§17. Ions in Strong Electric Fields

More, R. (LLNL, USA)
Kato, T.

Strong electric fields can produce significant modification of atomic structure and cause field-induced ionization. Fields strong enough to have such dramatic effects can occur in close collisions of ions or can be produced by focused electromagnetic radiation.

For many-electron ions strong-field effects can be studied by two-dimensional Thomas-Fermi calculations including an applied electric field. A weak field induces a dipole polarization of the ion. At high field there is a nonlinear dipole moment and also a quadrupole moment. At strong enough field, there is field-induced ionization, and our calculations determine the limiting electric field and provide a model for charge-transfer between many-electron ions.

The Thomas-Fermi solution should exactly obey several mathematical conditions. First, when the applied field is zero the two-dimensional solution should reduce to the well-known spherical solution. Second, there is a theorem which describes screening of the applied electric field $E(\infty)$ by bound electrons,

$$Z\,\vec{E}(0) = Q\,\vec{E}(\infty) \qquad (1)$$

Q is the ion charge and Z is the nuclear charge; E(0) is the field acting on the nucleus. Eq. (1) holds independent of the field strength. Third, the Virial theorem gives:

$$2K + U_{en} + U_{ee} - U_{eF} = 0 \quad (2)$$

where K = total kinetic energy of the bound electrons, U_{en} = electron-nucleus interaction energy, U_{ee} = electron-electron interaction energy, and U_{eF} = interaction with the applied field. Next, there is an equation derived from the condition that the solution should describe the ion ground state in the field. This equation reads

$$\frac{5}{3}K + U_{en} + 2U_{ee} + U_{eF} = (Z-Q)\mu \qquad (3)$$

where μ is the electron chemical potential. Fifth, there is the Thomas-Fermi scaling law: the solution for nuclear charge Z, ion charge Q in a field E is related by a simple change of variables to the solution for a scaled ion of charges Z', Q' = (Q Z'/Z) in an electric field $E' = E\,(Z'/Z)^{5/3}$. Finally there are equations which give the energy changes in terms of the ion polarizability $\alpha(Z,Q)$:

$$\delta K = -\frac{3}{2}\alpha E^2 \qquad \delta U_{eF} = -\alpha E^2$$

$$\delta E_{tot} = -\frac{1}{2}\alpha E^2 \qquad (4)$$

These formulas apply for small E. In Thomas-Fermi theory, the polarizability α scales as Z^{-1}. These exact properties of the solution provide tests of a numerical calculation, alongside the usual test for convergence with zoning. According to these tests, our 2D calculations are accurate to about 1/2 %. The numerical calculations determine the field-induced ionization state $Q_{min}(Z, E)$ and nonlinear polarizability. Detailed results will be presented elsewhere.