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:

h=6.626755×10^{-34} J s

k=1.380658×10^{-23} J K^{-1}

N_A=6.022137×10^{23} mol^{-1}

1 eV = 1.60219×10^{-19} J

$\hbar = h/(2\pi)$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$$

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\hat{H}|\psi\rangle = \frac{-\hbar}{i}\frac{\partial}{\partial t}|\psi\rangle$$

$$\Delta p \Delta x \geq \hbar/2$$

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

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:

   (a) increase (b) decrease (c) stay the same ________

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;

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

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.

$$\mathbf{H} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

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

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

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?

(a) $\begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$ (b) $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ (c) $\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ ________

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

(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