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Recoil in electron-atom scattering

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The attractive interaction between an atom and an electron or positron is described as a complex single-particle self-energy in which the effects of recoil and finite velocity are treated exactly. In addition to the well-known expansion for the potential in powers of the inverse separation distance $1/R$ with nonadiabatic corrections, we obtain a contribution due to the recoil of the electron as it exchanges virtual quanta with the atom.

The long-range attractive interaction between an electron and an atom or molecule has its origin in the polarization of the collective system by the approaching electron. For atoms or molecules without permanent dipole moments the force is entirely quantum mechanical in nature and is usually calculated in a development based on perturbation theory. The potential is determined as a power series in the inverse distance $1/R$ between the electron and the atom, the lowest-order term being $1/R^4$ and the next term is $1/R^6$ containing, in part, the nonadiabatic correction due to the inability of the atomic electron cloud to follow faithfully the motion of the electron.[1]

When a virtual quantum is exchanged both the atom and electron must recoil in order to conserve momentum. Even for the lightest atoms such as hydrogen or helium, the effect is negligibly small, but for the electron which has a very small mass, the recoil may cause measurable changes in the interaction. Motivation for this work comes partly from the analogous problem of the interaction of an electron with a solid surface. There, the effect of recoil is to modify strongly the classical $1/z$ self-energy and to cause it to saturate to a constant near the surface,[2,3] and this saturation of the interaction potential has been recently verified experimentally.[4]

Here we consider the interaction between an electron and an atom in a self-consistent many-body formalism which includes full three-dimensional recoil. The interaction potential is expressed as a complex self-energy and the formalism can be extended to all orders of perturbation theory. The formalism separates clearly the effects of electron recoil and the nonadiabatic contributions originating in atomic excitation, the latter being due to the inability of the atomic electron cloud to follow the motion of the scattering electron. To lowest order in our formalism the nonadiabatic effects appear as the velocity-dependent $1/R^6$ correction to the leading $1/R^4$ term. The effect of recoil of the scattering electron is to reduce the strength of the interaction, and for small separation, it causes the $1/R^4$ interaction to saturate to a $1/R^2$ form.

As a starting point for the calculations, let us consider the interaction between an electron and a hydrogenlike atom. The generalization to more complicated systems will become apparent shortly when the results are expressed in terms of polarization operators. We will also, for simplicity, neglect exchange. We take the unperturbed system to be an isolated atom and an electron for which the corresponding eigenstate is the product of an atomic function and two momentum functions.

$$|j\rangle = u_f(\mathbf{r}_1)\frac{e^{i\mathbf{K}_0\cdot\mathbf{R}_1}}{\sqrt{\Omega}}\frac{e^{i\mathbf{P}_0\cdot\mathbf{R}_2}}{\sqrt{\Omega}} \quad , \tag{1}$$

with corresponding unperturbed energy

$$E_j = \epsilon_f + \frac{1}{2(m_1+1)}K_0^2 + \tfrac{1}{2}P_0^2 \quad , \tag{2}$$

where ϵ_f is the unperturbed atomic energy measured from the ground state and atomic units are used throughout. If $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ are the vectors from the origin to the atomic nucleus and to the scattering electron, respectively, and if $\boldsymbol{\rho}_1$ is the vector to the atomic electron, the perturbing potential is then

$$H' = -\frac{1}{|\boldsymbol{\tau}_1-\boldsymbol{\tau}_2|} + \frac{1}{|\boldsymbol{\rho}_1-\boldsymbol{\tau}_2|} \quad . \tag{3}$$

The first nonvanishing contribution to the energy shift comes from second order in perturbation theory:

$$\Delta E = \sum_j |\langle j|H'|i\rangle|^2/(E_i - E_j) \quad . \tag{4}$$

This energy shift is expressed in terms of the spatial integral over an interaction self-energy

$$\Delta E = \int d\mathbf{R}\langle\mathbf{0}|\mathbf{R}\rangle\Sigma(\mathbf{R})\langle\mathbf{R}|\mathbf{0}\rangle \quad , \tag{5}$$

where $\langle\mathbf{R}|\mathbf{0}\rangle$ is the translational eigenstate of the electron-atom system in the center-of-mass reference frame. The self-energy $\Sigma(\mathbf{R})$ can be systematically generalized to all orders in perturbation theory,[3,5] although in the present case we stop with the second-order term which leads to

$$\Sigma(\mathbf{R}) = \sum_j \frac{\langle\mathbf{K}|\mathbf{R}\rangle}{\langle\mathbf{0}|\mathbf{R}\rangle}\frac{\langle i|H'|j\rangle\langle f,\mathbf{K}|H'|\mathbf{0},0\rangle}{E_i - E_j} \quad . \tag{6}$$

We evaluate the matrix elements by expanding to first order in the atomic operator $\mathbf{r}_1 = \boldsymbol{\rho}_1 - \boldsymbol{\tau}_1$ and obtain the expression

$$\Sigma(\mathbf{R}) = -(1/4\pi^4)\sum_f \int (d\mathbf{K}/K^2) e^{i\mathbf{K}\cdot\mathbf{R}} \mathbf{K}\cdot\langle f|\mathbf{r}_1|i\rangle \times \int (d\mathbf{Q}/Q^2) e^{i\mathbf{Q}\cdot\mathbf{R}} \mathbf{Q}\cdot\langle f|\mathbf{r}_1|i\rangle \left[-\epsilon_f + \frac{1}{2(m_1+1)}[K_i^2-(\mathbf{K}_i+\mathbf{K})^2] + \tfrac{1}{2}[P_i^2-(\mathbf{P}_i+\mathbf{K})^2]\right]^{-1} . \quad (7)$$

Clearly in the denominator, the recoil term involving m_1, the mass of the atom, is small with respect to the corresponding term for the electron. If we also neglect the terms in the velocity and recoil of the electron and approximate the denominator by the atomic energy exchange ϵ_f, we recover the familiar $1/R^4$ potential

$$\Sigma(R) = -\frac{1}{R^4}\sum_f \frac{|\langle f|z|i\rangle|^2}{\epsilon_f} , \quad (8)$$

where z is the polarization operator parallel to the direction of $\mathbf{R}$. (We have also made the tacit assumption that the atomic energies are independent of azimuthal quantum number.) However, because of the light mass of the electron, the neglect of its recoil in the denominator is valid only for asymptotically large values of R. This is most readily seen for the case in which the relative velocity of the system is small, i.e., $\mathbf{P}_i \to 0$. The self-energy can then be obtained in closed form and is

$$\Sigma(R) = -\frac{1}{R^2}\sum_f \frac{|\langle f|z|i\rangle|^2}{\epsilon_f}\left[\frac{1}{R^2} - \left(\frac{1}{R^2}+\frac{a}{R}\right)e^{-aR}\right] , \quad (9)$$

where

$$a^2 = \frac{2(m_1+1)}{m_1+2}\epsilon_f \approx 2\epsilon_f . \quad (10)$$

This clearly reduces to Eq. (8) as $aR \to \infty$. An interesting case which illustrates that recoil indeed causes a saturation of the self-energy is the limit $aR \to 0$ where we recover

$$\Sigma(R) \underset{aR\to 0}{\to} -\frac{1}{2R^2}\langle i|z^2|i\rangle \frac{2(m_1+1)}{m_1+2} \approx -\langle i|z^2|i\rangle/R^2 . \quad (11)$$

The effect of recoil as the system exchanges virtual quanta is to weaken or saturate the interaction to a $1/R^2$ form. The range of the effect is given by the parameter $\mathbf{a} \simeq \sqrt{2\epsilon_f}$, which can be several atomic units, as noted by estimating ϵ_f to be a typical atomic excitation energy. Although the limit of zero separation distance ($R = 0$) is certainly beyond the range of validity of the approximations used to develop Eq. (7) the expression shown in Eq. (11) is more than a mere academic exercise. It demonstrates that the inclusion of electronic recoil weakens the leading $1/R^4$ term (and will also act similarly on the higher-order terms as well) at separation distances where the effect can become noticeable. Furthermore, this effect is not expressible in terms of a power series in $1/R$.

If we now allow the system to have a finite relative velocity, Eq. (7) can again be readily evaluated in terms of complete and incomplete auxiliary functions to the sine integral.[6] When there is a finite relative velocity the self-energy becomes complex and the imaginary part can be further divided into conservative and nonconservative parts. The nonconservative part is finite only if the system has sufficient initial energy to create a real atomic excitation, i.e., if the energy is above the inelastic threshold. The asymptotic correction to the real part is velocity dependent and develops in a power series in $1/R^2$. Thus the lowest correction is of the same order in $1/R$ as the next term coming from the multipole expansion of the potential of Eq. (3). Restricting the development to the dipolar terms, the real part of the asymptotic form of Eq. (7) becomes

$$\mathrm{Re}\,\Sigma(R) = -\frac{1}{R^4}\sum_f \frac{|\langle f|z|i\rangle|^2}{\epsilon_f}\left(1 - \frac{6P_i^2}{R^2\epsilon_f^2} + \cdots\right) . \quad (12)$$

The correction term, proportional to the initial energy, is recognized as the first velocity-dependent nonadiabatic contribution.[1] The leading term in the low-energy conservative imaginary part is proportional to the electron velocity and is given by

$$\mathrm{Im}\,\Sigma(R) = \frac{2P_i}{R^5}\sum_f \frac{|\langle f|z|i\rangle|^2}{\epsilon_f^2} + \cdots . \quad (13)$$

We should emphasize the importance of keeping full three-dimensional recoil in these calculations. It is considerably simpler to neglect the longitudinal component and retain only the two-dimensional recoil in the directions transverse to the axis of relative motion. If this is done, one obtains erroneous recoil corrections to the $1/R^4$ potential which can be expanded in $1/R$ in the asymptotic region. However, the correct three-dimensional treatment gives the much faster exponential decay of recoil effects as illustrated in the case of Eq. (9).

We have shown in this article that the many-body interaction between an electron and an atom can be represented by a complex effective self-energy. This self-energy distinguishes very naturally between the effects due to recoil of the electron and the nonadiabatic contributions from the atomic electronic cloud. Although the effect of recoil decays exponentially with separation, we have shown that it can contribute to a significant weakening of the leading $1/R^4$ term in the potential and it will have a similar effect on the higher-order terms. Thus, considerations of recoil saturation of the potential can be important in the finite-range problem of electron-atom interactions. We note also that the expressions derived in this paper apply equally well to the low-energy interaction of a positron with an atom.

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