Quantum Mechanics **NAME:**

Homework 2a: 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. The time-independent Schrödinger equation is obtained from the full Schrödinger equation by:

   a) colloquialism. b) solution for eigenfunctions. c) separation of the x and y variables. d) separation of the space and time variables. e) expansion.

2. A system in a stationary state will:

   a) not evolve in time. b) evolve in time. c) both evolve and not evolve in time. d) occasionally evolve in time. e) violate the Heisenberg uncertainty principle.

3. For a Hermitian operator eigenproblem, one can always find (subject to some qualitifications perhaps—but which are just mathemtical hemming and hawwing) a complete set (or basis) of eigenfunctions that are:

   a) independent of the x-coordinate. b) orthonormal. c) collinear. d) pathological. e) righteous.

4. "Let's play *Jeopardy*! For $100, the answer is: If it shares the same same range as a basis set of functions and is at least piecewise continuous, then it can be expanded in the basis with a vanishing limit of the mean square error between it and the expansion."

   What is a/an ____________, Alex?

   a) equation b) function c) triangle d) deduction e) tax deduction

5. "Let's play *Jeopardy*! For $100, the answer is: The postulate that expansion coefficients of a wave function in the eigenstates of an observable are the probability amplitudes for wave function collapse to eigenstates of that observable."

   What is ____________, Alex?

   a) the special Born postulate b) the very special Born postulate c) normalizability d) the mass-energy equivalence e) the general Born postulate

6. The expansion of a wave function in an observable's basis (or complete set of eigenstates) is

   a) just a mathematical decomposition. b) useless in quantum mechanics. c) irrelevant in quantum mechanics. d) not just a mathematical decomposition since the expansion coefficients are probability amplitudes. e) just.

7. "Let's play *Jeopardy*! For $100, the answer is: A state that no macroscopic system can be in except arguably for states of Bose-Einstein condensates, superconductors, superfluids and maybe others sort of."

   What is a/an ____________, Alex?

   a) stationary state b) accelerating state c) state of the Union d) state of being e) state of mind

8. A stationary state is:

   a) just a special kind of classical state. b) more or less a kind of classical state. c) voluntarily a classical state. d) was originally not a classical state, but grew into one. e) radically unlike a classical state.

9. Except arguably for certain special cases (superconductors, superfluids, and Bose-Einstein condensates), no macroscopic system can be in a:

   a) mixed state. b) vastly mixed state. c) classical state. d) stationary state. e) state of the union.

10. "Let's play *Jeopardy*! For $100, the answer is: An equation that must hold in order for the non-relativistic Hamiltonian operator and the operator $i\hbar\partial/\partial t$ to both yield an energy expectation value for a wave function $\Psi(x,t)$."

    What is ____________, Alex?

    a) the continuity equation b) the Laplace equation c) Newton's 2nd law d) Schrödinger's equation e) Hamiton's equation

11. Can the gravitational potential cause quantization of energy states?

    a) No. b) It is completely uncertain. c) Theoretically yes, but experimentally no.
    d) Experimental evidence to date (post-2001) suggests it can.
    e) In principle there is no way of telling.

12. It follows from the general Born postulate that the expectation value of an observable Q is given by

$$\langle Q\rangle = \int_{-\infty}^{\infty} \Psi^* Q \Psi \, dx \ .$$

It's weird to call an operator an observable, but that is the convention (Co-137).

a) Write down the explicit expression for

$$\frac{d\langle Q\rangle}{dt} \ .$$

Recall Q in general can depend on time too.

b) Now use the Schrödinger equation

$$H\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

to eliminate partial time derivatives where possible in the expression for $d\langle Q\rangle/dt$. Remember how complex values behave when complex conjugated. You should use the angle bracket form for expectation values to simplify the expression where possible.

c) The commutator of two operators A and B is defined by

$$[A, B] = AB - BA \ ,$$

where it is always understood that the commutator and operators are acting on an implicit general function to the right. If you have trouble initially remembering the understood condition, you can write

$$[A, B]f = (AB - BA)f \ ,$$

where f is an explicit general function. Operators don't in general commute: i.e., $[A, B] = AB - BA \neq 0$ in general. Prove

$$\left[\sum_i A_i, \sum_j B_j\right] = \sum_{i,j}[A_i, B_j] \ .$$

d) Now show that $d\langle Q\rangle/dt$ can be written in terms of $\langle i[H, Q]\rangle$. The resulting important expression oddly enough doesn't seem to have a common name. I just call it the general time evolution formula. **HINTS:** First, V and Ψ^* do commute. Second, the other part of the Hamiltonian operator

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

can be put in the right place using integration by parts and the normalization condition on the wave function. Note T turns out to be the kinetic energy operator.

e) If $d\langle Q\rangle/dt = 0$, then Q is a quantum mechanical constant of the motion. It's weird to call an observable (which is a operator) a constant of the motion, but that is the convention (Co-247). Show that the operator $Q = 1$ (i.e., the unit operator) is a constant of the motion. What is $\langle 1\rangle$?

f) Find the expression for $d\langle x\rangle/dt$ in terms of what we are led to postulate as the momentum operator

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

The position operator x should be eliminated from the expression. **HINTS:** Note V and x commute, but T and x do not. Leibniz's formula (Ar-558) might be of use in evaluating the commutator $[T, x]$. The formula is

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

13. In one dimension, Ehrenfest's theorem in quantum mechanics is usually taken to consist of two formulae:

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p\rangle$$

and

$$\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x}\right\rangle ,$$

where the angle brackets indicate expectation values as usual.

a) From the general time evolution formula prove the 1st Ehrenfest formula. **HINTS:** Recall the general time evolution formula in non-relativistic quantum mechanics is

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

where Q is any observable and H is the Hamiltonian:

$$H = T + V(x) .$$

Also recall that quantum mechanical momentum operator and kinetic energy operator are given by

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad \text{and} \qquad T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} ,$$

respectively. Leibniz's formula (Ar-558) might be of use in evaluating some of the commutators:

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

b) From the general time evolution formula prove the 2nd Ehrenfest formula.

c) In the macroscopic limit, the expectation values become the classical dynamical variables by the correspondence principle (which is an auxiliary principle of quantum mechanics enunciated by Bohr in 1920 (Wikipedia: Correspondance principle)): i.e., $\langle x\rangle$ becomes x, etc. (Note we are allowing a common ambiguity in notation: x and p are both coordinates and, in the classical formalism, the dynamical variables describing the particle. Everybody does this: who are we do disagree.) Find the macroscopic limits of the Ehrenfest formulae and identify the macroscopic limits in the terminology of classical physics.

d) If you **ARE** writing a **TEST**, omit this part.
If one combines the two Ehrenfest formulae, one gets

$$m\frac{d^2\langle x\rangle}{dt^2} = -\left\langle \frac{\partial V}{\partial x}\right\rangle$$

which looks very like Newton's 2nd law in its $F = ma$ form for a force given by a potential. Using the correspondence priniciple, it does become the 2nd law in the macroscopic limit. However, an interesting question arises—well maybe not all that interesing—does the $\langle x\rangle$ (which we could call the center of the wave packet) actually obey the 2nd law-like expression

$$m\frac{d^2\langle x\rangle}{dt^2} = -\frac{\partial V(\langle x\rangle)}{\partial\langle x\rangle} \ ?$$

To disprove a general statement, all you need to do is find one counterexample. Consider a potential of the form $V(x) = Ax^\lambda$, and show that in general the $\langle x\rangle$ doesn't obey 2nd law-like expression given above. Then show that it does in three special cases of λ.

14. You are given a complete set of orthonormal stationary states (i.e., energy eigenfunctions) $\{\psi_n\}$ and a general wave equation $\Psi(x,t)$ that is for the same system as $\{\psi_n\}$: i.e., $\Psi(x,t)$ is detemined by the same

Hamiltonian as $\{\psi_n\}$. The set of eigen-energies of $\{\psi_n\}$ are $\{E_n\}$. The system is bounded in space by $x = -\infty$ and $x = \infty$.

a) Give the formal expansion expression of $\Psi(x, 0)$ (i.e., $\Psi(x, t)$ at time zero) in terms of $\{\psi_n\}$. Also give the formal expression for the coefficients of expansion c_n.

b) Now give the formal expansion for $\Psi(x, t)$ remembering that $\omega_n = E_n/\hbar$. Justify that this is the solution of the Schrödinger equation for the initial conditions $\Psi(x, 0)$.

c) Find the general expression, simplified as far as possible, for expectation value $\langle H^\ell \rangle$ in terms of the expansion coefficients, where ℓ is any positive (or zero) integer. Are these values time dependent?

d) Give the special cases for $\ell = 0$, 1, and 2, and the expression for the standard deviation for energy σ_E. **HINTS:** This should be a very short answer: 3 or 4 lines.

15. Classically $E \geq V_{\text{min}}$ for a particle in a conservative system.

a) Show that this classical result must be so. **HINT:** This shouldn't be a from-first-principles proof: it should be about one line.

b) The quantum mechanical analog is almost the same: $\bar{E} = \langle H \rangle > V_{\text{min}}$ for any normalizable state of the system considered. Note the equality $\bar{E} = \langle H \rangle = V_{\text{min}}$ never holds quantum mechanically. (There is an over-idealized exception, which we consider in part (e).) Prove the inequality. **HINTS:** The key point is to show that $\langle T \rangle > 0$ for all physically allowed states. Use integration by parts.

c) Now show that result $\bar{E} > V_{\text{min}}$ implies $E > V_{\text{min}}$, where E is any eigen-energy of the system considered. Note the equality $E = V_{\text{min}}$ never holds quantum mechanically (except for the over-idealized system considered in part (e)). In a sense, there is no rest state for quantum mechanical particle. This lowest energy is called the zero-point energy.

d) The $E > V_{\text{min}}$ result for an eigen-energy in turn implies a 3rd result: any ideal measurement always yields an energy greater than V_{min} Prove this by reference to a quantum mechanical postulate.

e) This part is **NOT** to be done on **EXAMS**: it's just too much (for the grader). There is actually an exception to $E > V_{\text{min}}$ result for an eigen-energy where $E = V_{\text{min}}$ occurs. The exception is for quantum mechanical systems with periodic boundary conditions and a constant potential. In ordinary 3-dimensional Euclidean space, the periodic boundary conditions can only occur for rings (1-dimensional systems) and sphere surfaces (2-dimensional systems) I believe. Since any real system must have a finite size in all 3 spatial dimensions, one cannot have real systems with only periodic boundary conditions. Thus, the exception to the $E > V_{\text{min}}$ result is for unrealistic over-idealized systems. Let us consider the idealized ring system as an example case. The Hamiltonian for a 1-dimensional ring with a constant potential is

$$H = -\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\phi^2} + V ,$$

where r is the ring radius, ϕ is the azimuthal angle, and V is the constant potential. Find the eigen-functions and eigen-energies for the Schrödinger equation for the ring system with periodic boundary conditions imposed. Why must one impose periodic boundary conditions on the solutions? What solution has eigen-energy $E = V_{\text{min}}$?

16. The constant energy of a classical particle in a conservative system is given by

$$E = T + V .$$

Since classically $T \geq 0$ always, a bound particle is confined by surface defined by $T = 0$ or $E = V(\vec{r})$. The points constituting this surface are called the turning points: a name which makes most sense in one dimension. Except for static cases where the turning point is trivially the rest point (and maybe some other weird cases), the particle comes to rest only for an instant at a turning point since the forces are unbalanced there. So it's a place where a particle "ponders for an instant before deciding where to go next". The region with $V > E$ is classically forbidden. Now for most quantum mechanical potential wells, the wave function extends beyond the classical turning point surface into the classical forbidden zone and, in fact, usually goes to zero only at infinity. If the potential becomes infinite somewhere (which is an idealization of course), the wave function goes to zero: this happens for the infinite square well for instance.

Let's write the 1-dimensional time-independent Schrödinger equation in the form

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m}{\hbar^2}(V - E)\psi \ .$$

a) Now solve for ψ for the region with $V > E$ with simplifying the assumption that V is constant in this region.

b) Can the solutions be normalized?

c) Can the solutions constitute an entire wave function? Can they be part of a wave function? In which regions?

d) Although we assumed constant V, what crudely is the behavior of the wave function likely to be like the regions with $V > E$.

e) For typical potentials considered at our level, qualitatively what is the likelihood of finding the particle in the classically forbidden region? Why?

17. If there are no internal degrees of freedom (e.g., spin) and they are **NORMALIZABLE**, then one-particle, 1-dimensional energy eigenstates are non-degenerate. We (that is to say you) will prove this.

Actually, we know already that any 2nd order ordinary linear differential equation has only two linearly independent solutions (Ar-402) which means, in fact, that from the start we know there is a degeneracy of 2 at most. Degeneracy count is the number of independent solutions. If there is more than one independent solution, then infinitely many linear combinations of solutions have the same energy. But in an expansion of wave function, only a set linear independent solutions is needed and thus the number of such solutions is the physically relevant degeneracy. Of course, our proof means that one of the linearly independent solutions is not normalizable.

a) Assume you have two degenerate 1-dimensional energy eigenstates for Hamiltonian H: ψ_1 and ψ_2. Prove that $\psi_1\psi_2' - \psi_2\psi_1'$ equals a constant where the primes indicate derivative with respect to x the spatial variable. **HINT:** Write down the eigenproblem for both ψ_1 and ψ_2 and do some multiplying and subtraction and integration.

b) Prove that the constant in part (a) result must be zero. **HINT:** To be physically allowable eigenstates, the eigenstates must be normalizable.

c) Integrate the result of the part (b) answer and show that the two assumed solutions are not physically distinct. Show for all x that

$$\psi_2(x) = C\psi_1(x) \ ,$$

where C is a constant. This completes the proof of non-degeneracy since eigenstates that differ by a multiplicative constant are not physically (i.e., expansion) distinct. **HINT:** You have to show that there is no other way than having $\psi_2(x) = C\psi_1(x)$ to satisfy the condition found in the part (b) answer. Remember the eigenproblem is a linear, homogeneous differential equation.

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

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

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

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

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

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

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

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

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5 Kronecker Delta and Levi-Civita Symbol

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

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

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6 Time Evolution Formulae

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

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

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

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7 Simple Harmonic Oscillator (SHO) Formulae

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

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

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

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

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

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\cos(\theta) \qquad Y_{1,\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin(\theta)e^{\pm i\phi}$$

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

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

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13 Hydrogenic Atom

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

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

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

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

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

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

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

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

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

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

14 General Angular Momentum Formulae

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

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

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

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

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

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

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

15 Spin 1/2 Formulae

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

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

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

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

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

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

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

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

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

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

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

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

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

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16 Time-Independent Approximation Methods

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

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

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

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

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

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

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

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17 Time-Dependent Perturbation Theory

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

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

18 Interaction of Radiation and Matter

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

19 Box Quantization

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

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

20 Identical Particles

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

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

21 Second Quantization

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

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

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

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

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

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

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

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

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

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

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

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

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

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

22 Klein-Gordon Equation

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

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

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

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

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