

## Homework 04

Name: \_\_\_\_\_

### Problem 1 (10 points)

Consider the infinite one dimensional square well, with

$$U(x) = \begin{cases} 0 & \text{if } |x| \leq a; \\ \infty & \text{if } |x| > a \end{cases}$$

Use the variational principle and guess/trial/ansatz function  $\Psi(x) = C(a - |x|)^b$ , where  $b > 0$  is a variable parameter and  $C$  is the normalization constant, to find the estimate of the ground level energy.

### Problem 2 (10 points)

Consider a harmonic oscillator

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2}m\omega^2\hat{\mathbf{x}}^2 \quad (1)$$

Apply the variational principle to find the ground state energy estimate. Use the guess/trial/ansatz function

$$\Psi(x) = \frac{C}{x^2 + b^2}$$

where  $C$  is normalization constant and  $b$  is variable parameter.

### Problem 3 (10 points)

Consider a particle of mass  $m$  and charge  $q$  (sign is unknown) is moving in one dimension ('x') and influenced by the electric field

$$\vec{E}(x) = \begin{cases} E_0\vec{x} & \text{if } x > 0; \\ -E_0\vec{x} & \text{if } x < 0; \end{cases}$$

Here,  $\vec{x}$  stands for unit vector along 'x' direction.

Consider a trial  $\Psi(x) = C \exp(-a|x|)$  and estimate the ground-state energy by minimizing the expectation value of the energy with respect to parameter  $a$ .

For which sign of charge  $q$  the bound state can exist.

### Problem 4 (10 points)

Generally, we do not know the ground level eigen state  $|\psi_g\rangle$ . However, if we have some information about  $|\psi_g\rangle$  and can guess a function  $|\psi\rangle$  such that  $\langle\psi|\psi_g\rangle = 0$ . Show that in this case  $\langle\psi|\hat{H}|\psi\rangle \geq E_{fe}$ , where  $E_{fe}$  is the energy of the first excited state.

### Problem 5 (10 points)

If the potential is even then the ground state function is even too. For example, ground state of the harmonic oscillator (Eq. 1) is even. Thus based on the result of the previous problem, we can use an odd trial function to estimate the energy of the first excited state.

Apply this idea to the Hamiltonian from the problem 2 and its ansatz function for the ground state. This time use the trial function

$$\Psi(x) = x \frac{C}{x^2 + b^2}$$

and estimate  $E_{fe}$ . You should arrive to somewhat useless result, which will teach you about one more condition required for the use the theorem outlined in Problem 4. Discuss this condition.

**Bonus 10 points:** modify the ansatz function, and get a better estimate of the first excited state energy.