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Comments upon bound-state charges in electric fields

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Abstract

A short review is done of the effect electric fields may have upon bound-state electrical charges.

Introduction. A non-relativistic charge q with mass m in an electric field $\mathbf{E}$ and potential $V(\mathbf{r})$ is governed by the dipole hamiltonian

$$H_d = \frac{1}{2m}p^2 - q\mathbf{E}\mathbf{r} + V(\mathbf{r}) \tag{1}$$

or the standard non-relativistic hamiltonian

$$H_s = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + V(\mathbf{r}) \quad , \tag{2}$$

where $\mathbf{p}$ is momentum and $\mathbf{A}$ is the vector potential; for external fields we may take a zero scalar potential, $div\mathbf{A} = 0$ and $\mathbf{E} = -(1/c)\partial\mathbf{A}/\partial t$. We limit ourselves to static fields or to a radiation field of the form $\mathbf{A} = \mathbf{A}_0\cos(\omega t - \mathbf{kr})$, which, for non-relativistic charges, may be approximated by $\mathbf{A} = \mathbf{A}_0\cos\omega t$, since the variations of the spatial phase $kr = \omega r/c$ are much smaller than those of the temporal phase ωt; ω is the frequency, $\mathbf{k}$ is the wavevector and c denotes the speed of light in vacuum; the non-relativistic approximation is ensured by $qA_0/mc^2 \ll 1$.

We note that $\mathbf{p} = m\mathbf{v}$ in equation (1) and $\mathbf{p} = m\mathbf{v} + q\mathbf{A}/c$ in equation (2); the former is the mechanical momentum, the latter includes the electromagnetic momentum. Consequently, in equation (2) the charge is immersed in the electromagnetic field, in equation (1) the electric field may be localized and for some time disentangled from the charge. The electric field in equation (1) may be unbounded in space. In general, motion in limited space regions requires special considerations.

The two hamiltonians given by equations (1) and (2) are related by the unitary (canonical) Goeppert-Mayer transform;[1] the initial moment of time is important in this equivalence. There is a further canonical transform, called the Kramers-Henneberger transform,[2]-[5] which takes the hamiltonian H_s into $p^2/2m + \widetilde{V}(\mathbf{r})$, where $\widetilde{V}(\mathbf{r}) = V(\mathbf{r} + \boldsymbol{\zeta})$ is the radiation-dressed potential; $\boldsymbol{\zeta} = q\mathbf{E}t^2/2m$ for a static field and $\boldsymbol{\zeta} = -q\mathbf{E}_0/m\omega^2$ for an oscillating field $\mathbf{E} = \mathbf{E}_0\sin\omega t$. The former transform highlights the gauge character of the electromagnetic field, while the latter transform includes, partly, the motion of the charge in the field.

Static fields. Historically, the problem of bound charges in electric field appeared first for the hydrogen atom, and light atoms, in low, static electric fields. A high electric field among the static

electric fields available in laboratory is typically $10^{-1} statvolt/cm$ $(3kV/m)$; its mechanical work qEa upon an electron in atom is extremely small in comparison with the atomic energies; here $q = -4.8 \times 10^{-10} statcoulomb$ is the electron charge, E is the magnitude of the electric field and $a = 10^{-8}$ is the atom radius. Consequently, the field polarizes the atom, usually in the second-order of the perturbation theory (except for hydrogen, where the polarization occurs in the first order). The polarization is computed by time-independent perturbation theory, conveniently using the hamiltonian given by equation (1). The use of the perturbation theory presumes an adiabatic application of the field, which preserves the stationary states, causing at most linear combinations of them. And, of course, the interaction strength should be small, such that the energy levels are little chaged. Adiabatic introduction of the interaction is only possible for weak interaction, as required by the perturbation theory. The adiabatic application of weak static electric fields is achievable by experimental means (*e.g.*, between the plates of a capacitor slowly charging). Moreover, another problem may appear: the interaction energy $-q\mathbf{Er}$, where $\mathbf{r}$ is the charge position, exhibits a particularity: it is unbounded, which makes questionable the application of the perturbation theory; the hydrogen atom and the light atoms are "spatially extended", since the charges interact by long-range Coulomb potentials. This means, in fact, that the charge states are metastable, and the charge may go out from the atom under the action of the electric field; this is the (static) field-assisted atom ionization, treated in classical works.[5]-[8] We note that the field introduces a potential barrier (besides the "ion" potential barrier), which may be tunneled by the electron. The tunneling through the barrier proceeds by in and out propagating wavefunctions; this again presuposes an adiabatic application of the field. The adiabatic hypothesis means that the rate of introducing the field is slower than time $\hbar/\Delta\mathcal{E}$, where $\Delta\mathcal{E}$ is the mean inter-spacing of the energy levels, such that the interaction does not produce transitions between the states.[9] The ionization rate is proportional to $e^{-cons/E}$, for small E; it is very small.

This is valid for the hydrogen atom, and, to some extent, for light atoms; these bound assemblies have well-separated energy levels and long-range Coulomb interaction. Heavy atoms and, in general, many-particle assemblies require a special discussion. Bound many-particle assemblies have at least two particularities. First, their single-particle levels are rather dense, almost, in some cases, they form a continuum of relevant single-particle states. It is convenient to work with single-particle states, as generated by a mean-field potential, as they govern the single-particle class of elementary excitations in these assemblies, the only relevant states for our problem. A convenient picture for heavy atoms is provided by the Thomas-Fermi model. In this circumstance, any perturbation, of a reasonably small magnitude, is rather rapidly accommodated as a valid stationary state, such that the effect of the electric field is rather fastly incorporated in the stationary states; accordingly, the electric field produces polarization. In a heavy atom and neutral many-charge bound states the Coulomb interaction is screened to short-range forces, such that these assemblies may be viewed as "spatially finite"; consequently, the unboundedness of the interaction potential does not matter too much. This "finiteness" of these assemblies is their second particularity. Tunneling through the potential barrier of the electric field may appear, in a field-assisted ionization (decay, charge emission, dissociation, fragmentation). Some bound many-particle assemblies may exhibit spontaneous decay, like the nuclear alpha-particle decay or proton disintegration (emission). It is worth stressing the fact that the inclusion of the field in the energy levels may be done by perturbation theory.

The above considerations apply, in general, to heavy atoms and bound many-particle assemblies like molecules and atomic clusters, or atomic nuclei. Small molecules may be viewed as a particular case of heavy atoms, large molecules and atomic clusters look more close to solids, with extended electron states and (bounding, screened) short-range inter-nuclear potentials; spontaneous charge emission from these bound states, both electronic and ionic charges, is little knwon, ion fragmen-

tation has an extremely small rate. Low static electric fields produce mainly polarization of these assemblies. It is worth noting that the adiabatic hypothesis holds for low fields applied to these assemblies.

Oscillating fields. The advent of high-power lasers brings three important new circumstances in this problem. First, the field is oscillating,, second, it may be high and, thirdly, it is applied suddenly. The experiments with laser beams proceed by placing a collection of bound charges (atoms, molecules, atomic clusters, atomic nuclei, ...) in the laser focus and firing up the laser pulse upon that collection of particles. Initially, the laser beams were not focused, they were lasting long, their succession was slow and the field intensity was low, in comparison with the field frequency. In this case, the charges may be viewed as fully immersed in the radiation field; the standard non-relativistic hamiltonian given by equation (2) may be used. The particles are (dynamically) polarized, may be ionized, and the radiation may affect the scattering cross-section of collisions, by absorbing and emitting multiple photons; this later process is the well-known Kroll-Watson effect. The calculations are done by time-dependent perturbation-theoretical methods, which lead to transitions among non-stationary states, or tunneling through classically unavailable states, as in the imaginary-time tunneling method; the ionization rate is of the same form $\sim e^{-const/E_0}$ as for static fields; the underlying presuposition is the adiabatic introduction of the (weak) interaction.[10]-[14]

Nowadays, the laser beams are focused; consequently, the particles may collide upon the laser focus, exchanging multiple photons; this is a new scattering process; the dipole hamiltonian given by equation (1) is suitable for this problem.[15] Laser beams introduce an important new feature: the interaction is applied in this case suddenly. Indeed, the time of setting up the interaction with the electromagnetic radiation upon a particle in a laser beam is of order a/c, where a is the dimension of the particle; for atoms $a/c \simeq 10^{-19}s$ ($a = 10^{-8}cm$), for atomic nuclei $a/c \simeq 10^{-24}s$ ($a = 10^{-13}cm$). These are very short times in comparison with any relevant time. They produce perturbation energies of the order $\hbar c/a \simeq 10keV$ for atoms and $\hbar c/a \simeq 10Mev$ for atomic nuclei; these energy uncertainties are much larger than mean inter-separation between energy levels, at least for the relevant single-particle states; the single-particle states are mixed up and, in fact, undefined, a circumstance which precludes any application of the perturbation theory at this stage.

In the subsequent duration of time, after the sudden application of the interaction, the assembly of charges may follow two distinct courses. If the field strength is small, the charges oscillate, emit higher-order harmonics of electromagnetic radiation, according to the variation of the dressed potential $\widetilde{V}(\mathbf{r}) = V(\mathbf{r}+\boldsymbol{\zeta})$ and may tunnel;[16]-[19] if there exists a spontaneous ionization (decay, charge emission), the decay rate is affected;[20] after each process of this type, the charges are re-arranged (reconfigured), the mean-field potential is modified, and the radiation-dressing process is resumed. These processes imply a gradual accommodation of the charges to the interaction, which becomes incorporated in the assembly's dynamics. The accommodation proceeds in a long time (since the perturbation is small), but more rapidly in many-particle assemblies, where the perturbation has the chance to be close to a quasi-stationary state. The calculations in this case proceed by slowly time-depending quasi-stationary states, linear combinations of these states, slow transition rates responsible of radiation emission, tunneling, etc, generally, perturbation-theoretical type of calculations. The adiabatic hypothesis holds in this regime.

If the field strength is large, the charges bound state is rapidly dissociated (ionized, fragmented);[21] the criterion of separation between the two regimes, of weak and high field intensity, is provided by comparing ζ with the dimension of the bound state; for a reasonably large ζ, the ejected charge is taken and removed by the electric fields of extraction, employed in this kind of experiments.

References

[1] M. Goeppert-Mayer, "Uber Elementarakte mit zwei Quantensprungen", Ann. Physik **401** 273-294 (1931).

[2] W. C. Henneberger, "Perturbation method for atoms in intense light beams", Phys. Rev. Lett. **21** 838-840 (1968).

[3] H. A. Kramers, "Non-relativistic quantum-electrodynamics and the correspondence principle", Solvay Congress 1948, in *Collected Scientific Papers*, North-Holland, Amsterdam (1956), p. 845.

[4] N. G. van Kampen, "Contribution to the quantum theory of light scattering", Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **26** (15) (1951).

[5] W. Pauli and M. Fierz, "Zur Theorie der Emission langwelliger Lichtquanten", Nuovo Cimento **15**, 167-188 (1938).

[6] J. R. Oppenheimer, "Three notes on the quantum theory of aperiodic effects", Phys. Rev. **13** 66-81 (1928).

[7] C. Lanczos, "Zur Intensitatsschwachung der Spektrallinien in hohen elektrischen Feldern", Z. Phys. **68** 204-232 91931).

[8] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, Springer, Berlin (1957).

[9] A. M. Dykhne, "Quantum transitions in the adiabatic approximation", Sov. Phys.-JETP **11** 411-415 (1960) (ZHETF **38** 570-578 (1960)).

[10] L. V. Keldysh, "Ionization in the field of a strong electromagnetic wave", Sov. Phys.-JETP **20** 1307-1314 (1965) (ZhETF **47** 1945-1957 (1965)).

[11] A. M. Perelomov, V. S. Popov and M. V. Terentiev, "Ionization of atoms in an alternating electric field", Sov. Phys.-JETP **23** 924-934 (1966) (ZhETF **50** 1393-1409 (1966)).

[12] A. I. Nikishov and V. I. Ritus, "Ionization of systems bound by short-range forces by the field of an electromagnetic wave", Sov. Phys.-JETP **23** 168-177 (1966) (ZhETF **50** 255-270 (1966)).

[13] M. V. Ammosov, N. B. Delone and V. P. Krainov, "Tunnel ionization of complex atoms and of atomic ions in an alternating electromagnetic field", Sov. Phys.-JETP **64** 1191-1194 (1986) (ZhETF **91** 2008-2013 (1986)).

[14] H. R. Reiss, "Complete Keldysh theory and its limiting cases", Phys. Rev. **A42** 1476-1486 (1990).

[15] M. Apostol, "Scattering of non-relativistic charged particles by electromagnetic radiation", Z. Naturforschung **A72** 1173-1177 (2017).

[16] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier and P. B. Corkum, "Theory of high-harmonics generation by low-frequency laser fields", Phys. Rev. **A49** 2117-2132 (1994).

[17] B. A. Zon, "Many-electron tunneling in atoms", J. Exp. Theor. Phys. **89** 219-222 (1999).

[18] B. A. Zon, "Tunneling ionization of atoms with excitation of the core", J. Exp. Theor. Phys. **91** 899-904 (2000).

[19] M. Gavrila, "Atomic stabilization in superintense laser fields", J. Phys. B: At. Mol. Opt. Phys. **35** R147-R193 (2002).

[20] M. Apostol, "Some comments on the bound-state disintegration by electromagnetic radiation (electromagnetic effect on the alpha decay)", J. Theor. Phys. **275** (2017).

[21] M. Apostol, "A note on the ionization of atoms by electromagnetic radiation", J. Theor. Phys. **273** (2017).

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