero temperature. The second term of (11) is the level-independent energy shift, which comes from the change in the electron mass at finite temperature.[3–5] Although this term has the same magnitude as the result of Ref. 2, it has quite different origin. In Refs. 1 and 2, the temperature effects are computed by nonrelativistic perturbation theory using the interaction Hamiltonian

$$H_{\text{int}}=-\frac{e}{m}\mathbf{A}\cdot\mathbf{P}+\frac{e^2}{2m}A^2\ .$$

In Ref. 2, however, the effect of only the first term is computed for the Lamb shift. As has been shown in Ref. 1, the order-α contribution of the second term exactly cancels that of the first term. Therefore, there is no temperature-dependent contribution of order α from the above interaction Hamiltonian.

Now one has to ask whether the third term of (11) is reliable. In our calculation the approximation in Eqs. (10) and (11) solely comes from the approximate calculation of $\Sigma(p)$ and Γ^μ, which is done at a one-loop level. Therefore, it appears that the third term of (11), which is of order α^3, is not reliable. The reason is that if we compute Σ_β up to α^2 order the dominant contribution of the α^2 term to E_{nj} could be of order α^2. But this term, which comes from the temperature dependence of electron mass, would be level independent. The level-dependent contribution of α^2 terms in Σ_β starts from the term of order α^4. If we consider the energy difference between levels, therefore,

$$E_{nj}-E_{n'j'}=(E_{nj}^0-E_{n'j'}^0)-\frac{11m}{18}\frac{Z^2\alpha^3}{\beta^2 m^2}\left(\frac{1}{n^2}-\frac{1}{n'^2}\right)+O(\alpha^4)\ , \tag{12}$$

the $\alpha^3(T/m)^2$ term is reliable. Thus, the level-dependent finite-temperature effects on the hydrogenlike atoms are given by (12). When the temperature is 1 eV, the temperature-dependent term of (12) is about 10^{-10} times the fine-structure splitting, and therefore is too small to be observable.

We finally comment on the temperature effect on the hyperfine structure, which arises from the interaction between the magnetic moment of the nucleus and the magnetic moment of the electron. Therefore, the hyperfine splitting is proportional to the magnetic dipole moment of electron. The electron magnetic moment in the low-temperature limit is given by[3,4]

$$\boldsymbol{\mu}=\frac{e}{2m_\beta}\boldsymbol{\sigma}\left(1+\frac{\alpha}{2\pi}-\frac{2\pi\alpha}{9m^2\beta^2}\right)\ .$$

Therefore, the finite-temperature effect on the magnetic moment is about 10^{-11} percent at $T=1$ eV, and similarly for the hyperfine splitting.

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