Quantum Mechanics 3, Spring 2012 CMI

Problem set 9

Due by beginning of class on Monday Mar 19, 2012

Variational principle and approximations

1. $\langle 12 \rangle$ Suppose $H = (H_{jk})$ is a hermitian hamiltonian on the complex hilbert space $\mathbb{C}^n$ and $z = (z_k = x_k + iy_k)$ a state vector $1 \le j, k \le n$. We wish to extremize $z^\dagger H z$ subject to the constraint $z^\dagger z = 1$.

   (a) $\langle 2 \rangle$ Formulate this variational problem as the extremization of a new functional $\mathcal{E}$ by the method of Lagrange multipliers.

   (b) $\langle 5 \rangle$ Find the conditions for an extremum with respect to variations in the real and imaginary parts x_p and y_p.

   (c) $\langle 2 \rangle$ Combine these conditions to show that they imply the Schrödinger eigenvalue problem and its adjoint.

   (d) $\langle 3 \rangle$ Treat z_k and z_k^* as independent variables. Find the conditions for $\mathcal{E}$ to be extremal with respect to z_k and z_k^* and compare with the previous results.

2. $\langle 14 \rangle$ Consider the anharmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + gx^4$. We wish to get a variational upper bound for the g.s. energy using the normalized trial wave function (α is a variational parameter.)

$$\psi(x) = Ae^{-\alpha x^2/2}, \quad A = \left(\frac{\alpha}{\pi}\right)^{1/4}, \quad \alpha > 0, g > 0, m > 0, \omega > 0. \tag{1}$$

   (a) $\langle 5 \rangle$ Find the expectation value $\langle H \rangle$ in the trial state. Show that you get

$$\langle H \rangle = \frac{\hbar^2 \alpha}{4m} + \frac{m\omega^2}{4\alpha} + \frac{3g}{4\alpha^2}. \tag{2}$$

   (b) $\langle 3 \rangle$ Show that the optimal value of α is determined by the condition

$$f(\alpha) = \frac{\hbar^2}{m}\alpha^3 - m\omega^2\alpha - 6g = 0 \tag{3}$$

   Argue that there is precisely one positive root α^* of this cubic equation.

   (c) $\langle 1 \rangle$ For the numerical values $\hbar = 1, m = 1, \omega = 1, g = \frac{1}{10}$ find the variational estimate E_0^V for g.s. energy. You may use the fact that the positive zero of $\alpha^3 - \alpha - 6g = 0$ occurs at $\alpha_* = 1.2212$ when $g = 1/10$.

   (d) $\langle 1 \rangle$ Recall that the g.s. energy to first order in perturbation theory around the SHO is

$$E_0^P = \frac{1}{2}\hbar\omega + \frac{3g\hbar^2}{4m^2\omega^2} + \cdots \tag{4}$$

   For the same numerical values find the g.s. energy E_0^P by 1st order perturbation theory.

   (e) $\langle 4 \rangle$ Compare the results of perturbation theory and variational approximation. Which is better? Explain why one is less than the other.