# 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.

	a	b	с	d	е		a	b	с	d	е
1.	0	0	0	0	Ο	16.	0	Ο	0	0	0
2.	0	0	0	0	0	17.	0	0	Ο	Ο	Ο
3.	0	0	0	0	0	18.	0	Ο	Ο	0	Ο
4.	0	0	0	0	0	19.	0	0	0	0	0
5.	0	0	Ο	Ο	Ο	20.	0	0	Ο	0	0
6.	0	Ο	Ο	Ο	Ο	21.	0	Ο	Ο	Ο	Ο
7.	0	0	0	0	0	22.	0	0	0	0	0
8.	0	0	Ο	Ο	Ο	23.	0	0	Ο	0	0
9.	0	0	0	0	0	24.	0	0	0	0	0
10.	0	Ο	Ο	Ο	Ο	25.	0	Ο	Ο	Ο	Ο
11.	0	Ο	Ο	Ο	Ο	26.	0	0	Ο	Ο	Ο
12.	0	Ο	Ο	Ο	Ο	27.	0	Ο	Ο	Ο	Ο
13.	0	Ο	Ο	Ο	Ο	28.	0	Ο	Ο	Ο	Ο
14.	0	0	0	0	0	29.	0	0	0	0	Ο
15.	0	0	Ο	Ο	Ο	30.	0	0	Ο	0	0

# Answer Table for the Multiple-Choice Questions

002 qmult 00080 1 1 2 easy memory: wave-particle duality

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.

## SUGGESTED ANSWER: (b)

The wave-particle duality is isn't really a law of nature because you can't really derive anything from it, it seems. I think it's just a helpful description. Griffiths (p. 420) believes it's anti-helpful. But it's historical. Niels Bohr liked it a lot.

#### Wrong answers:

e) Oh, c'mon.

Redaction: Jeffery, 2001jan01

002 qmult 00090 1 4 5 easy deducto-memory: Sch eqn

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

#### SUGGESTED ANSWER: (e)

#### Wrong answers:

d) The Dirac equation for electrons includes relativistic effects.

Redaction: Jeffery, 2001jan01

002 qmult 00100 1 1 1 easy memory: Sch eqn compact form

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)  $H^{-1}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ .

### SUGGESTED ANSWER: (a)

#### Wrong Answers:

- b) The i is missing.
- c) The  $\hbar$  is missing.

Redaction: Jeffery, 2001jan01

002 qmult 00110 1 1 3 easy memory: Hamiltonian operator

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

## SUGGESTED ANSWER: (c)

#### Wrong answers:

- a) This another operator in quantum field theory or a function in classical mechanics.
- b) This the  $\nabla^2$  operator.
- d) Neptune was originally named Georgium Sidus (George's Star) by William Herschel, its discoverer. He was honoring his patron George III. I think I've seen Neptune referred to

as the Georgian in very old books. Anyway, other astronomers thought Georgium Sidus was too Britannic and settled on Neptune.

e) An inhabitant of Toronto.

Redaction: Jeffery, 2008jan01

002 qmult 00200 143 easy deducto-memory: Born postulate

**Extra keywords:** mathematical physics

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 ideab) Einstein's notionc) Born's postulated) Dirac's hypothesise) Death's conclusion

## SUGGESTED ANSWER: (c)

I think one should think of the particle as being in a superposition of places and interpret  $\Psi(\vec{r})$  as the weighting for the particle at  $\vec{r}$ .

'Measurement' is a euphemism for wave function collapse in my opinion.

### Wrong answers:

a) As Lurch would say AAAARGH.

Redaction: Jeffery, 2008jan01

## 002 qmult 00210 1 1 1 easy memory: QM probability density

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

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

e) a negative probability.

## SUGGESTED ANSWER: (a)

## Wrong answers:

- b) The probability amplitude is  $\Psi$  itself.
- e) A nonsense answer.

Redaction: Jeffery, 2001jan01

# 002 qmult 002<br/>20 115 easy memory: probability of finding particle in dx

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)  $\Psi(x,t)^* \Psi(x,t) dx = |\Psi(x,t)|^2 dx$ .

### SUGGESTED ANSWER: (e)

#### Wrong Answers:

a) I'm always making this mistake when the wave function is pure real.

Redaction: Jeffery, 2001jan01

002 qmult 00300 1 4 5 easy deducto-memory: observable defined

Extra keywords: See Co-137, Gr-104

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) intaglible b) intaglio c) obtainable d) oblivion e) observable

SUGGESTED ANSWER: (e)

## Wrong answers:

a) As Lurch would say AAAARGH.

Redaction: Jeffery, 2008jan01

002 qmult 00310 1 1 3 easy memory: expectation value defined

- 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.

### SUGGESTED ANSWER: (c)

Why do we use this funny jargon term expectation value in quantum mechanics? Who knows. We're stuck with it though.

Remember the expectation values are ensemble means: i.e., the means for an infinite ensemble of identical systems measured at the same time in their evolution.

#### Wrong Answers:

e) No. The probability density is for an ensemble of identical states all at one time.

Redaction: Jeffery, 2001jan01

002 qmult 00320 1 1 3 easy memory: expectation value notation 10. The expectation value of operator Q for some wave function is often written:

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

## SUGGESTED ANSWER: (c)

### Wrong Answers:

- d) This is expectation value of the operator f(Q).
  - e) This is the operator f(Q).

Redaction: Jeffery, 2001jan01

002 qmult 00400 1 1 1 easy memory: physical requirments Extra keywords: Gr-11

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.

## SUGGESTED ANSWER: (a)

#### Wrong answers:

b) So-so guess.

Redaction: Jeffery, 2008jan01

002 qmult 00410 1 1 4 easy memory: normalization requirement

12. A physical requirement on wave functions is that they should be:

a) reliable. b) friable. c) certifiable. d) normalizable. e) retriable.

SUGGESTED ANSWER: (d)

### Wrong Answers:

e) C'mon.

#### Redaction: Jeffery, 2001jan01

002 qmult 00500 1 1 2 easy memory: the momentum operator defined 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)  $\hbar \frac{\partial}{\partial t}$ 

SUGGESTED ANSWER: (b)

#### Wrong Answers:

e) C'mon.

Redaction: Jeffery, 2001jan01

002 qmult 00510 1 1 4 easy memory: constant of the motion

- 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.

**SUGGESTED ANSWER:** (d): It may seem strange to call an operator a constant of the motion rather than it's expectation value, but that is the jargon used by M1-512 and Co-248. Mike Claude ought to know.

#### Wrong Answers:

e) Say what.

Redaction: Jeffery, 2001jan01

002 qmult 00520 1 4 5 easy deducto-memory: Ehrenfest's theorem

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.

### SUGGESTED ANSWER: (e)

See Co-242 for Ehrenfest's theorem.

It's only a partial connection. The world is still waiting for the consensus theory of how classical physics emerges as a limiting form of quantum mechanics. At least that is the impression I get.

### Wrong Answers:

d) The world is still waiting for this connection.

Redaction: Jeffery, 2001jan01

002 qmult 00600 1 4 5 easy deducto-memory: uncertainty principle 1

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

# SUGGESTED ANSWER: (e)

#### Wrong answers:

a) Tarkovsky, you should be living in this hour.

Redaction: Jeffery, 2001jan01

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

## SUGGESTED ANSWER: (e)

#### Wrong answers:

a) Tarkovsky, you should be living in this hour.

Redaction: Jeffery, 2001jan01

002 qfull 00100 1 3 0 easy math: probability and age distribution

Extra keywords: (Gr-10:1.1)

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

$\begin{array}{c} \text{Age} \\ \text{(years)} \end{array}$	Frequency	
14	2	
15	1	
16	6	
22	2	
24	2	
25	5	

**SUGGESTED ANSWER:** The normalization is 1/18, the mean 19.56, the variance 18.36, and the standard deviation 4.28. The mode is 16. Because of the sparseness of the data, the median is somewhat ill-defined. One could put it anywhere from 16 to 22. The middle of this range 19 is probably most sensible.

### Fortran Code

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\*

```
program ages
 parameter (nage=6)
 dimension age(2, nage)
 data age/14.,2., 15.,1., 16.,6., 22.,2.,
&
          22.,2., 25.,5./
 sum0=0.
 sum1=0.
 sum 2=0.
 do i=1,nage
 sum0=sum0+age(2,i)
  sum1=sum1+age(1,i)*age(2,i)
  sum2=sum2+age(1,i)**2*age(2,i)
 end do
 xmean=sum1/sum0
 var=sum2/sum0-xmean**2
 stdev=sqrt(var)
 print*,'sum0,xmean,var,stdev'
 print*, sum0, xmean, var, stdev
        18. 19.5555553 18.3580322 4.28462744
```

end

Redaction: Jeffery, 2001jan01

002 qfull 00200 2 3 0 moderate math: probability needle 1

Extra keywords: (Gr-10:1.3) probability and continuous variables

- 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  $\theta$  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  $\langle \cos^2 \theta \rangle$ .

### SUGGESTED ANSWER:

a) The probability density is

$$\rho(\theta) = \begin{cases} \frac{1}{\pi} , & \theta \in [0, \pi]; \\ 0 , & \text{otherwise.} \end{cases}$$

Note that the density is normalized: i.e., the zeroth moment of the distribution is

$$1 = \left< \theta^0 \right> = \int_0^\pi \rho(\theta) \, d\theta \; .$$

The sketch you will just have to imagine.

b) The items are

$$\begin{split} \langle \theta \rangle &= \int_0^\pi \frac{\theta}{\pi} \, d\theta = \frac{1}{\pi} \left( \frac{\theta^2}{2} \right) \Big|_0^\pi = \frac{\pi}{2} \; ,\\ \langle \theta^2 \rangle &= \int_0^\pi \frac{\theta^2}{\pi} \, d\theta = \frac{1}{\pi} \left( \frac{\theta^3}{3} \right) \Big|_0^\pi = \frac{\pi^2}{3} \; ,\\ \sigma^2 &= \langle \theta^2 \rangle - \langle \theta \rangle^2 = \frac{\pi^2}{3} - \left( \frac{\pi}{2} \right)^2 = \frac{\pi^2}{12} \; ,\\ \sigma &= \frac{\pi}{2} \; . \end{split}$$

and

$$\sigma = \frac{\pi}{2\sqrt{3}} \; .$$

Note that the general nth moment expression is

$$\langle \theta^n \rangle = \int_0^\pi \frac{\theta^n}{\pi} d\theta = \frac{1}{\pi} \left( \frac{\theta^{n+1}}{n+1} \right) \Big|_0^\pi = \frac{\pi^n}{n+1} \; .$$

c) The items are

$$\begin{split} \langle \sin \theta \rangle &= \int_0^\pi \frac{\sin \theta}{\pi} \, d\theta = \frac{-\cos \theta}{\pi} \Big|_0^\pi = \frac{2}{\pi} \approx \frac{2}{3} \;, \\ \langle \cos \theta \rangle &= \int_0^\pi \frac{\cos \theta}{\pi} \, d\theta = \frac{\sin \theta}{\pi} \Big|_0^\pi = 0 \;, \\ \langle \sin^2 \theta \rangle &= \int_0^\pi \frac{\sin^2 \theta}{\pi} \, d\theta = \frac{1}{\pi} \int_0^\pi \frac{1}{2} [1 - \cos(2\theta)] \, d\theta = \frac{1}{2\pi} \left[ \theta - \frac{\sin(2\theta)}{2} \right] \Big|_0^\pi = \frac{1}{2} \;, \\ \langle \cos^2 \theta \rangle &= \int_0^\pi \frac{\cos^2 \theta}{\pi} \, d\theta = \frac{1}{\pi} \int_0^\pi \frac{1}{2} [1 + \cos(2\theta)] \, d\theta = \frac{1}{2\pi} \left[ \theta + \frac{\sin(2\theta)}{2} \right] \Big|_0^\pi = \frac{1}{2} \;. \end{split}$$

and

$$\langle \cos^2 \theta \rangle = \int_0^\pi \frac{\cos^2 \theta}{\pi} \, d\theta = \frac{1}{\pi} \int_0^\pi \frac{1}{2} [1 + \cos(2\theta)] \, d\theta = \frac{1}{2\pi} \left[ \theta + \frac{\sin(2\theta)}{2} \right] \Big|_0^\pi = \frac{1}{2} \, .$$

Redaction: Jeffery, 2001jan01

002 qfull 00220 1 3 0 easy math: Gaussian probability density Extra keywords: (Gr-11:1.6)

20. Consider the Gaussian probability density

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

where A, a, and  $\lambda$  are constants.

- a) Determine the normalization constant A.
- b) The nth 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, mediam, variance  $\sigma^2$ , and standard deviation (or dispersion)  $\sigma$ .
- d) Sketch the Gaussian probability density.

## SUGGESTED ANSWER:

a) Behold:

$$1 = \int_{-\infty}^{\infty} \rho(x) \, dx = A \int_{-\infty}^{\infty} e^{-\lambda(x-a)^2} \, dx = A \sqrt{\frac{\pi}{\lambda}} \, ,$$

where we have used a table integral. Thus the

$$A = \sqrt{\frac{\lambda}{\pi}} \; .$$

b) Behold:

$$\langle x^0 \rangle = \int_{-\infty}^{\infty} \rho(x) \, dx = 1 ,$$

$$\langle x^1 \rangle = \int_{-\infty}^{\infty} x \rho(x) \, dx = \int_{-\infty}^{\infty} [(x-a)+a]\rho(x) \, dx = a ,$$
and
$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \rho(x) \, dx = \int_{-\infty}^{\infty} (x-a+a)^2 \rho(x) \, dx = \int_{-\infty}^{\infty} [(x-a)^2 + 2(x-a)a + a^2]\rho(x) \, dx = 0$$

a

$$\begin{split} \langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 \rho(x) \, dx = \int_{-\infty}^{\infty} (x - a + a)^2 \rho(x) \, dx = \int_{-\infty}^{\infty} [(x - a)^2 + 2(x - a)a + a^2] \rho(x) \, dx \\ &= \int_{-\infty}^{\infty} y^2 \sqrt{\frac{\lambda}{\pi}} e^{-\lambda y^2} \, dy + a^2 \\ &= \frac{\sqrt{\pi}}{2} \frac{1}{\lambda^{3/2}} \sqrt{\frac{\lambda}{\pi}} + a^2 = \frac{1}{2\lambda} + a^2 \; , \end{split}$$

where we have used MAT.

c) The mean is the first moment of the density: i.e., a. By symmetry and the fact that the mean is a global maximum for the density, it follows at once that the mode and median are also a. From the part (b) answer it follows that

$$\sigma^2 = \langle (x-a)^2 \rangle = \langle x^2 \rangle - a^2 = \frac{1}{2\lambda}$$
, and so  $\sigma = \frac{1}{\sqrt{2\lambda}}$ .

d) You will have to imagine the sketch. The density is symmetric about point a where the maximum is located. Near the maximum the curve is parabolic:

$$e^{-(x-a)^2/(2\sigma^2)} \approx 1 - \frac{(x-a)^2}{2\sigma^2}$$

for  $|x - a| \ll \sigma$ . This region is the Gaussian core. Far from a (i.e.,  $|x - a| \gtrsim \sigma$ ) the curve declines rapidly: these regions are the Gaussian wings.

Redaction: Jeffery, 2001jan01

002 qfull 00310 2 5 0 moderate thinking: probability conservation **Extra keywords:** (Gr-13:1.9) probability current

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

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

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

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

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

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

**HINT:** Note that

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

- 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  $\rho$  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)?

## SUGGESTED ANSWER:

a) Behold:

$$\begin{split} \frac{\partial P(a,t)}{\partial t} &= \frac{\partial}{\partial t} \int_{-\infty}^{a} |\Psi(x,t)|^2 \, dx = \int_{-\infty}^{a} \frac{\partial}{\partial t} |\Psi(x,t)|^2 \, dx \\ &= \int_{-\infty}^{a} \left( \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \right) \, dx \, \,, \end{split}$$

where the partial derivative operator can be put inside the integral since the end points don't depend on t. Recall x is a coordinate here, **NOT** a dynamical variable. So x does **NOT** depend on t.

Now from the Schrödinger equation

$$\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar} H \Psi = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi$$

and

$$\frac{\partial \Psi^*}{\partial t} = -\frac{1}{i\hbar}H\Psi^* = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \; ,$$

where we only consider real potentials as usual. It now follows that

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{i\hbar}{2m} \left(\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2}\right) = \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)$$

We can now integrate the expression for the time derivative of the cumulative probability function to get

$$\frac{\partial P(a,t)}{\partial t} = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \Big|_{-\infty}^a = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \Big|_{x=a} ,$$

where we have assumed the wave function is normalizable, and so the term evaluated at  $-\infty$  is zero as it must be for any normalizable wave function.

Now converting a to the general x gives

$$\frac{\partial P(x,t)}{\partial t} = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \ ,$$

where the x dependence of the right-hand side is implicit. Note that  $\partial P(x,t)/\partial t$  is pure real. b) Begorra:

$$\begin{aligned} \frac{\partial P(x,t)}{\partial t} &= \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) = \frac{i\hbar}{2m} \left( \Psi^* \frac{i}{\hbar} p_{\rm op} \Psi - \Psi \frac{i}{\hbar} p_{\rm op} \Psi^* \right) \\ &= -\frac{1}{2m} \left( \Psi^* p_{\rm op} \Psi - \Psi p_{\rm op} \Psi^* \right) = -\frac{1}{2m} \left[ \Psi^* p_{\rm op} \Psi + \Psi (p_{\rm op} \Psi)^* \right] \\ &= -\frac{1}{m} \operatorname{Re}(\Psi^* p_{\rm op} \Psi) \;. \end{aligned}$$

Now isn't this a cute, compact formula.

c) If the wave function is normalizable at time t, it must go to zero at  $x = \pm \infty$  and for any physically reasonable wave function the spatial derivative of the wave function must also go to zero  $x = \pm \infty$ . Then from the part (b) answer, it follows that

$$\frac{\partial P(\infty, t)}{\partial t} = 0$$

Thus  $P(\infty, t)$  is a constant at time t.

The above proof shows that if  $P(\infty, t)$  is finite, then it's a constant at time t. But if it's finite at time t, it will stay finite as time advances and therefore stay a constant as time advances. So, in fact, if  $P(\infty, t)$  is finite at time t, it stays finite and a constant forever.

If the last argument seems too tricky, then make the assumption that  $P(\infty, t)$  is always finite. Then it is always constant by our first proof and our assumption is consistent and verified a posteriori.

To conclude,  $P(\infty, t)$  is a constant at all times. Thus, total probability is conserved and a normalizable wave function stays normalizable. If the wave function is, in fact, normalized,  $P(\infty, t) = 1$  for all time, of course.

Actually, we've only shown that probability is conserved for all time while Schrödinger equation evolution is occurring. In wave function collapse, people believe that probability is

conserved too, but what the proof for that is is beyond me—any maybe everyone since there is no definite theory of wave function collapse if it happens at all really.

d) We now define

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

Since  $\partial P(x,t)/\partial t$  is the rate of probability increase in the region  $[-\infty, x], -\partial P(x,t)/\partial t$  is the rate of probability decrease in that region. Since the total probability is conserved for a normalizable wave function as we showed in the part (c) answer, the decrease in probability in region  $[-\infty, x]$  demands an increase in region  $[x, \infty]$ . Thus, J(x, t) is the rate of probability flow from  $[-\infty, x]$  to  $[x, \infty]$ . It's only sensible then to call J(x, t) a probability current.

Using the part (b) answer, we find

$$J(x,t) = \frac{1}{m} \operatorname{Re}(\Psi^* p_{\rm op} \Psi)$$

(CT-239 agrees). Note J(x,t) is a pure real. This formula has a neat correspondence to classical current density: e.g.,  $\vec{v}\rho$ . The  $\Psi^*\Psi$  corresponds to density and  $p_{\rm op}/m$  corresponds to velocity. A correspondance is all I think that one can suggest without doing anything more.

But say we integrated J(x,t) over all x? Well

$$\begin{split} \int_{-\infty}^{\infty} J(x,t) \, dx &= -\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \int_{-\infty}^{x} |\Psi(x')|^2 \, dx' \, dx \\ &= -\frac{\partial}{\partial t} \left[ \left( x \int_{-\infty}^{x} |\Psi(x')|^2 \, dx' \right) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} x |\Psi(x)|^2 \, dx \right] \\ &= -\frac{\partial}{\partial t} \left( \infty - \int_{-\infty}^{\infty} \Psi^* x \Psi \, dx \right) \\ &= \frac{\partial}{\partial t} \langle x \rangle \;, \end{split}$$

where we have rather embarrasingly set the time derivative of a constant infinity equal to zero—it must be the right limiting behavior. So we have to prove

$$\lim_{x \to \infty} x \frac{\partial P(x,t)}{\partial t} = 0$$

Probably, there is no general proof other than to assert that the wave function goes to zero rapidly enough as  $x \to \infty$  that  $\partial P(x,t)/\partial t$  goes to zero fast enough to cancel x going to infinity.

And well

$$\langle p_{\rm op} \rangle = \int_{-\infty}^{\infty} \Psi^* p_{\rm op} \Psi \, dx = \int_{-\infty}^{\infty} [\operatorname{Re}(\Psi^* p_{\rm op} \Psi) + \operatorname{Im}(\Psi^* p_{\rm op} \Psi)] \, dx = \int_{-\infty}^{\infty} \operatorname{Re}(\Psi^* p_{\rm op} \Psi) \, dx$$

since the expectation value of an observable is a pure real. So we find that

$$\frac{\partial}{\partial t} \langle x \rangle = \frac{\langle p_{\rm op} \rangle}{m}$$

which is just the Ehrenfest theorem first equation (CT-242). The correspondence to the classical result

$$v = \frac{p}{m}$$

is obvious.

e) Given

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

it follows that probability density  $|\Psi|^2$  is time independent and that

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}|\psi|^2 = 0$$

identically. Then probability function P(x,t) and probability current J(x,t) are actually time independent: i.e.,

$$\frac{\partial P(x,t)}{\partial t} = 0$$
 and  $J(x,t) = 0$ 

identically. The wave function in this case is a called a stationary state or an eigen-energy state. The  $\omega = E/\hbar$ , where E is the eigen-energy of the time-independent Schrödinger equation.

Proving that J(x,t) = 0 for a stationary state directly from the formula

$$J(x,t) = \frac{1}{m} \operatorname{Re}(\Psi^* p_{\mathrm{op}} \Psi)$$

looks impossible. Maybe the only proof is to reverse the steps and find that

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

and thus is zero.

**NOTE:** Some idle thoughts occur to me.

First if  $\Psi$  is pure real, then J=0. In this case,

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

implies that

$$H\Psi = 0$$

The solutions in this case would be zero energy stationary states. They can happen.

Second, what if the time dependence of  $\Psi$  can be entirely confined to phase factor: i.e., one must be able to write

$$\Psi(x,t) = R(x)e^{i\theta(x,t)} .$$

This wave function would not be what we ordinarily call a stationary state unless  $\theta(x,t) = Et/\hbar$ . But it would have

$$|\Psi(x,t)|^2 = |R(x)|^2$$

which is a constant with time. If  $|\Psi(x,t)|^2$  is a constant with time, then the current should be zero everywhere. Can we find this from the explicit current formula? Using the part (d) answer, we find

$$\begin{split} J(x,t) &= \frac{1}{m} \operatorname{Re}(\Psi^* p_{\mathrm{op}} \Psi) \\ &= \frac{1}{m} \operatorname{Re}\left[ R^* e^{-i\theta} \left( \frac{\hbar}{i} \frac{\partial R}{\partial x} + R \hbar \frac{\partial \theta}{\partial x} \right) e^{i\theta} \right] \\ &= \frac{\hbar}{m} \operatorname{Re}\left( -iR^* \frac{\partial R}{\partial x} + |R|^2 \frac{\partial \theta}{\partial x} \right) \;, \end{split}$$

Well the last expression is not zero in general as far as I can see. It's zero if R is only complex through a coefficient which is true of stationary states and if  $\theta$  has no spatial dependence which is also true of stationary states. It may be that  $\Psi(x,t) = R(x)e^{i\theta(x,t)}$  is not in general an allowed from of a solution. Maybe there is some other way of thinking of things, but that's all for on 2011jan21.

Redaction: Jeffery, 2001jan01

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

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

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

# 4 Some Operators

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

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

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

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

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

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

5 Kronecker Delta and Levi-Civita Symbol

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & \text{otherwise} \end{cases} \quad \varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic}; \\ -1, & ijk \text{ anticyclic}; \\ 0, & \text{if two indices the same.} \end{cases}$$
$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell} \qquad (\text{Einstein summation on } i)$$

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  $\frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{m} \langle \vec{p} \rangle$  and  $\frac{d\langle \vec{p} \rangle}{dt} = -\langle \nabla V(\vec{r}) \rangle$   
 $|\Psi(t)\rangle = \sum_{j} c_{j}(0)e^{-iE_{j}t/\hbar} |\phi_{j}\rangle$ 

7 Simple Harmonic Oscillator (SHO) Formulae

$$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi = E\psi$$
$$\beta = \sqrt{\frac{m\omega}{\hbar}} \qquad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}}H_n(\beta x)e^{-\beta^2 x^2/2} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$
$$H_0(\beta x) = H_0(\xi) = 1 \qquad H_1(\beta x) = H_1(\xi) = 2\xi$$

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

8 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \qquad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m}$$
$$|\Psi(p,t)|^2 dp = |\Psi(k,t)|^2 dk \qquad \Psi(p,t) = \frac{\Psi(k,t)}{\sqrt{\hbar}}$$
$$x_{\text{op}} = x \qquad p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x} \qquad Q\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}, t\right) \qquad \text{position representation}$$
$$x_{\text{op}} = -\frac{\hbar}{i} \frac{\partial}{\partial p} \qquad p_{\text{op}} = p \qquad Q\left(-\frac{\hbar}{i} \frac{\partial}{\partial p}, p, t\right) \qquad \text{momentum representation}$$
$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar} dp \qquad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi} dk$$
$$\Psi(x,t) = \int_{-\infty}^{\infty} \Psi(p,t) \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}} dp \qquad \Psi(x,t) = \int_{-\infty}^{\infty} \Psi(k,t) \frac{e^{ikx}}{(2\pi)^{1/2}} dk$$
$$\Psi(p,t) = \int_{-\infty}^{\infty} \Psi(x,t) \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{3/2}} d^3p \qquad \Psi(\vec{r},t) = \int_{\text{all space}}^{\infty} \Psi(\vec{r},t) \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3r$$
$$\Psi(\vec{p},t) = \int_{\text{all space}}^{\infty} \Psi(\vec{r},t) \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3r \qquad \Psi(\vec{k},t) = \int_{\text{all space}}^{\infty} \Psi(\vec{r},t) \frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3r$$

9 Commutator Formulae

$$[A, BC] = [A, B]C + B[A, C] \qquad \left[\sum_{i} a_{i}A_{i}, \sum_{j} b_{j}B_{j}\right] = \sum_{i,j} a_{i}b_{j}[A_{i}, b_{j}]$$
  
if  $[B, [A, B]] = 0$  then  $[A, F(B)] = [A, B]F'(B)$   
 $[x, p] = i\hbar \qquad [x, f(p)] = i\hbar f'(p) \qquad [p, g(x)] = -i\hbar g'(x)$   
 $[a, a^{\dagger}] = 1 \qquad [N, a] = -a \qquad [N, a^{\dagger}] = a^{\dagger}$ 

<sup>10</sup> Uncertainty Relations and Inequalities

$$\sigma_x \sigma_p = \Delta x \Delta p \ge \frac{\hbar}{2} \qquad \sigma_Q \sigma_Q = \Delta Q \Delta R \ge \frac{1}{2} \left| \langle i[Q, R] \rangle \right|$$
$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \ge \frac{\hbar}{2}$$

# 11 Probability Amplitudes and Probabilities

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

## 12 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \qquad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$
$$L^2 Y_{\ell m} = \ell(\ell+1)\hbar^2 Y_{\ell m} \qquad L_z Y_{\ell m} = m\hbar Y_{\ell m} \qquad |m| \le \ell \qquad m = -\ell, -\ell+1, \dots, \ell-1, \ell$$
$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & \dots \\ s & p & d & f & g & h & i & \dots \end{pmatrix}$$

13 Hydrogenic Atom

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

$$a_{z} = \frac{a}{Z} \left( \frac{m_{e}}{m_{\text{reduced}}} \right) \qquad a_{0} = \frac{\hbar}{m_{e}c\alpha} = \frac{\lambda_{C}}{2\pi\alpha} \qquad \alpha = \frac{e^{2}}{\hbar c}$$

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

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

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

 $L_q(x) = e^x \left(\frac{d}{dx}\right)^q \left(e^{-x}x^q\right)$  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

$$\begin{split} [J_i, J_j] &= i \hbar \varepsilon_{ijk} J_k \quad \text{(Einstein summation on } k) \qquad [J^2, \vec{J}] = 0 \\ J^2 |jm\rangle &= j(j+1) \hbar^2 |jm\rangle \qquad J_z |jm\rangle = m \hbar |jm\rangle \\ J_{\pm} &= J_x \pm i J_y \qquad J_{\pm} |jm\rangle = \hbar \sqrt{j(j+1) - m(m\pm 1)} |jm\pm 1\rangle \\ J_{\left\{\frac{x}{y}\right\}} &= \left\{\frac{1}{2\frac{1}{2i}}\right\} (J_{\pm} \pm J_{-}) \qquad J_{\pm}^{\dagger} J_{\pm} = J_{\mp} J_{\pm} = J^2 - J_z (J_z \pm \hbar) \\ [J_{fi}, J_{gj}] &= \delta_{fg} i \hbar \varepsilon_{ijk} J_k \qquad \vec{J} = \vec{J_1} + \vec{J_2} \qquad J^2 = J_1^2 + J_2^2 + J_{1+} J_{2-} + J_{1-} J_{2+} + 2J_{1z} J_{2z} \\ J_{\pm} &= J_{1\pm} + J_{2\pm} \qquad |j_1 j_2 jm\rangle = \sum_{m_1 m_2, m = m_1 + m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 jm\rangle j_1 j_2 jm\rangle \\ |j_1 - j_2| \leq j \leq j_1 + j_2 \qquad \sum_{|j_1 - j_2|}^{j_1 + j_2} (2j+1) = (2j_1 + 1)(2j_2 + 1) \end{split}$$

15 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$$
$$|\pm\rangle_x = \frac{1}{\sqrt{2}} \left(|+\rangle \pm |-\rangle\right) \qquad |\pm\rangle_y = \frac{1}{\sqrt{2}} \left(|+\rangle \pm i|-\rangle\right) \qquad |\pm\rangle_z = |\pm\rangle$$

 $|++\rangle = |1,+\rangle|2,+\rangle \qquad |+-\rangle = \frac{1}{\sqrt{2}} \left(|1,+\rangle|2,-\rangle \pm |1,-\rangle|2,+\rangle\right) \qquad |--\rangle = |1,-\rangle|2,-\rangle$   $\sigma_x = \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$   $\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k \qquad [\sigma_i,\sigma_j] = 2i\varepsilon_{ijk}\sigma_k \qquad \{\sigma_i,\sigma_j\} = 2\delta_{ij}$   $(\vec{A}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma}) = \vec{A}\cdot\vec{B} + i(\vec{A}\times\vec{B})\cdot\vec{\sigma}$ 

$$\frac{d(\vec{S}\cdot\hat{n})}{d\alpha} = -\frac{i}{\hbar}[\vec{S}\cdot\hat{\alpha},\vec{S}\cdot\hat{n}] \qquad \vec{S}\cdot\hat{n} = e^{-i\vec{S}\cdot\vec{\alpha}}\vec{S}\cdot\hat{n}_0e^{i\vec{S}\cdot\vec{\alpha}} \qquad |\hat{n}_{\pm}\rangle = e^{-i\vec{S}\cdot\vec{\alpha}}|\hat{z}_{\pm}\rangle$$

$$e^{ixA} = \mathbf{1}\cos(x) + iA\sin(x) \quad \text{if } A^2 = \mathbf{1} \qquad e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} = \mathbf{1}\cos(x) - i\vec{\sigma}\cdot\hat{\alpha}\sin(x)$$
$$\sigma_i f(\sigma_j) = f(\sigma_j)\sigma_i\delta_{ij} + f(-\sigma_j)\sigma_i(1-\delta_{ij})$$
$$\mu_{\text{Bohr}} = \frac{e\hbar}{2m} = 0.927400915(23) \times 10^{-24} \text{ J/T} = 5.7883817555(79) \times 10^{-5} \text{ eV/T}$$
$$g = 2\left(1 + \frac{\alpha}{2\pi} + \dots\right) = 2.0023193043622(15)$$

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

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

# 16 Time-Independent Approximation Methods

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

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

$$\begin{split} |\psi_{n}^{1\text{st}}\rangle &= |\psi_{n}^{(0)}\rangle + \lambda \sum_{\text{all } k, \ k \neq n} \frac{\left\langle \psi_{k}^{(0)} | H^{(1)} | \psi_{n}^{(0)} \right\rangle}{E_{n}^{(0)} - E_{k}^{(0)}} |\psi_{k}^{(0)}\rangle \\ E_{n}^{1\text{st}} &= E_{n}^{(0)} + \lambda \left\langle \psi_{n}^{(0)} | H^{(1)} | \psi_{n}^{(0)} \right\rangle \\ E_{n}^{2\text{nd}} &= E_{n}^{(0)} + \lambda \left\langle \psi_{n}^{(0)} | H^{(1)} | \psi_{n}^{(0)} \right\rangle + \lambda^{2} \sum_{\text{all } k, \ k \neq n} \frac{\left| \left\langle \psi_{k}^{(0)} | H^{(1)} | \psi_{n}^{(0)} \right\rangle \right|^{2}}{E_{n}^{(0)} - E_{k}^{(0)}} \\ E(\phi) &= \frac{\left\langle \phi | H | \phi \right\rangle}{\left\langle \phi | \phi \right\rangle} \qquad \delta E(\phi) = 0 \\ H_{kj} &= \left\langle \phi_{k} | H | \phi_{j} \right\rangle \qquad H\vec{c} = E\vec{c} \end{split}$$

# 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

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

19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm 1, \pm 2, \dots \qquad k = \frac{2\pi n}{L} \qquad \Delta k_{\text{cell}} = \frac{2\pi}{L} \qquad \Delta k_{\text{cell}}^3 = \frac{(2\pi)^3}{V}$$
$$dN_{\text{states}} = g \frac{k^2 \, dk \, d\Omega}{(2\pi)^3/V}$$

# 20 Identical Particles

$$\begin{split} |a,b\rangle &= \frac{1}{\sqrt{2}} \left( |1,a;2,b\rangle \pm |1,b;2,a\rangle \right) \\ \psi(\vec{r}_1,\vec{r}_2) &= \frac{1}{\sqrt{2}} \left( \psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2) \right) \end{split}$$

# 21 Second Quantization

$$\begin{split} & [a_i, a_j^{\dagger}] = \delta_{ij} \qquad [a_i, a_j] = 0 \qquad [a_i^{\dagger}, a_j^{\dagger}] = 0 \qquad |N_1, \dots, N_n\rangle = \frac{(a_n^{\dagger})^{N_n}}{\sqrt{N_n!}} \dots \frac{(a_1^{\dagger})^{N_1}}{\sqrt{N_1!}} |0\rangle \\ & \{a_i, a_j^{\dagger}\} = \delta_{ij} \qquad \{a_i, a_j\} = 0 \qquad \{a_i^{\dagger}, a_j^{\dagger}\} = 0 \qquad |N_1, \dots, N_n\rangle = (a_n^{\dagger})^{N_n} \dots (a_1^{\dagger})^{N_1} |0\rangle \\ & \Psi_s(\vec{r}')^{\dagger} = \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}^{\dagger} \qquad \Psi_s(\vec{r}\,) = \sum_{\vec{p}} \frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}^{\dagger} \\ & [\Psi_s(\vec{r}\,), \Psi_{s'}(\vec{r}\,')]_{\mp} = 0 \qquad [\Psi_s(\vec{r}\,)^{\dagger}, \Psi_{s'}(\vec{r}\,')^{\dagger}]_{\mp} = 0 \qquad [\Psi_s(\vec{r}\,), \Psi_{s'}(\vec{r}\,')^{\dagger}]_{\mp} = \delta(\vec{r} - \vec{r}\,')\delta_{ss'} \\ & |\vec{r}_1s_1, \dots, \vec{r}_ns_n\rangle = \frac{1}{\sqrt{n!}}\Psi_{s_n}(\vec{r}\,_n)^{\dagger} \dots \Psi_{s_n}(\vec{r}\,_n)^{\dagger} |0\rangle \\ & \Psi_s(\vec{r}\,')^{\dagger}|\vec{r}_1s_1, \dots, \vec{r}_ns_n\rangle\sqrt{n+1}|\vec{r}_1s_1, \dots, \vec{r}_ns_n, \vec{r}s\rangle \\ & |\Phi\rangle = \int d\vec{r}_1 \dots d\vec{r}_n \ \Phi(\vec{r}_1, \dots, \vec{r}_n)|\vec{r}_1s_1, \dots, \vec{r}_ns_n\rangle \\ & 1_n = \sum_{s_1\dots s_n} \int d\vec{r}_1 \dots d\vec{r}_n \ |\vec{r}_1s_1, \dots, \vec{r}_ns_n\rangle\langle\vec{r}_1s_1, \dots, \vec{r}_ns_n| \qquad 1 = |0\rangle\langle 0| + \sum_{n=1}^{\infty} 1_n \end{split}$$

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

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

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

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

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

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

22 Klein-Gordon Equation

$$\begin{split} E &= \sqrt{p^2 c^2 + m^2 c^4} \qquad \frac{1}{c^2} \left( i\hbar \frac{\partial}{\partial t} \right)^2 \Psi(\vec{r}, t) = \left[ \left( \frac{\hbar}{i} \nabla \right)^2 + m^2 c^2 \right] \Psi(\vec{r}, t) \\ &\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left( \frac{mc}{\hbar} \right)^2 \right] \Psi(\vec{r}, t) = 0 \\ \rho &= \frac{i\hbar}{2mc^2} \left( \Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right) \qquad \vec{j} = \frac{\hbar}{2im} \left( \Psi^* \nabla \Psi - \Psi \nabla \Psi^* \right) \\ &\frac{1}{c^2} \left( i\hbar \frac{\partial}{\partial t} - e\Phi \right)^2 \Psi(\vec{r}, t) = \left[ \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right)^2 + m^2 c^2 \right] \Psi(\vec{r}, t) \\ &\Psi_+(\vec{p}, E) = e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar} \qquad \Psi_-(\vec{p}, E) = e^{-i(\vec{p}\cdot\vec{r} - Et)/\hbar} \end{split}$$