

Answers to these problems will be collected in class on Sept. 21.

1. Prove that  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  commutes with the Dirac Hamiltonian.
2. Show that Eqs.(2.124-5) in the Lecture Notes reduce to Eqs.(2.135-6).
3. Thomas-Fermi Model Potential Example:
  - (a) Download and compile the routines `thomas.f` and `nrelMP.f`
  - (b) Use the routine `thomas` to determine  $\phi(r)$ ,  $N(r)$ , and  $Z_{\text{eff}}(r)$  for Na ( $Z=11$ ). Submit a plot of the data.
  - (c) Edit the output data set “`thomas.dat`” from the above step to make a two column file: `r` vs. `zeff`. Name the resulting data set “`zeff.dat`”. This data set will be used as input to `nrelMP`.
  - (d) Create an input file “`mod.in`” (standard input unit 5) in the form:

```
Z
n1  l1  e1
n2  l2  e2
n3  l3  e3
etc.
```

where  $Z=11$  for Na, where `n1`, `l1` are quantum numbers of energy levels of Na and `e1` is an estimate of the energy. For example, the row  
(3, 0, -0.2)  
would correspond to a 3s state with a guess of -0.2 au for the energy. Use the routine `nrelMP` to evaluate energies of the seven lowest levels of Na.
  - (e) Compare your calculated energy levels with spectroscopic data. this data is available from <http://physics.nist.gov> under the heading Physical Reference Data, subheading Atomic Spectroscopy Database [Version 3.0] The energies in this database are relative to the atomic ground state. The theoretical energies are relative to the ionization limit. To compare the measured energies with calculations, you must subtract the ionization limit from the measured values and convert to atomic units!