Chemistry 120A

Spring Semester, 2013; Prof. Head-Gordon 1st Mid-Term Exam

Friday February 22

Name: _ **Instructions:** (1) The best of good luck and good fortune to everyone! (2) The exam is closed book. (3) The exam has 4 pages plus 2 blanks for extra scratch paper. Grade: Problem 1: General (7 points) Problem 2: Particle in a box (6 points) Problem 3: Two-level system (8 points) Total (21 points) **Useful facts and figures:** $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ *h*=6.626755×10⁻³⁴ J s $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ $k=1.380658\times10^{-23}$ J K⁻¹ $\hat{H}|\psi\rangle = \frac{-\hbar}{i} \frac{\partial}{\partial t} |\psi\rangle$ $N_A = 6.022137 \times 10^{23} \text{ mol}^{-1}$ $1 \text{ eV} = 1.60219 \times 10^{-19} \text{ J}$ $\Delta p \Delta x \ge \hbar / 2$ $\begin{bmatrix} \hat{A}, \hat{B} \end{bmatrix} = \hat{A}\hat{B} - \hat{B}\hat{A}$ $\hbar = h/(2\pi)$

Question I: General Multiple choice problems: 7 points

Mark your answer on the line to the right of each problem

- 1. At a finite potential step, the 1st derivative of the wavefunction, $\partial \Psi / \partial x$, exhibits:
 - (a) continuity(b) a finite step(c) an infinite step
- 2. All else constant, a larger force constant for the harmonic oscillator will cause the wavelength corresponding to the energy difference between levels to:

3. Can a particle in quantum mechanics be reflected by a potential barrier that is smaller than its kinetic energy?

	(a) yes	(b) no		
4.	Which of the following is the quantity $ \phi\rangle\langle\psi $?			
	(a) a number	(b) a ket	(c) an operator	
5.	Which of the following is the quantity $\langle \phi \psi \rangle$?			
	(a) a number	(b) a ket	(c) an operator	
6.	All else being equal, if one compares two wavefunctions, the one with the larger curvature $(\partial^2 \Psi / \partial x^2)$ will have an energy which is :			
	(a) higher	(b) lower		
7.	Which of the following has the shortest de Broglie wavelength?			
	(a) a 1eV He atom	(b) a 1 eV photon	(c) a 1eV electron	

Question II. The particle in a 1-dimensional box of length *L* with potential:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x \le 0, \ x \ge L \end{cases}$$

The energy eigenvalues and normalized eigenfunctions are as follows;

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}; \qquad \phi_n(x) = \sqrt{\frac{2}{L} \sin \frac{n\pi x}{L}} \qquad n = 1, 2, 3...$$

Suppose now that a particle in a box is described by the following state at time zero: $|\Psi(t=0)\rangle = |\phi_{n=1}\rangle - 2|\phi_{n=3}\rangle$

8. If its position is measured at t = 0, where is the particle more likely to be?

(a) left half of box (b) right half (c) both equally likely

9. If its position is measured at a later time, t, the probability that the particle is more likely to be on the right hand side will never vary from the result at t = 0.

(a) true (b) false

10. The statement given in (9) above is true for any superposition, rather than just the particular state given above.

(a) true

(b) false

- 11. The scale factor by which to multiply the ket $|\Psi(t=0)\rangle$ so that it is normalized is:
 - (a) 1/5 (b) 1/3 (c) $1/\sqrt{5}$
- 12. If the energy is measured at t = 0, the probability of measuring the energy $2\pi^2 \hbar^2 / mL^2$ is:
 - (a) 0 (b) 1/5 (c) 1/3
- 13. The average energy obtained from measurements at time t = 0 on large numbers of systems prepared in the state $|\Psi(t=0)\rangle$ is:
 - (a) $17\pi^2\hbar^2/10mL^2$ (b) $37\pi^2\hbar^2/10mL^2$ (c) $44\pi^2\hbar^2/10mL^2$

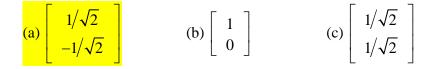
Question III. A two-level system has the following Hamiltonian in the basis of eigenvectors, $\{|1\rangle, |2\rangle\}$, of an observable A.

$$\mathbf{H} = \left[\begin{array}{rrr} 1 & 1 \\ 1 & 1 \end{array} \right]$$

Suppose that a particle is described by the following state at time zero:

$$\left|\Psi(t=0)\right\rangle = \frac{3}{5}\left|1\right\rangle - \frac{4}{5}\left|2\right\rangle$$

- 14. What are the energy eigenvalues?
 - (a) -1, 3 (b) 0, 2 (c) 1, 1
- 15. What is the eigenvector belonging to the lowest eigenvalue?



16. If the eigenvalues of A are 1 and 2, do the operators \hat{A} and \hat{H} commute (i.e $\left[\hat{H}, \hat{A}\right] = 0$)?

(a) yes (b) no

17. If the eigenvalues of A are both equal to 2, do the operators \hat{A} and \hat{H} commute?

(a) yes (b) no

18. The average value of the energy for $|\Psi(t=0)\rangle$ is:

(a) 0 (b) 0.04 (c) 0.4

19. If the energy is measured for $|\Psi(t=0)\rangle$, the probability of the higher eigenvalue is:

- (a) 0 (b) 0.02 (c) 0.2
- 20. Is the probability of measuring the lowest energy eigenvalue time-dependent?
 - (a) yes (b) no
- 21. If the value of \hat{A} was measured (and its eigenvalues are non-degenerate), would the probability of getting the lowest eigenvalue be time-dependent?

(a) yes (b) no

Mean 15.12 Median 15.16 **Standard Deviation 2.21**

