Return answers to Johnson mailbox in Room 225 NSH before 10:30 AM, Dec 14, 2005.

1. (50%) The r.m.s. radius of an atom is $R_{\rm rms} = \sqrt{\langle \boldsymbol{R}^2 \rangle}$ where

$$\boldsymbol{R} = \sum_i \boldsymbol{r}_i.$$

   (a) Write out the expression for $\boldsymbol{R}^2$ in second quantized form. (Take care! This operator is a combination of one- and two-particle operators.)

   (b) Express each part of the $\boldsymbol{R}^2$ operator in normal order with respect to a closed core.

   (c) Write down explicit formulas for the first-order matrix element of $\langle v|\boldsymbol{R}^2|v\rangle$ in an atom with one valence electron. (Keep in mind the fact that $\boldsymbol{R}^2$ is an irreducible tensor operator of rank 0.)

   (d) Evaluate $R_{\rm rms}$ to first-order for the $2p$ state of Li using screened Coulomb wave functions for the core and valence electrons: $Z_{1s} = 3 - 5/16$ and $Z_{2p} = 1.25$.

2. (25%) Consider an atom with one valence electron that is described in lowest order by a local potential $U(r) \neq V_{\rm HF}$.

   (a) Write out the expressions for first- and second-order matrix elements $\langle \Psi_w|T|\Psi_v\rangle$ of the dipole transition operator $T(\omega)$, being careful to account for $\Delta = V_{\rm HF} - U$ and to include terms arising from the energy dependence of T.

   (b) Show that both first- and second-order matrix elements of T are gauge-independent.

3. (25%) In a classical picture, the valence electron in Li induces a dipole moment $\boldsymbol{p} = \alpha \boldsymbol{E}$ in the heliumlike core, where $\boldsymbol{E}$ is the electric field produced by the valence electron at the origin, and α is the core polarizability ($\alpha = 0.189 a_0^3$ for Li^+).

   (a) Show that the classical interaction energy of the valence electron with the induced dipole field is

$$\delta W = -\frac{e^2}{8\pi\epsilon_0}\frac{\alpha}{r^4}$$

(b) Determine numerically the energy correction $\langle v|\delta W|v\rangle$ for $3d$ and $4f$ states of Li using wave functions in a screened Coulomb potential ($Z_{1s} = 3 - 5/16$ and $Z_{3d,4f} = 1$). Compare your answers with the following results from second-order MBPT:

$$E^{(2)}_{3d} = -4.07 \times 10^{-5}\text{a.u.} \qquad E^{(2)}_{4f} = -2.93 \times 10^{-6}\text{a.u.}$$