

Quantum Mechanics**NAME:**

Homework 1: Schrödinger's Equation and the Wave Function: 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.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	16.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
2.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	17.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
3.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	18.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
4.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	19.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
5.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	20.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
6.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	21.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
7.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	22.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
8.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	23.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
9.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	24.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
10.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	25.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
11.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	26.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
12.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	27.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
13.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	28.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
14.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	29.	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
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1. The nebulous (and sometimes disparaged) concept that all microscopic physical entities have both wave and particle properties is called the wave-particle:

a) singularity. b) duality. c) triality. d) infinality. e) nullility.

2. “Let’s play *Jeopardy!* For \$100, the answer is: The equation that governs (or equations that govern) the time evolution of quantum mechanical systems in the non-relativistic approximation.”

What is/are _____, Alex?

a) $\vec{F}_{\text{net}} = m\vec{a}$ b) Maxwell’s equations c) Einstein’s field equations of general relativity
d) Dirac’s equation e) Schrödinger’s equation

3. The full Schrödinger’s equation in compact form is:

a) $H\Psi = i\hbar \frac{\partial\Psi}{\partial t}$. b) $H\Psi = \hbar \frac{\partial\Psi}{\partial t}$. c) $H\Psi = i \frac{\partial\Psi}{\partial t}$. d) $H\Psi = i\hbar \frac{\partial\Psi}{\partial x}$.
e) $H^{-1}\Psi = i\hbar \frac{\partial\Psi}{\partial t}$.

4. The energy operator in quantum mechanics,

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

(here given for 1 particle in one dimension) is called the:

a) Lagrangian b) Laplacian c) Hamiltonian d) Georgian e) Torontonian

5. “Let’s play *Jeopardy!* For \$100, the answer is: The postulate that the wave function $\Psi(\vec{r})$ is quantum mechanics is a probability amplitude and $|\Psi(\vec{r})|^2$ is a probability density for localizing a particle at \vec{r} on a ‘measurement’.”

What is _____, Alex?

a) Schrödinger’s idea b) Einstein’s notion c) Born’s postulate d) Dirac’s hypothesis
e) Death’s conclusion

6. In the probabilistic interpretation of wave function Ψ , the quantity $|\Psi|^2$ is:

a) a probability density. b) a probability amplitude. c) 1. d) 0.
e) a negative probability.

7. The probability of finding a particle in differential region dx is:

a) $\Psi(x, t) dx$. b) $\Psi(x, t)^* dx$. c) $[\Psi(x, t)^*/\Psi(x, t)] dx$. d) $\Psi(x, t)^2 dx$.
e) $\Psi(x, t)^*\Psi(x, t) dx = |\Psi(x, t)|^2 dx$.

8. “Let’s play *Jeopardy!* For \$100, the answer is: It is an Hermitian operator that governs (or represents in some people’s jargon) a dynamical variable in quantum mechanics.”

What is an _____, Alex?

a) intangible b) intaglio c) obtainable d) oblivion e) observable

9. In quantum mechanics, a dynamical variable is governed by a Hermitian operator called an observable that has an expectation value that is:

a) the most likely value of the quantity given by the probability density: i.e., the mode of the probability density.
b) the median value of the quantity given by the probability density.
c) the mean value of the quantity given by the probability density.
d) any value you happen to measure.
e) the time average of the quantity.

10. The expectation value of operator Q for some wave function is often written:

a) Q . b) $\rangle Q \langle$. c) $\langle Q \rangle$. d) $\langle f(Q) \rangle$. e) $f(Q)$.

11. These quantum mechanical entities must be (with some exceptions):

- i) Single-valued (and their derivatives too).
- ii) finite (and their derivatives too).
- iii) continuous (and their derivatives too).
- iv) normalizable or square-integrable.

They are:

- a) wave functions. b) observables. c) expectation values. d) wavelengths.
 - e) wavenumbers.
12. A physical requirement on wave functions is that they should be:
- a) reliable. b) friable. c) certifiable. d) normalizable. e) retrievable.
13. The momentum operator in one-dimension is:
- a) $\hbar \frac{\partial}{\partial x}$. b) $\frac{\hbar}{i} \frac{\partial}{\partial x}$. c) $\frac{i}{\hbar} \frac{\partial}{\partial x}$. d) $\frac{i}{\hbar} \frac{\partial}{\partial t}$. e) $\hbar \frac{\partial}{\partial t}$.
14. If an observable has no explicit time dependence and it commutes with the Hamiltonian, then it is a quantum mechanical:
- a) fudge factor. b) dynamical variable. c) universal constant.
 - d) constant of the motion. e) constant of the stagnation.
15. Ehrenfest's theorem partially shows the connection between quantum mechanics and:
- a) photonics. b) electronics. c) special relativity. d) general relativity.
 - e) classical mechanics.
16. "Let's play *Jeopardy!* For \$100, the answer is: It describes a fundamental limitation on the accuracy with which we can know position and momentum simultaneously."
- What is _____, Alex?
- a) Tarkovsky's doubtful thesis b) Rublev's ambiguous postulate
 - c) Kelvin's nebulous zeroth law d) Schrödinger's wild hypothesis
 - e) Heisenberg's uncertainty principle
17. "Let's play *Jeopardy!* For \$100, the answer is: It describes a fundamental limitation on the accuracy with which we can know position and momentum simultaneously."
- What is _____, Alex?
- a) Tarkovsky's doubtful thesis b) Rublev's ambiguous postulate
 - c) Kelvin's nebulous zeroth law d) Schrödinger's wild hypothesis
 - e) Heisenberg's uncertainty principle
18. Given the following age distribution, compute its the normalization (i.e., the factor that normalizes the distribution), mean, variance, and standard deviation. Also give the mode (i.e., the age with highest frequency) and median. **HINT:** Doing the calculation with a small computer code would be the efficient way to answer the problem.

Table: Age Distribution

Age (years)	Frequency
14	2
15	1
16	6
22	2
24	2
25	5

19. An indicator needle on a semi-circular scale (e.g., like a needle on car speedometer) bounces around and comes to rest with equal probability at any angle θ in the interval $[0, \pi]$.

- a) Give the probability density $\rho(\theta)$ and sketch a plot of it.
- b) Compute the 1st and 2nd moments of the distribution (i.e., $\langle\theta\rangle$ and $\langle\theta^2\rangle$) and the variance and standard deviation.
- c) Compute $\langle\sin\theta\rangle$, $\langle\cos\theta\rangle$, $\langle\sin^2\theta\rangle$, and $\langle\cos^2\theta\rangle$.

20. Consider the Gaussian probability density

$$\rho(x) = Ae^{-\lambda(x-a)^2},$$

where A , a , and λ are constants.

- a) Determine the normalization constant A .
- b) The n th moment of a probability density is defined by

$$\langle x^n \rangle = \int_{-\infty}^{\infty} x^n \rho(x) dx.$$

Determine the 0th, 1st, and 2nd moments of the Gaussian probability density.

- c) For the Gaussian probability density determine the mean, mode, median, variance σ^2 , and standard deviation (or dispersion) σ .
- d) Sketch the Gaussian probability density.
21. The expression for the probability that a particle is in the region $[-\infty, x]$ (i.e., the cumulative probability distribution function) is

$$P(x, t) = \int_{-\infty}^x |\Psi(x', t)|^2 dx'.$$

- a) Find an explicit, non-integral formula for $\partial P(x, t)/\partial t$ given that the wave function is normalizable at time t . Simplify the formula as much as reasonably possible. **HINT:** Make use of the physics: i.e., the Schrödinger equation itself. This is a common trick in quantum mechanics and, *mutatis mutandis*, throughout physics. It probably helps to let the dummy variable in the integral be x and the endpoint a while doing the math.
- b) Recall momentum observable is

$$p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x}.$$

Substitute p_{op} into the formula derived in part (a) and simplify as much as possible. In the simplification, make use of the real-part function Re which has the property that

$$\text{Re}(z)$$

is the real part of complex variable z . For example, if $z = x + iy$, then

$$\text{Re}(z) = \text{Re}(x + iy) = x.$$

HINT: Note that

$$-p_{\text{op}}\Psi^* = (p_{\text{op}}\Psi)^*.$$

- c) If the wave function is normalizable at time t , show that $P(\infty, t)$ is a constant with respect to time: i.e., total probability is conserved.
- d) The probability current is defined

$$J(x, t) = -\frac{\partial P(x, t)}{\partial t}.$$

Argue that this is a sensible definition. Then using the part (b) answer write an explicit formula for $J(x, t)$ in terms of the wave function. Discuss how this formula corresponds to a classical current density: e.g.,

$$\vec{v}\rho$$

where \vec{v} is velocity and ρ is a density of something.

e) Given

$$\Psi(x, t) = \psi(x)e^{-i\omega t} ,$$

what can one say about the probability density $|\Psi|^2$, the cumulative probability function $P(x, t)$, and the probability current $J(x, t)$?

22. “God does not play dice”—Einstein. Discuss.

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

2 Some Useful Formulae

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

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

3 Schrödinger's Equation

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

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

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

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

4 Some Operators

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

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

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

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

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

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

5 Kronecker Delta and Levi-Civita Symbol

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

$$\varepsilon_{ijk} \varepsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \quad (\text{Einstein summation on } i)$$

6 Time Evolution Formulae

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

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

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

7 Simple Harmonic Oscillator (SHO) Formulae

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

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

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

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

8 Position, Momentum, and Wavenumber Representations

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

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

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

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

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

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

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

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

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

9 Commutator Formulae

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

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

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

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

10 Uncertainty Relations and Inequalities

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

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

11 Probability Amplitudes and Probabilities

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

12 Spherical Harmonics

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

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

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

13 Hydrogenic Atom

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

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

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

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

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

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

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

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

$$\text{Nodes} = (n-1) - \ell \quad \text{not counting zero or infinity}$$

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

14 General Angular Momentum Formulae

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

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

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

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

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

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

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

15 Spin 1/2 Formulae

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

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

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

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

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

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

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

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

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

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

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

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

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

16 Time-Independent Approximation Methods

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

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

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

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

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

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

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

17 Time-Dependent Perturbation Theory

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

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

18 Interaction of Radiation and Matter

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

19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm 1, \pm 2, \dots \quad k = \frac{2\pi n}{L} \quad \Delta k_{\text{cell}} = \frac{2\pi}{L} \quad \Delta k_{\text{cell}}^3 = \frac{(2\pi)^3}{V}$$

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

20 Identical Particles

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

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

21 Second Quantization

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

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

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

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

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

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

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

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

$$N = \sum_{\vec{p}s} a_{\vec{p}s}^\dagger a_{\vec{p}s} \quad T = \sum_{\vec{p}s} \frac{p^2}{2m} a_{\vec{p}s}^\dagger a_{\vec{p}s}$$

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

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

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

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

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

22 Klein-Gordon Equation

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

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

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

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

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