Quantum Mechanics **NAME:**

Homework 2b: Solving the Schrödinger's Equation: Homeworks are not handed in or marked. But you get a mark for reporting that you have done them. Once you've reported completion, you may look at the already posted supposedly super-perfect solutions.

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	16.	O	O	O	O	O
2.	O	O	O	O	O	17.	O	O	O	O	O
3.	O	O	O	O	O	18.	O	O	O	O	O
4.	O	O	O	O	O	19.	O	O	O	O	O
5.	O	O	O	O	O	20.	O	O	O	O	O
6.	O	O	O	O	O	21.	O	O	O	O	O
7.	O	O	O	O	O	22.	O	O	O	O	O
8.	O	O	O	O	O	23.	O	O	O	O	O
9.	O	O	O	O	O	24.	O	O	O	O	O
10.	O	O	O	O	O	25.	O	O	O	O	O
11.	O	O	O	O	O	26.	O	O	O	O	O
12.	O	O	O	O	O	27.	O	O	O	O	O
13.	O	O	O	O	O	28.	O	O	O	O	O
14.	O	O	O	O	O	29.	O	O	O	O	O
15.	O	O	O	O	O	30.	O	O	O	O	O

1. In quantum mechanics, the infinite square well can be regarded as the prototype of:

   a) all bound systems. b) all unbound systems. c) both bound and unbound systems. d) neither bound nor unbound systems. e) Prometheus unbound.

2. In the infinite square well problem, the wave function and its first spatial derivative are:

   a) both continuous at the boundaries.
   b) continuous and discontinuous at the boundaries, respectively.
   c) both discontinuous at the boundaries.
   d) discontinuous and continuous at the boundaries, respectively.
   e) both infinite at the boundaries.

3. Meeting the boundary conditions of bound quantum mechanical systems imposes:

   a) Heisenberg's uncertainty principle. b) Schrödinger's equation. c) quantization. d) a vector potential. e) a time-dependent potential.

4. At energies higher than the bound stationary states there:

   a) are between one and several tens of unbound states. b) are only two unbound states. c) is a single unbound state. d) are no states. e) is a continuum of unbound states.

5. "Let's play *Jeopardy*! For \$100, the answer is: This effect occurs because wave functions can extend (in an exponentially decreasing way albeit) into the classically forbidden region: i.e., the region where a classical particle would have negative kinetic energy."

   What is ____________, Alex?

   a) stimulated radiative emission b) quantum mechanical tunneling c) quantization d) symmetrization e) normalization

6. A simple model of the outer electronic structure of a benzene molecule is a 1-dimensional infinite square well with:

   a) vanishing boundary conditions. b) periodic boundary conditions. c) aperiodic boundary conditions. d) no boundary conditions. e) incorrect boundary conditions.

7. You are given the time-independent Schrödinger equation

$$H\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

   and the infinite square well potential

$$V(x) = \begin{cases} 0\,, & x \in [0, a]; \\ \infty & \text{otherwise.} \end{cases}$$

a) What must the wave function be outside of the well (i.e., outside of the region $[0, a]$) in order to satisfy the Schrödinger equation? Why?

b) What boundary conditions must the wave function satisfy? Why must it satisfy these boundary conditions?

c) Reduce Schrödinger's equation inside the well to an equation of the same form as the **CLASSICAL** simple harmonic oscillator differential equation with all the constants combined into a factor of $-k^2$, where k is newly defined constant. What is k's definition?

d) Solve for the general solution for a **SINGLE** k value, but don't impose boundary conditions or normalization yet. A solution by inspection is adequate. Why can't we allow solutions with $E \leq 0$? Think carefully: it's not because k is imaginary when $E < 0$.

e) Use the boundary conditions to eliminate most of the solutions with $E > 0$ and to impose quantization on the allowed set of distinct solutions (i.e., on the allowed k values). Give the general wave function with the boundary conditions imposed and give the quantization rule for k in terms of a dimensionless quantum number n. Note that the multiplication of a wave function by an arbitrary global phase factor

$e^{i\phi}$ (where ϕ is arbitrary) does not create a physically distinct wave function (i.e., does not create a new wave function as recognized by nature.) (Note the orthogonality relation used in expanding general functions in eigenfunctions also does not distinguish eigenfunctions that differ by global phase factors either: i.e., it gives the expansion coefficients only for distinct eigenfunctions. So the idea of distinct eigenfunctions arises in pure mathematics as well as in physics.)

f) Normalize the solutions.

g) Determine the general formula for the eigenenergies in terms of the quantum number n.

8. Calculate $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, σ_x, and σ_p for the 1-dimensional infinite square well with range $[0,a]$. Recall the general solution is

$$\psi = \sqrt{\frac{2}{a}}\sin(kx) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) ,$$

where $n = 1, 2, 3, \ldots$. Also check that the Heisenberg uncertainty principle is satisfied.

9. A particle is in a mixed state in a 1-dimensional infinite square well where the well spans $[0,a]$ and the solutions are in the standard form of Gr-26. At time zero the state is

$$\Psi(x,0) = A\left[\psi_1(x) + \psi_2(x)\right] ,$$

where $\psi_1(x)$ and $\psi_2(x)$ are the time-independent 1st and 2nd stationary states of the infinite square well.

a) Determine the normalization constant A. Remember the stationary states are orthonormal. Also is the normalization a constant with time? Prove this from the general time evolution equation

$$\frac{d\langle Q\rangle}{dt} = \left\langle\frac{\partial Q}{\partial t}\right\rangle + \frac{1}{\hbar}\langle i[H,Q]\rangle .$$

b) Now write down $\Psi(x,t)$. Give the argument for why it is the solution. As a simplfication in the solution use

$$\omega_1 = \frac{E_1}{\hbar} = \frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 ,$$

where E_1 is the ground state energy of the infinite square well.

c) Write out $|\Psi(x,t)|^2$ and simplify it so that it is clear that it is pure real. Make use Euler's formula: $e^{ix} = \cos x + i\sin x$. What's different about our mixed state from a stationary state?

d) Determine $\langle x\rangle$ for the mixed state. Note that the solution is oscillatory. What is the angular frequency $w_{\rm q}$ and amplitude of the oscillation. Why would you be wrong if your amplitude was greater than $a/2$.

e) Determine $\langle p\rangle$ for the mixed state. As Peter Lorre (playing Dr. Einstein—Herman Einstein, Heidelberg 1919) said in *Arsenic and Old Lace* "the quick way, Chonny."

f) Determine $\langle H\rangle$ for the mixed state. How does it compare to E_1 and E_2?

g) Say a classical particle had kinetic energy equal to the energy $\langle H\rangle$ found in the part (f) answer. The particle is bounces back and forth between the walls of the infinite square well. What would its angular frequency be in terms of $\omega_{\rm q}$ and the angular frequency found in the part (d) answer.

10. "Let's play *Jeopardy*! For \$100, the answer is: $\hbar\omega$.

a) What is the energy difference between adjacent simple harmonic ocsillator energy levels, Alex?
b) What is the energy difference between adjacent infinite square well energy levels, Alex?
c) What is the energy difference between most adjacent infinite square well energy levels, Alex?
d) What is the energy difference between the first two simple harmonic ocsillator energy levels **ONLY,** Alex?
e) What is the bar where physicists hang out in Las Vegas, Alex?

11. The simple harmonic oscillator (SHO) ground state is

$$\Psi_0(x,t) = Ae^{-\beta^2 x^2/2 - iE_0 t/\hbar} \ ,$$

where

$$E_0 = \frac{\hbar\omega}{2} \qquad \text{and} \qquad \beta = \sqrt{\frac{m\omega}{\hbar}} \ .$$

   a) Verify that the wave function satisfies the full Schrödinger equation for the SHO. Recall that the SHO potential is $V(x) = (1/2)m\omega^2 x^2$.

   b) Determine the normalization constant A.

   c) Calculate the expectation values of x, x^2, p, and p^2.

   d) Calculate σ_x and σ_p, and show that they satisfy the Heisenberg uncertainty principle.

12. A particle in a simple harmonic oscillator (SHO) potential has initial wave function

$$\Psi(x,0) = A\left[\psi_0 + \psi_1\right] \ ,$$

where A is the normalization constant and the ψ_i are the standard form 0th and 1st SHO eigenstates. Recall the potential is

$$V(x) = \frac{1}{2}m\omega^2 x^2 \ .$$

Note ω is just an angular frequency parameter of the potential and not **NECESSARILY** the frequency of anything in particular. In the classical oscillator case ω is the frequency of oscillation, of course.

   a) Determine A assuming it is pure real as we are always free to do.

   b) Write down $\Psi(x,t)$. There is no need to express the ψ_i explicitly. Why must this $\Psi(x,t)$ be the solution?

   c) Determine $|\Psi(x,t)|^2$ in simplified form. There should be a sinusoidal function of time in your simplified form.

   d) Determine $\langle x\rangle$. Note that $\langle x\rangle$ oscillates in time. What is its angular frequency and amplitude.

   e) Determine $\langle p\rangle$ the quick way using the 1st formula of Ehrenfest's theorem. Check that the 2nd formula of Ehrenfest's theorem holds.

13. Say you have the potential

$$V(x) = \begin{cases} \infty \ , & x < 0; \\ \frac{1}{2}m\omega^2 x^2 & x \geq 0. \end{cases}$$

   a) By reflecting on the nature of the potential **AND** on the boundary conditions, identify the set of Schrödinger equation eigenfunctions satisfy this potential. Justify your answer. **HINTS:** Don't try solving the Schrödinger equation directly, just use an already known set of eigenfunctions to identify the new set. This shouldn't take long.

   b) What is the expression for the eigen-energies of your eigenfunctions?

   c) What factor must multiply the already-known (and already normalized) eigenfunctions you used to construct the new set you found in part (a) in order to normalize the new eigenfunctions? **HINT:** Use the evenness or oddness (i.e., definite parity) of the already-known set.

   d) Show that your new eigenfunctions are orthogonal. **HINT:** Use orthogonality and the definite parity of the already-known set.

   e) Show that your eigenfunctions form a complete set given that the already-known set was complete. **HINTS:** Remember completeness only requires that you can expand any suitably well-behaved function (which means I think it has to be piecewise continuous (Ar-435) and square-integrable (CT-99) satisfying the same boundary conditions as the set used in the expansion. You don't have to be able to expand any function. Also, use the completeness of the already-known set.

14. The generating function method is a powerful method for obtaining the eigenfunctions of Sturm-Liouville Hermitian operators and some of their general properties. One can possibly obtain with only moderately arduous labor some special values, the norm value, a general series formula for the eigenfunctions, and recurrence relations for iteratively constructing the complete set of eigenfunctions. The only problem is who the devil thought up the generating function?

    In the case of Hermite polynomials, the generating function—which may or may not have been thought up by French mathematician Charles Hermite (1822–1901)—is

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n \frac{t^n}{n!}$$

(Ar-609ff; WA-644). The H_n are the Hermite polynomials: they are functions of x and n is their order.

    Actually, the **HERMITE EQUATION** needs a weight function e^{-x^2} to be put in Sturm-Liouville self-adjoint form (Ar-426, WA-486). Alternatively, the Hermite polynomials times $e^{-x^2/2}$ satisfy a Sturm-Liouville Hermitian operator equation which happens to be the time-independent Schrödinger equation for the 1-dimensional quantum mechanical simple harmonic oscillator (Ar-612, WA-638). The 1-dimensional quantum mechanical simple harmonic oscillator is one of those few quantum mechanical systems with an analytic solution.

    NOTE: The parts of this question are independent: i.e., you should be able to do any of the parts without having done the other parts.

    a) Find the 1st recurrence relation

    $$H_{n+1} = 2xH_n - 2nH_{n-1}$$

    by differentiating both the generating function and its and series expansion with respect to t. This recurrence relation provides a means of finding any order of Hermite polynomial. **HINT:** You will need to re-index summations and make use of the uniqueness theorem of power series.

    b) Find the 2nd recurrence relation

    $$H_n' = 2nH_{n-1}$$

    by differentiating both the generating function and its and series expansion with respect to x. **HINT:** You will need to re-index summations and make use of the uniqueness theorem of power series.

    c) Use the 1st recurrence relation to work out and tabulate the polynomials up to 3rd order: i.e., find H_0, H_1, H_2, and H_3. You can find the first two polynomials (i.e., the 0th and 1st order polynomials) needed to start the recurrence process by a simple Taylor's series expansion of generating function.

    d) Use the 1st recurrence relation to prove that the order of a Hermite polynomial agrees with its polynomial degree (which is the degree of its highest degree term) and that even order Hermite polynomials are even functions and the odd order ones are odd functions. The last result means that the Hermite polynomials have definite parity (i.e., are either even or odd functions). **HINT:** Use proof by induction and refer to collectively to the results to be proven as "the results to be proven". If you didn't get H_0 and H_1 explicitly in part (c), you can assume H_0 has degree 0 and H_1 has degree 1.

15. A free particle is:

    a) bound. b) unbound. c) both bound and unbound. d) neither bound nor unbound.
    e) neither here nor there.

16. The free particle system is one with where the potential is:

    a) the simple harmonic oscillator potential (SHO). b) a quasi-SHO potential.
    c) an infinite square well potential. d) a finite square well potential.
    e) zero (or a constant) everywhere.

17. The general expression for the free particle energy eigenfunction in 1-dimension is:

    a) e^{ikx}, where $k = \pm E$. b) e^{kx}, where $k = \pm E$. c) e^{kx}, where $k = \pm\sqrt{2mE/\hbar^2}$.
    d) e^{ikx}, where $k = \pm\sqrt{2mE/\hbar^2}$. e) e^{kx^2}, where $k = \pm\sqrt{2mE/\hbar^2}$.

18. The free particle energy eigenfunctions are not physical states that a particle can actually be in because they:

    a) can't be normalized (i.e., they arn't square-integrable).
    b) can be normalized (i.e., they are square-integrable).
    c) are growing exponentials.
    d) don't exist.
    e) do exist.

19. The initial wave function of a free particle is

$$\Psi(x,0) = \begin{cases} A\ , & x \in [-a,a]; \\ 0\ , & \text{otherwise,} \end{cases}$$

where a and A are positive real numbers. The particle is in a completely zero potential environment since it is a free particle.

    a) Determine A from normalization.

    b) Determine $\psi(k) = \Psi(k,0)$ the time-zero wavenumber representation of the particle state. It is the Fourier transform of $\Psi(x,0)$. What is $\Psi(k,t)$? Sketch $\psi(k)$. Locate the global maximum and the zeros of $\psi(k)$. Give the expression for the zeros (i.e., for the location of the zeros).

    c) Determine the wavenumber space probability density $|\Psi(k,t)|^2$ and show then that $\Psi(k,t)$ is normalized in wavenumber space. (You can use a table integral.) Sketch $|\Psi(k,t)|^2$ and locate the global maximum and the zeros. Give the expression for the zeros.

    d) Crudely estimate and then calculate exactly σ_x, σ_k, and σ_p for time zero. Are the results consistent with the Heisenberg uncertainty principle?

Appendix 2 Quantum Mechanics Equation Sheet

Note: This equation sheet is intended for students writing tests or reviewing material. Therefore it neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things.

1 Constants not to High Accuracy

Constant Name	Symbol	Derived from CODATA 1998
Bohr radius	$a_{\mathrm{Bohr}} = \dfrac{\lambda_{\mathrm{Compton}}}{2\pi\alpha}$	$= 0.529\,\text{Å}$
Boltzmann's constant	k	$= 0.8617 \times 10^{-6}\,\mathrm{eV\,K^{-1}}$ $= 1.381 \times 10^{-16}\,\mathrm{erg\,K^{-1}}$
Compton wavelength	$\lambda_{\mathrm{Compton}} = \dfrac{h}{m_e c}$	$= 0.0246\,\text{Å}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5\,\mathrm{eV}$
Elementary charge squared	e^2	$= 14.40\,\mathrm{eV}\,\text{Å}$
Fine Structure constant	$\alpha = \dfrac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\dfrac{\hbar^2}{2m_e}$	$= 3.81\,\mathrm{eV}\,\text{Å}^2$
	$\dfrac{\hbar^2}{m_e}$	$= 7.62\,\mathrm{eV}\,\text{Å}^2$
Planck's constant	h	$= 4.15 \times 10^{-15}\,\mathrm{eV}$
Planck's h-bar	$\hbar$	$= 6.58 \times 10^{-16}\,\mathrm{eV}$
	hc	$= 12398.42\,\mathrm{eV}\,\text{Å}$
	$\hbar c$	$= 1973.27\,\mathrm{eV}\,\text{Å}$
Rydberg Energy	$E_{\mathrm{Ryd}} = \dfrac{1}{2} m_e c^2 \alpha^2$	$= 13.606\,\mathrm{eV}$

2 Some Useful Formulae

Leibniz's formula
$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n} \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

Normalized Gaussian
$$P = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2}\right]$$

3 Schrödinger's Equation

$$H\Psi(x,t) = \left[\frac{p^2}{2m} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$$H\psi(x) = \left[\frac{p^2}{2m} + V(x)\right]\psi(x) = E\psi(x)$$

$$H\Psi(\vec{r},t) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \qquad H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle$$

$$H\psi(\vec{r}) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \qquad H|\psi\rangle = E|\psi\rangle$$

4 **Some Operators**

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

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

$$p = \frac{\hbar}{i}\nabla \qquad p^2 = -\hbar^2\nabla^2$$

$$H = \frac{p^2}{2m} + V(\vec{r}\,) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}\,)$$

$$\nabla = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\theta}\frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

5 **Kronecker Delta and Levi-Civita Symbol**

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & \text{otherwise} \end{cases} \qquad \varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic;} \\ -1, & ijk \text{ anticyclic;} \\ 0, & \text{if two indices the same.} \end{cases}$$

$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell} \qquad \text{(Einstein summation on } i\text{)}$$

6 **Time Evolution Formulae**

$$\text{General} \qquad \frac{d\langle A\rangle}{dt} = \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{\hbar}\langle i[H(t), A]\rangle$$

$$\text{Ehrenfest's Theorem} \qquad \frac{d\langle\vec{r}\rangle}{dt} = \frac{1}{m}\langle\vec{p}\rangle \qquad \text{and} \qquad \frac{d\langle\vec{p}\rangle}{dt} = -\langle\nabla V(\vec{r}\,)\rangle$$

$$|\Psi(t)\rangle = \sum_j c_j(0)e^{-iE_jt/\hbar}|\phi_j\rangle$$

7 **Simple Harmonic Oscillator (SHO) Formulae**

$$V(x) = \frac{1}{2}m\omega^2x^2 \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\psi = E\psi$$

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \qquad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}}H_n(\beta x)e^{-\beta^2x^2/2} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$H_0(\beta x) = H_0(\xi) = 1 \qquad H_1(\beta x) = H_1(\xi) = 2\xi$$

$$H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 \qquad H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi$$

8 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \qquad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m}$$

$$|\Psi(p,t)|^2\,dp = |\Psi(k,t)|^2\,dk \qquad \Psi(p,t) = \frac{\Psi(k,t)}{\sqrt{\hbar}}$$

$$x_{\text{op}} = x \qquad p_{\text{op}} = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}, t\right) \qquad \text{position representation}$$

$$x_{\text{op}} = -\frac{\hbar}{i}\frac{\partial}{\partial p} \qquad p_{\text{op}} = p \qquad Q\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p, t\right) \qquad \text{momentum representation}$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar}\,dp \qquad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi}\,dk$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \Psi(p,t)\frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}}\,dp \qquad \Psi(x,t) = \int_{-\infty}^{\infty} \Psi(k,t)\frac{e^{ikx}}{(2\pi)^{1/2}}\,dk$$

$$\Psi(p,t) = \int_{-\infty}^{\infty} \Psi(x,t)\frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}}\,dx \qquad \Psi(k,t) = \int_{-\infty}^{\infty} \Psi(x,t)\frac{e^{-ikx}}{(2\pi)^{1/2}}\,dx$$

$$\Psi(\vec{r},t) = \int_{\text{all space}} \Psi(\vec{p},t)\frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\,d^3p \qquad \Psi(\vec{r},t) = \int_{\text{all space}} \Psi(\vec{k},t)\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}\,d^3k$$

$$\Psi(\vec{p},t) = \int_{\text{all space}} \Psi(\vec{r},t)\frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\,d^3r \qquad \Psi(\vec{k},t) = \int_{\text{all space}} \Psi(\vec{r},t)\frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}\,d^3r$$

9 Commutator Formulae

$$[A, BC] = [A, B]C + B[A, C] \qquad \left[\sum_i a_i A_i, \sum_j b_j B_j\right] = \sum_{i,j} a_i b_j [A_i, b_j]$$

$$\text{if} \qquad [B, [A, B]] = 0 \qquad \text{then} \qquad [A, F(B)] = [A, B]F'(B)$$

$$[x, p] = i\hbar \qquad [x, f(p)] = i\hbar f'(p) \qquad [p, g(x)] = -i\hbar g'(x)$$

$$[a, a^\dagger] = 1 \qquad [N, a] = -a \qquad [N, a^\dagger] = a^\dagger$$

10 Uncertainty Relations and Inequalities

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2} \qquad \sigma_Q \sigma_Q = \Delta Q \Delta R \geq \frac{1}{2} \left| \langle i[Q,R] \rangle \right|$$

$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \geq \frac{\hbar}{2}$$

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11 Probability Amplitudes and Probabilities

$$\Psi(x,t) = \langle x|\Psi(t)\rangle \qquad P(dx) = |\Psi(x,t)|^2\,dx \qquad c_i(t) = \langle \phi_i|\Psi(t)\rangle \qquad P(i) = |c_i(t)|^2$$

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12 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \qquad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$

$$L^2 Y_{\ell m} = \ell(\ell+1)\hbar^2 Y_{\ell m} \qquad L_z Y_{\ell m} = m\hbar Y_{\ell m} \qquad |m| \leq \ell \qquad m = -\ell, -\ell+1, \ldots, \ell-1, \ell$$

0	1	2	3	4	5	6	...
s	p	d	f	g	h	i	...

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13 Hydrogenic Atom

$$\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta,\phi) \qquad \ell \leq n-1 \qquad \ell = 0, 1, 2, \ldots, n-1$$

$$a_z = \frac{a}{Z}\left(\frac{m_e}{m_{\text{reduced}}}\right) \qquad a_0 = \frac{\hbar}{m_e c \alpha} = \frac{\lambda_{\text{C}}}{2\pi\alpha} \qquad \alpha = \frac{e^2}{\hbar c}$$

$$R_{10} = 2a_Z^{-3/2} e^{-r/a_Z} \qquad R_{20} = \frac{1}{\sqrt{2}} a_Z^{-3/2} \left(1 - \frac{1}{2}\frac{r}{a_Z}\right) e^{-r/(2a_Z)}$$

$$R_{21} = \frac{1}{\sqrt{24}} a_Z^{-3/2} \frac{r}{a_Z} e^{-r/(2a_Z)}$$

$$R_{n\ell} = -\left\{ \left(\frac{2}{na_Z}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^\ell L_{n+\ell}^{2\ell+1}(\rho) \qquad \rho = \frac{2r}{nr_Z}$$

$$L_q(x) = e^x \left(\frac{d}{dx}\right)^q \left(e^{-x} x^q\right)$$ Rodrigues's formula for the Laguerre polynomials

$$L_q^j(x) = \left(\frac{d}{dx}\right)^j L_q(x)$$ Associated Laguerre polynomials

$$\langle r \rangle_{n\ell m} = \frac{a_Z}{2}\left[3n^2 - \ell(\ell+1)\right]$$

Nodes $= (n-1) - \ell$ not counting zero or infinity

$$E_n = -\frac{1}{2} m_e c^2 \alpha^2 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -E_{\text{Ryd}} \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -13.606 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} \text{ eV}$$

14 General Angular Momentum Formulae

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \qquad \text{(Einstein summation on } k\text{)} \qquad [J^2, \vec{J}] = 0$$

$$J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle \qquad J_z|jm\rangle = m\hbar|jm\rangle$$

$$J_\pm = J_x \pm iJ_y \qquad J_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}|jm\pm 1\rangle$$

$$J_{\left\{ {x \atop y} \right\}} = \left\{ \begin{matrix} \frac{1}{2} \\ \frac{1}{2i} \end{matrix} \right\} (J_+ \pm J_-) \qquad J_\pm^\dagger J_\pm = J_\mp J_\pm = J^2 - J_z(J_z \pm \hbar)$$

$$[J_{fi}, J_{gj}] = \delta_{fg} i\hbar\varepsilon_{ijk}J_k \qquad \vec{J} = \vec{J}_1 + \vec{J}_2 \qquad J^2 = J_1^2 + J_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

$$J_\pm = J_{1\pm} + J_{2\pm} \qquad |j_1 j_2 jm\rangle = \sum_{m_1 m_2, m=m_1+m_2} |j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2|j_1 j_2 jm\rangle j_1 j_2 jm\rangle$$

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \qquad \sum_{|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1)$$

15 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}\left(|+\rangle \pm |-\rangle\right) \qquad |\pm\rangle_y = \frac{1}{\sqrt{2}}\left(|+\rangle \pm i|-\rangle\right) \qquad |\pm\rangle_z = |\pm\rangle$$

$$|++\rangle = |1,+\rangle|2,+\rangle \qquad |+-\rangle = \frac{1}{\sqrt{2}}\left(|1,+\rangle|2,-\rangle \pm |1,-\rangle|2,+\rangle\right) \qquad |--\rangle = |1,-\rangle|2,-\rangle$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k \qquad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

$$(\vec{A}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma}) = \vec{A}\cdot\vec{B} + i(\vec{A}\times\vec{B})\cdot\vec{\sigma}$$

$$\frac{d(\vec{S}\cdot\hat{n})}{d\alpha} = -\frac{i}{\hbar}[\vec{S}\cdot\hat{\alpha}, \vec{S}\cdot\hat{n}] \qquad \vec{S}\cdot\hat{n} = e^{-i\vec{S}\cdot\vec{\alpha}}\vec{S}\cdot\hat{n}_0 e^{i\vec{S}\cdot\vec{\alpha}} \qquad |\hat{n}_\pm\rangle = e^{-i\vec{S}\cdot\vec{\alpha}}|\hat{z}_\pm\rangle$$

$$e^{ixA} = \mathbf{1}\cos(x) + iA\sin(x) \quad \text{if } A^2 = \mathbf{1} \qquad\qquad e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} = \mathbf{1}\cos(x) - i\vec{\sigma}\cdot\hat{\alpha}\sin(x)$$

$$\sigma_i f(\sigma_j) = f(\sigma_j)\sigma_i\delta_{ij} + f(-\sigma_j)\sigma_i(1-\delta_{ij})$$

$$\mu_{\text{Bohr}} = \frac{e\hbar}{2m} = 0.927400915(23)\times 10^{-24}\,\text{J/T} = 5.7883817555(79)\times 10^{-5}\,\text{eV/T}$$

$$g = 2\left(1 + \frac{\alpha}{2\pi} + \ldots\right) = 2.0023193043622(15)$$

$$\vec{\mu}_{\text{orbital}} = -\mu_{\text{Bohr}}\frac{\vec{L}}{\hbar} \qquad \vec{\mu}_{\text{spin}} = -g\mu_{\text{Bohr}}\frac{\vec{S}}{\hbar} \qquad \vec{\mu}_{\text{total}} = \vec{\mu}_{\text{orbital}} + \vec{\mu}_{\text{spin}} = -\mu_{\text{Bohr}}\frac{(\vec{L}+g\vec{S})}{\hbar}$$

$$H_\mu = -\vec{\mu}\cdot\vec{B} \qquad H_\mu = \mu_{\text{Bohr}}B_z\frac{(L_z + gS_z)}{\hbar}$$

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16 **Time-Independent Approximation Methods**

$$H = H^{(0)} + \lambda H^{(1)} \qquad |\psi\rangle = N(\lambda)\sum_{k=0}^{\infty}\lambda^k|\psi_n^{(k)}\rangle$$

$$H^{(1)}|\psi_n^{(m-1)}\rangle(1-\delta_{m,0}) + H^{(0)}|\psi_n^{(m)}\rangle = \sum_{\ell=0}^{m}E^{(m-\ell)}|\psi_n^{(\ell)}\rangle \qquad |\psi_n^{(\ell>0)}\rangle = \sum_{m=0,\ m\neq n}^{\infty}a_{nm}|\psi_n^{(0)}\rangle$$

$$|\psi_n^{1\text{st}}\rangle = |\psi_n^{(0)}\rangle + \lambda\sum_{\text{all } k,\ k\neq n}\frac{\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle$$

$$E_n^{1\text{st}} = E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle$$

$$E_n^{2\text{nd}} = E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle + \lambda^2\sum_{\text{all } k,\ k\neq n}\frac{\left|\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$E(\phi) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} \qquad \delta E(\phi) = 0$$

$$H_{kj} = \langle\phi_k|H|\phi_j\rangle \qquad H\vec{c} = E\vec{c}$$

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17 **Time-Dependent Perturbation Theory**

$$\pi = \int_{-\infty}^{\infty}\frac{\sin^2(x)}{x^2}\,dx$$

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|H_{\rm perturbation}|0\rangle|^2\delta(E_n - E_0)$$

18 Interaction of Radiation and Matter

$$\vec{E}_{\rm op} = -\frac{1}{c}\frac{\partial\vec{A}_{\rm op}}{\partial t} \qquad \vec{B}_{\rm op} = \nabla\times\vec{A}_{\rm op}$$

19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm1, \pm2, \ldots \qquad k = \frac{2\pi n}{L} \qquad \Delta k_{\rm cell} = \frac{2\pi}{L} \qquad \Delta k^3_{\rm cell} = \frac{(2\pi)^3}{V}$$

$$dN_{\rm states} = g\frac{k^2\,dk\,d\Omega}{(2\pi)^3/V}$$

20 Identical Particles

$$|a,b\rangle = \frac{1}{\sqrt{2}}\left(|1,a;2,b\rangle \pm |1,b;2,a\rangle\right)$$

$$\psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)$$

21 Second Quantization

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i, a_j] = 0 \qquad [a_i^\dagger, a_j^\dagger] = 0 \qquad |N_1,\ldots,N_n\rangle = \frac{(a_n^\dagger)^{N_n}}{\sqrt{N_n!}}\cdots\frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1!}}|0\rangle$$

$$\{a_i, a_j^\dagger\} = \delta_{ij} \qquad \{a_i, a_j\} = 0 \qquad \{a_i^\dagger, a_j^\dagger\} = 0 \qquad |N_1,\ldots,N_n\rangle = (a_n^\dagger)^{N_n}\ldots(a_1^\dagger)^{N_1}|0\rangle$$

$$\Psi_s(\vec{r}\,)^\dagger = \sum_{\vec{p}}\frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}}a^\dagger_{\vec{p}s} \qquad \Psi_s(\vec{r}\,) = \sum_{\vec{p}}\frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}}a_{\vec{p}s}$$

$$[\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')]_\mp = 0 \qquad [\Psi_s(\vec{r})^\dagger, \Psi_{s'}(\vec{r}\,')^\dagger]_\mp = 0 \qquad [\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')^\dagger]_\mp = \delta(\vec{r}-\vec{r}\,')\delta_{ss'}$$

$$|\vec{r}_1 s_1,\ldots,\vec{r}_n s_n\rangle = \frac{1}{\sqrt{n!}}\Psi_{s_n}(\vec{r}_n)^\dagger\ldots\Psi_{s_n}(\vec{r}_n)^\dagger|0\rangle$$

$$\Psi_s(\vec{r}\,)^\dagger|\vec{r}_1 s_1,\ldots,\vec{r}_n s_n\rangle\sqrt{n+1}|\vec{r}_1 s_1,\ldots,\vec{r}_n s_n,\vec{r}s\rangle$$

$$|\Phi\rangle = \int d\vec{r}_1\ldots d\vec{r}_n\,\Phi(\vec{r}_1,\ldots,\vec{r}_n)|\vec{r}_1 s_1,\ldots,\vec{r}_n s_n\rangle$$

$$1_n = \sum_{s_1\ldots s_n}\int d\vec{r}_1\ldots d\vec{r}_n\,|\vec{r}_1 s_1,\ldots,\vec{r}_n s_n\rangle\langle\vec{r}_1 s_1,\ldots,\vec{r}_n s_n| \qquad 1 = |0\rangle\langle 0| + \sum_{n=1}^\infty 1_n$$

$$N = \sum_{\vec{p}s} a^\dagger_{\vec{p}s} a_{\vec{p}s} \qquad T = \sum_{\vec{p}s} \frac{p^2}{2m} a^\dagger_{\vec{p}s} a_{\vec{p}s}$$

$$\rho_s(\vec{r}\,) = \Psi_s(\vec{r}\,)^\dagger \Psi_s(\vec{r}\,) \qquad N = \sum_s \int d\vec{r}\, \rho_s(\vec{r}\,) \qquad T = \frac{1}{2m} \sum_s \int d\vec{r}\, \nabla\Psi_s(\vec{r}\,)^\dagger \cdot \nabla\Psi_s(\vec{r}\,)$$

$$\vec{j}_s(\vec{r}\,) = \frac{1}{2im} \left[\Psi_s(\vec{r}\,)^\dagger \nabla\Psi_s(\vec{r}\,) - \Psi_s(\vec{r}\,) \nabla\Psi_s(\vec{r}\,)^\dagger \right]$$

$$G_s(\vec{r} - \vec{r}\,') = \frac{3n}{2} \frac{\sin(x) - x\cos(x)}{x^3} \qquad g_{ss'}(\vec{r} - \vec{r}\,') = 1 - \delta_{ss'} \frac{G_s(\vec{r} - \vec{r}\,')^2}{(n/2)^2}$$

$$v_{\text{2nd}} = \frac{1}{2} \sum_{ss'} \int d\vec{r} d\vec{r}\,'\, v(\vec{r} - \vec{r}\,') \Psi_s(\vec{r}\,)^\dagger \Psi_{s'}(\vec{r}\,')^\dagger \Psi_{s'}(\vec{r}\,') \Psi_s(\vec{r}\,)$$

$$v_{\text{2nd}} = \frac{1}{2V} \sum_{pp'qq'} \sum_{ss'} v_{\vec{p}-\vec{p}\,'} \delta_{\vec{p}+\vec{q},\vec{p}\,'+\vec{q}\,'} a^\dagger_{\vec{p}s} a^\dagger_{\vec{q}s'} a_{\vec{q}\,'s'} a_{\vec{p}\,'s} \qquad v_{\vec{p}-\vec{p}\,'} = \int d\vec{r}\, e^{-i(\vec{p}-\vec{p}\,')\cdot\vec{r}} v(\vec{r}\,)$$

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22 **Klein-Gordon Equation**

$$E = \sqrt{p^2c^2 + m^2c^4} \qquad \frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} \right)^2 \Psi(\vec{r}, t) = \left[\left(\frac{\hbar}{i} \nabla \right)^2 + m^2c^2 \right] \Psi(\vec{r}, t)$$

$$\left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar} \right)^2 \right] \Psi(\vec{r}, t) = 0$$

$$\rho = \frac{i\hbar}{2mc^2} \left(\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right) \qquad \vec{j} = \frac{\hbar}{2im} \left(\Psi^* \nabla \Psi - \Psi \nabla \Psi^* \right)$$

$$\frac{1}{c^2} \left(i\hbar \frac{\partial}{\partial t} - e\Phi \right)^2 \Psi(\vec{r}, t) = \left[\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right)^2 + m^2c^2 \right] \Psi(\vec{r}, t)$$

$$\Psi_+(\vec{p}, E) = e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar} \qquad \Psi_-(\vec{p}, E) = e^{-i(\vec{p}\cdot\vec{r} - Et)/\hbar}$$