INDIAN INSTITUTE OF TECHNOLOGY MANDI

QUIZ - 2

Introduction to Theoretical Chemistry (CY 704)

Full Marks: 20 **Date: 04.11.2011** **Time 50 min.**

Answer *ALL* Questions:

1. What are the energy eigenfunctions and eigenvalues for the one dimensional box problem discussed in the class if the ends of the box are at x= –L/2 and x= +L/2. What will happen to those eigenfunctions and eigenvalues, if we add one repulsive Dirac Delta Potential at x = 0 to the above mentioned (particle in a one dimensional box) problem ?

[6]

2. (a) Show that for a particle in a one dimensional box, in an arbitrary state $\Psi(x,0)$,

$< E > > E1$

(b) Under what condition does the equality maintain?

[3]

3. A particle in the one-dimensional box with walls at x = 0 and x = L, is in the ground state. One of the wall of the box is moved to the position x = 2L, in a time short compared to the natural period $2\pi/\omega_1$, where $\hbar\omega_1 = E_1$. If the energy of the particle is measured soon after this expansion, what value of energy is most likely to be found ? How does this energy compare to the particle's initial energy (E_1)?

[3]

4. At t = 0 it is known that of 1000 neutrons in a one dimensional box of width 10^{-5} cm, 100 have energy $4E_1$, and 900 have energy $225\ E_1$.
   (a) Construct a state function that has these properties.
   (b) How many neutrons are in the left half of the "box"?

[4]

5. What is the expectation value of momentum for a particle in the state

$$\Psi(x,t)=A\, e^{i\,\omega\, t}\, Cos[x],$$

where A is a real constant.

[2]

6. For what values of the real angle θ will be constant $C = \frac{1}{2}(e^{i\theta}-1)$ have no effect in calculation involving the modulus $|C\Psi|$?

[1]

7. Give an argument in support of the statement that one cannot measure the momentum of a particle in a one dimensional box, with absolute accuracy.

[1]