PHY 6646 Spring 2003 – Homework 4

Due by 5 p.m. on Friday, February 7. Partial credit will be available for solutions submitted by 5 p.m. on Monday, February 10.

Answer all questions. To gain maximum credit you should explain your reasoning and show all working. Please write neatly and include your name on the front page of your answers.

- 1. Shankar Exercise 16.1.2.
- 2. Revisit the previous question with a trial wave function

$$\psi(x,\alpha) = C(a^2 - x^2)(a^2 - \alpha x^2),$$

where α is real, and C is a positive, real normalization constant. Note that for $\alpha = 0$, this wave function reduces to that used in the previous question.

- (a) Calculate the energy expectation value $E(\alpha)$.
- (b) Obtain a variational upper bound E(α_{min}) on the ground-state energy E₀. You should obtain the numerical value α_{min} = 0.220750... Since you know E₀ for this problem, calculate the numerical value of E(α_{min})/E₀. Compare it with the answer you obtained in Question 1, and verify that your variational procedure has lowered the upper bound on E₀.
- (c) Calculate the overlap $F(\alpha) = |\langle \psi_0 | \psi(\alpha) \rangle|$ between the trial wave function $\psi(x, \alpha)$ and the true ground-state wave function $\psi_0(x)$.
- (d) Obtain an expression for the value $\alpha = \alpha_{\text{max}}$ that maximizes $F(\alpha)$. You should obtain the numerical value $\alpha_{\text{max}} = 0.223216...$
- (e) Compare the numerical values of $F(\alpha_{\min})$ and $F(\alpha_{\max})$. You should find that in this problem, the best variational estimate of the ground-state energy is *not* obtained from the trial wave function that has the greatest overlap with the true ground-state wave function.
- 3. Consider a family of trial wave functions $\psi(x, \alpha) = C(1 + \alpha x^2) \exp(-\alpha x^2)$ for the harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$.
 - (a) Use the variational method to obtain an upper bound $E(\alpha_0)$ on the ground-state energy.
 - (b) Calculate the energy uncertainty $\Delta E(\alpha)$ in the state $\psi(x, \alpha)$, and hence obtain a rigorous lower bound E_{low} for an energy eigenvalue of the harmonic potential. Pretending that we did not know the exact solutions for this potential, explain carefully the precise interpretation we should place on E_{low} .