PHYS 580 Homework 6 - due 5 pm Fri Dec 6, 2019

All questions are worth 10 points, irrespectively of complexity or length. Please submit all your solutions on paper, and make sure to include the same list of basic ingredients in all your solutions as in earlier homeworks (for economy of space, the list is omitted here).

1) Problem 10.5 (p.322) in the Giordano-Nakanishi textbook.

2) Problem 10.12 (p.333).

3) Write a matching method program to study the coupling between two one-dimensional quantum mechanical systems in neighboring square wells that are separated by a small, square barrier (cf. Figs. 10.11 and 10.12 of the textbook). In particular, observe how identical *unperturbed* states in each well get mixed due to being coupled through the finite barrier. Demonstrate numerically, for at at least two different examples (such as the two ground states and then two excited states), that the initially equal energy levels split up. Namely, the parity even mixture moves down in energy, while the parity odd one moves up. This phenomenon is discussed in Chapter 10 of the book (p.318-320).

4) Obtain a *deterministic* variational estimate for the ground state energy and wave function of a particle in a 1D Lennard-Jones potential with $\varepsilon = 10$, $\sigma = 1$ (remember, $m = 1$, $\hbar = 1$ units are used). Compare the obtained energy value and the wave function to what you have found in Lab 13, part 2.

The complexity of the calculation, of course, very much depends on how good your variational basis is, so my suggestion is that you use

$$\psi_n(x) = \begin{cases} const \times \left(x - \frac{3}{4}\right)^n e^{-ax} & , \quad \text{if } x > \frac{3}{4} \\ 0 & , \quad \text{otherwise} \end{cases} \qquad (a > 0)$$

Set $n = 3$, i.e., keep only one basis function ψ_3, and optimize a such that the estimated ground state energy is minimized.

[Optional: why did I suggest keeping ψ_3, and not, ψ_2 or ψ_4, for example?]

Note the errata pages for the textbook:

`http://www.physics.purdue.edu/~hisao/book/www/errata.pdf`
`http://www.physics.purdue.edu/~isao/book/www/errata.html`