PHYS 622: Quantum Mechanics II
Due date: Thursday, February 20, 2014

Problem Set #5

Sakurai and Napolitano problems:
5.20 [5.20], 5.21 [5.21]
The old (red) Sakurai (revised, 1st ed.) problems are listed in brackets.

1. Helium interaction term
Show that the helium interaction term in the Hamiltonian is

$$\langle \psi_{1s}(\vec{r}_1)|\langle \psi_{1s}(\vec{r}_2)|\frac{e^2}{|\vec{r}_2-\vec{r}_1|}|\psi_{1s}(\vec{r}_2)\rangle|\psi_{1s}(\vec{r}_1)\rangle = \frac{5}{8}Z\frac{e^2}{a_0}$$

2. Bouncing quantum particle
Consider a quantum particle of mass m in a constant gravitational field $\vec{g} = -g\hat{z}$ and constrained to move only along the z-axis, while being subject to a hard barrier at z=0 from below (i.e. potential energy $U(z\to 0^-)=+\infty$).

a) Write down the Schrodinger equation for the particle and any boundary conditions that it is subject to.

b) Estimate the energy of the ground state of the system using the variational method and your reasonable best choice of a trial function of your choosing.

c) Estimate the energy of the first excited state.

3. Minimax principle for the second excited state
Formulate the minimax principle for the second excited state and prove it.

4. More variational method
ψ_1 and ψ_2 are any two wavefunctions (not necessarily normalized and orthogonal). Consider the sub-Hilbert space spanned by these two wave functions (i.e. $\alpha\psi_1 + \beta\psi_2$). The expectation of the Hamiltonian H in this subspace is given by $\langle H\rangle=N/D$, where

$$N = (\alpha^* \ \beta^*)\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$D = (\alpha^* \ \beta^*)\begin{pmatrix} <\psi_1|\psi_1> & <\psi_1|\psi_2> \\ <\psi_2|\psi_1> & <\psi_2|\psi_2> \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$H_{ij} = <\psi_i|H|\psi_j>$$

Show that when α and β are varied, the extrema of $\langle H\rangle$ is given by the solutions of λ of the equation

$$\det\left[\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} - \lambda\begin{pmatrix} <\psi_1|\psi_1> & <\psi_1|\psi_2> \\ <\psi_2|\psi_1> & <\psi_2|\psi_2> \end{pmatrix}\right] = 0$$

These are the energy values in the sub-Hilbert space under consideration.

Note: You are essentially proving the Ritz theorem in this special case, so you should not use it explicitly to solve this problem.