PHAS3226: Quantum Mechanics

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Contents

1	Fun	damentals 3
	1.1	Dirac Notation
		1.1.1 Dual Space
2	Bas	ic Stuff We Have to Memorize 4
	2.1	Important Mathematical Curiosities
		2.1.1 Properties of Commutators
		2.1.2 Resolution of the Identity
		2.1.3 Operator Properties
3	Ras	ic Stuff We Have to Do
	3.1	Position Representation
	3.2	Change of Basis
	3.3	Uncertainty
	$\frac{3.3}{3.4}$	Matrix Representations of Operators
	0.4	Matrix Representations of Operators
4	Qua	antum Harmonic Oscillator 5
5	Ang	gular Momentum 7
	5.1	Orbital Angular Momentum
	5.2	Central Potentials
	5.3	Generalised Angular Momentum
		5.3.1 Ladder Operators
	5.4	Spin Operator
6	Spir	n 1/2 Systems
U	6.1	Spin-1/2 Properties
	6.2	Pauli Matrices
	0.2	Taun Matrices
7	App	proximate Methods and Many-Body Systems 10
	7.1	Perturbation Theory
		7.1.1 General Idea
		7.1.2 First Order
		7.1.3 Second Order
		7.1.4 Trivia
		7.1.5 Degenerate Eigenvalues
	7.2	The Variational Principle
		7.2.1 Proof
	7.3	Pauli Exclusion Principle
	7.4	THE REST OF THE STUFF?!

1 Fundamentals

1.1 Dirac Notation

Before we begin, it seems useful to just introduce Dirac notation. It's far more concise, powerful, and globally understood than any other notation - so there's no point in doing any recap of last year without it.

Dirac notation's inception can be found in the expansion postulate:

$$\psi = \sum_{n} a_n \phi_n$$

Where the set $\{\phi_n\}$ is a complete basis. From now on, we will the Einstein summation convention, wherein all summation signs are dropped and repeated indices (dummy indices) are assumed to be summed over. The expansion postulate now looks like this:

$$\psi = a_n \phi_n$$

This sort of gives ψ the appearance of a vector! It's just a linear weighted sum of the basis 'vectors'. For example, for the set $\{\phi_n\} = \{\phi_0, \phi_1, \phi_2\}$, the expansion postulate looks alarmingly like a position vector in \mathbb{R}^3 :

$$\psi = a_0\phi_0 + a_1\phi_1 + a_2\phi_2$$
$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$

Functionally, all Dirac notation is is the full, powerful method of treating states like 'vectors' in the 'vector space' defined by the basis states. We call these 'vectors' "kets" or "ket vectors", and denote them as follows:

$$\phi_n \to |\phi_n\rangle$$

In this notation (with the Einstein summation convention), our original expansion postulate looks wonderfully elegant:

$$|\psi\rangle = a_n |\phi_n\rangle$$

We can instantly see which symbols refer to states/basis states, and which refer to coefficients. More conveniences similar to this will become more and more evident.

1.1.1 Dual Space

Now, in order to actually do anything in quantum mechanics, we need to define complex conjugates of every ket. Implicitly, this means only defining the complex conjugates of the basis kets (as we can make any ket from a complete set of basis kets). This is quite easily done:

$$\phi_n^* \to \langle \phi_n |$$

These 'vectors' are given a different name - "bras" or "bra vectors".

The reasoning for this is quite elegant. For every basis ket, we have a corresponding basis bra - however we cannot go continuously from one set to the other. The basis bras define a 'vector space' that is related to but not the same as the basis kets. For this reason, we call the bra space 'dual' to the ket space. The 'dual space' can refer to either the bra space, or the ket space (as they are dual to each other) or the combination of the two. For the purposes of this document, the precise meaning of 'dual' will be made explicit whenever it is used.

A more precise definition of dual space is as follows:

For a given vector space V, the dual space V^* is defined as the set of all objects that (when combined with the vectors in space V using an operator) produces the scalar field of V.

Basically, all vector spaces have a corresponding set of scalars that we care about. For the vector space defined by column vectors for example, the dual space is the row vectors, and when you use the dot product operator, you get their inner product!

For a matrix space, the dual space is column vectors for matrix multiplication on the right, or row vectors for matrix multiplication on the left.

In the case of Dirac notation, there's a bra space, a ket space that's dual to it, and when you stick them together (inner product) you get a scalar (typically interpreted by the Born rule as the probability of some experimental outcome).

2 Basic Stuff We Have to Memorize

2.1 Important Mathematical Curiosities

2.1.1 Properties of Commutators

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

 $[A, B + C] = [A, B] + [A, C]$
 $[A, BC] = [A, B] C + B[A, C]$

2.1.2 Resolution of the Identity

fill this in

2.1.3 Operator Properties

• Hermitian if \hat{Q} satisfies:

$$\langle \phi | \hat{Q} | \psi \rangle = \left(\langle \psi | \hat{Q} | \phi \rangle \right)^*$$

This subsequently implies that the following quantity is always real:

$$\langle \phi | \hat{Q} | \phi \rangle$$

3 Basic Stuff We Have to Do

3.1 Position Representation

DO THIS

3.2 Change of Basis

DO THIS

3.3 Uncertainty

Uncertainty in some measurement operator \hat{Q} is given by:

$$\Delta Q^2 = \left< \hat{Q}^2 \right> - \left< \hat{Q} \right>^2$$

Practically, to calculate these values we apply identical arbitrary wavefunctions to either side of the operator, and divide by their inner product:

$$\left\langle f\left(\hat{Q}\right)\right\rangle _{\phi}=\frac{\left\langle \phi\right| f\left(\hat{Q}\right)\left|\phi\right\rangle}{\left\langle \phi\right|\phi\right\rangle}$$

For the uncertainty relation between two operators:

$$\Delta A \Delta B \geqslant \frac{1}{2} \left| \left\langle \left[A, B \right] \right\rangle \right|$$

Know how to derive this?!

3.4 Matrix Representations of Operators

For a given operator \hat{A} , we have to be able to show that it's operation on any complete orthonormal basis $\{|\phi_j\rangle\}$ can be represented as a matrix with elements A_{ij} . To to this we first expand each $|\phi_j\rangle$ as in the basis of eigenfunctions of \hat{A} : $\{|\alpha_n\rangle\}$:

$$|\phi_j\rangle = \sum_n \alpha_{in} |\alpha_n\rangle$$

Then we compute:

$$\langle \phi_i | \hat{A} | \phi_j \rangle = \sum_m \alpha_{im}^* \langle \alpha_m | \hat{A} \sum_n \alpha_{jn} | \alpha_n \rangle$$

$$= \sum_m \sum_n \alpha_{im}^* \alpha_{jn} \langle \alpha_m | \hat{A} | \alpha_n \rangle$$

$$= \sum_m \sum_n \alpha_{im}^* \alpha_{jn} a_n \langle \alpha_m | \alpha_n \rangle$$

$$= \sum_m \sum_n \alpha_{im}^* \alpha_{jn} a_n \delta_{mn}$$

$$= \sum_m \alpha_{im}^* \alpha_{jm} a_m = \text{constant}$$

$$= A_{ij}$$

Hence, in any given orthonormal basis $\{|\phi_j\rangle\}$, any operator \hat{A} can be represented as a matrix with elements:

$$A_{ij} = \langle \phi_i | \hat{A} | \phi_j \rangle$$

4 Quantum Harmonic Oscillator

The Quantum Harmonic Oscillator (QHO) is retrieved by taking the Hamiltonian of the classical Simple Harmonic Oscillator (SHO), and replacing x and p with their corresponding quantum operators:

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Which sort of looks like a difference of two squares of the form:

$$\hat{a}_{+}\hat{a}_{-} = (a\hat{x} - ib\hat{p})(a\hat{x} + ib\hat{p})$$

However, since \hat{x} and \hat{p} don't commute, this yields:

$$\hat{a}_{+}\hat{a}_{-} = b^{2}\hat{p}^{2} + a^{2}\hat{x}^{2} + iab(\hat{x}\hat{p} - \hat{p}\hat{x})$$

Which, by the commutator of \hat{x} and \hat{p} , and the definition of the QHO Hamiltonian:

$$\hat{a}_{+}\hat{a}_{-} = \lambda \hat{\mathcal{H}} - ab\hbar \tag{1}$$

Where λ is a scaling factor that can help us conveniently define a and b. For convenience, setting λ to $1/\hbar\omega$ yields¹:

$$a^{2} = \frac{1}{2}m\omega^{2}\lambda$$
$$a = \sqrt{\frac{m\omega}{2\hbar}}$$
$$b^{2} = \frac{1}{2m}\lambda$$
$$b = \sqrt{\frac{1}{2m\hbar\omega}}$$

 $^{^{1}}$ Any value of λ will eventually yield the following results, but they'll be much harder to work with.

Such that we can conveniently define a new variable $\alpha = \sqrt{m\omega/\hbar}$ such that:

$$a = \frac{1}{\sqrt{2}}\alpha$$

$$b = \frac{1}{\sqrt{2}} \frac{1}{\hbar \alpha}$$

Thus allowing us to write equation 1 as:

$$\hat{\mathcal{H}} = \left(\hat{a}_{+}\hat{a}_{-} + \frac{1}{2}\right)\hbar\omega$$

Where:

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2}} \left(\alpha \hat{x} \mp \frac{i}{\hbar \alpha} \hat{p} \right)$$

Which clearly corresponds to the energy eigenvalues of the QHO:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Such that we can define the number operator \hat{N} with eigenvalues n and the same eigenfunctions as the Hamiltonian as:

$$\hat{N} = \hat{a}_{+}\hat{a}_{-}$$

Some important things to note are that:

- \hat{a}_+ (step-up) and \hat{a}_- (step-down) are hermitian conjugates of each other.
- They conceptually correspond to the addition or removal of a single quanta of energy to the system $(\pm\hbar\omega)$.
- Their commutator equals unity:

$$[\hat{a}_+, \hat{a}_-] = 1$$

• Their eigenvalue equations are:

$$\hat{a}_{+} = \sqrt{n+1} |\phi_{n+1}\rangle$$
$$\hat{a}_{-} = \sqrt{n} |\phi_{n-1}\rangle$$

Which change the principal quantum number (energy level) n of the state $\phi_{n,...}$ accordingly.

• Their commutator with the Hamiltonian is:

$$\left[\hat{\mathcal{H}}, \hat{a}_{\pm}\right] = \pm \hbar \omega \hat{a}_{\pm}$$

• Any state $|\phi_n\rangle$ can be written as the (normalised) repeated application of the step-up operator to the vacuum state $|\phi_0\rangle$:

$$|\phi_1\rangle = \left(\frac{1}{\sqrt{1}}\hat{a}_+\right)|\phi_0\rangle$$

$$|\phi_2\rangle = \left(\frac{1}{\sqrt{2}}\hat{a}_+\right)|\phi_1\rangle$$

Such that:

$$|\phi_n\rangle = \frac{\hat{a}_+^n}{\sqrt{n!}} |\phi_0\rangle$$

• The position and momentum operators can be rewritten in terms of the step-up and step-down operators by adding/subtracting them and scaling appropriately.

5 Angular Momentum

5.1 Orbital Angular Momentum

From the postulates of QM we can define the orbital angular momentum operator by replacing the position and momentum in the classical relation with the position and momentum operators:

$$\hat{L} = \hat{r} \times \hat{p}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

Where:

$$\hat{L} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$$

$$\hat{r} = (\hat{x}, \hat{y}, \hat{z})$$

$$\hat{p} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

This has some pretty useful consequences:

• The commutators of the components of \hat{L} are as follows:

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar \hat{L}_z$$

And cyclic permutations of x, y, z. These can all be encapsulated by:

$$\hat{L} \times \hat{L} = i\hbar \hat{L}$$

• The commutator of any component of \hat{L} with \hat{L}^2 is zero:

$$\left[\hat{L}_{x/y/z}, \hat{L}^2\right] = 0$$

- As a result of the previous two facts, we can measure the square of the magnitude of \hat{L} in the form of \hat{L}^2 , as well as a single component of \hat{L} at the same time. This component is conventionally the \hat{L}_z component, and is the projection of \hat{L} onto the z-axis. Both of these operators operate exclusively on the angular coordinates in polar coordinates.
- The eigenvalue equations for these two quantities are as follows:

$$\hat{L}^2 |\phi\rangle = l(l+1) |\phi_{n,l}\rangle$$

$$\hat{L}_z \left| \phi \right\rangle = m_l \hbar \left| \phi_{n,l} \right\rangle$$

And the eigenfunctions are the spherical harmonics.

• The components of \hat{L} , and \hat{L} itself are hermitian.

5.2 Central Potentials

For a central potential (one that is independent of the angular coordinates), the Hamiltonian can be separated into a function of the radial coordinate and the orbital angular momentum operator alone

This implies that the Hamiltonian of a central potential commutes with both \hat{L}^2 and \hat{L}_z . DO WE NEED TO MATHEMATICALLY KNOW THIS

5.3 Generalised Angular Momentum

For quantum systems, there is also an intrinsic moment called 'spin' which has no classical analogue, but shares many of the properties of classical orbital angular momentum. For this reason it is useful to define a 'generalized' angular momentum \hat{J} which has the same properties as the orbital angular momentum, and which represents both the orbital angular momentum and spin in tandem.

The definition of \hat{J} is any operator which satisfies the orbital angular momentum commutator:

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hbar \hat{J}_z$$

And any cyclic permutations thereof. This basically means it has the same properties, eigenvalues, eigenfunctions, and commutators as \hat{L} , but with all L denoted as J and all l denoted as j. Do we need to be able to derive eigenvalues for the generalized angular momentum?

5.3.1 Ladder Operators

It may be useful to create operators akin to the step-up/step-down operators, which increase or decrease the generalized angular momentum quantum number j in quantized steps.

This is quite easy to do^2 :

$$\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$$

Which are not hermitian, but each is the hermitian conjugate of the other by inspection. The commutator relations of these new ladder operators are - by brute computation:

$$\begin{bmatrix} \hat{J}^2, \hat{J}_{\pm} \end{bmatrix} = 0$$
$$\begin{bmatrix} \hat{J}_{\pm}, \hat{J}_{\mp} \end{bmatrix} = \pm 2\hbar \hat{J}_z$$
$$\begin{bmatrix} \hat{J}_z, \hat{J}_{\pm} \end{bmatrix} = \pm \hbar \hat{J}_{\pm}$$

For convenience, $|\phi_{n,l,s,j}\rangle$ will now be represented by the relevant quantum numbers alone, and their projections along the z-axis. For example: when we're only dealing with j and m_j , we will use the ket $|j, m_j\rangle$.

The action of the ladder operators on a general eigenfunction $|\phi_{n,l,j}\rangle$ of \hat{L}_z is as follows:

$$\hat{J}_{+} |j, m_{j}\rangle = [j(j+1) - m_{j}(m_{j}+1)]^{\frac{1}{2}} |j, m_{j}+1\rangle$$

$$\hat{J}_{-} |j, m_{j}\rangle = [j(j+1) - m_{j}(m_{j}-1)]^{\frac{1}{2}} |j, m_{j}-1\rangle$$

5.4 Spin Operator

The spin operator \hat{S} has the same eigenvalues as \hat{L} and \hat{J} .

6 Spin 1/2 Systems

We will also only consider spin-1/2 systems ($s = 1/2, m_s = \pm 1/2$) which are some of the most useful systems to consider. Electrons and protons, for example, are spin-1/2, and this section will be presented w.r.t. them.

For spin-1/2 particles, there are two possible state kets, one for each of the two possible values of m_s : spin-up and spin-down:

$$|\uparrow\rangle = |\alpha\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle = \begin{bmatrix}1\\0\end{bmatrix}$$
$$|\downarrow\rangle = |\beta\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

Such that any general state $|\chi\rangle$ can be written as a superposition of both:

$$|\chi\rangle = a |\alpha\rangle + b |\beta\rangle$$

Note that, as the spin operator has the form of an angular momentum operator, it has the same properties as the generalized angular momentum operator \hat{J} , but for the quantum numbers s and m_s .

6.1 Spin-1/2 Properties

By applying operators to the up and down state kets, it is possible to construct general relations for spin-1/2 systems.

²Notice that the \pm sign in the definition is opposite to the \mp sign in the definition of \hat{a}_{\pm} .

• Ladder Operators, by definition:

$$\hat{S}_{\pm} \left| \alpha \right\rangle = \left[\frac{3}{4} - \frac{1}{2} \left(\frac{1}{2} \pm 1 \right) \right]^{\frac{1}{2}} \left| \frac{1}{2}, \frac{1}{2} \pm 1 \right\rangle$$

$$\hat{S}_{\pm} \left| \beta \right\rangle = \left\lceil \frac{3}{4} - \frac{1}{2} \left(-\frac{1}{2} \pm 1 \right) \right\rceil^{\frac{1}{2}} \left| \frac{1}{2}, -\frac{1}{2} \pm 1 \right\rangle$$

Direct computation yields:

$$\hat{S}_{-} |\beta\rangle = \hat{S}_{+} |\alpha\rangle = 0$$
$$\hat{S}_{+} |\beta\rangle = \hbar |\alpha\rangle$$
$$\hat{S}_{-} |\alpha\rangle = \hbar |\beta\rangle$$

Which makes sense, as you can't raise a spin-up to a spin-up-up, nor lower a spin-down to a spin-down-down if we're only dealing with spin-1/2 systems.

• From the above equations (for any state ket):

$$\hat{S}_{+}^{2}\left|\chi\right\rangle = 0$$

• From the above equation, and by subbing in $\hat{S}_{+} = \hat{S}_{x} \pm i\hat{S}_{y}$:

$$\left\{\hat{S}_x, \hat{S}_y\right\} = 0$$

Where the curly braces are the anticommutator.

• By definition, the commutator is:

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar \hat{S}_z$$

Such that (by combining it with the anticommutator):

$$\hat{S}_x \hat{S}_y = i \frac{\hbar}{2} \hat{S}_z$$

• Spin x-y operators, by definition:

$$\hat{S}_x = \frac{1}{2} \left(\hat{S}_+ + \hat{S}_- \right)$$

$$\hat{S}_y = \frac{1}{2i} \left(\hat{S}_+ - \hat{S}_- \right)$$

Subbing in the values obtained above for the ladder operators yields a whole bunch of stuff.

• The magnitude (for any state ket) is just a number:

$$\hat{S}^2 \left| \chi \right\rangle = \frac{3}{4} \hbar^2 \left| \chi \right\rangle$$

6.2 Pauli Matrices

Matrix representations of any of the above operators can be found easily by applying the basis kets (spin-up and spin-down) to either side:

$$\langle s, m_s | \hat{A} | s, m_s \rangle$$

This yields the following matrix representations of the spin-1/2 operators:

$$\hat{S}^2 = \frac{3}{4}\hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{3}{4}\hbar^2 \hat{I}$$
 $\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{\hbar}{2}\hat{\sigma}_x$

$$\hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \frac{\hbar}{2} \hat{\sigma}_y \qquad \hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\hbar}{2} \hat{\sigma}_z$$

Since any 2×2 matrix can be expanded in terms of the \hat{S}^2 and $\hat{S}_{x/y/z}$ operator: we can define an operator space using what are known as the 'Pauli Matrices':

$$\hat{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Which any 2×2 operator can be expanded in terms of. Note that, in some literature, the Pauli Matrices are also labelled: $\hat{I} \to \hat{\sigma}_0$ and $\hat{\sigma}_{x/y/z} \to \hat{\sigma}_{1/2/3}$. The traces of the Pauli Matrices are zero, and the determinants of the Pauli Matrices are -1.

7 Approximate Methods and Many-Body Systems

7.1 Perturbation Theory

Perturbation theory basically says that we can take a system Hamiltonian \mathcal{H} which isn't analytically solvable but is very close to one that is $\mathcal{H}^{(0)}$, and just add on corrections of decreasing size to the energy levels and eigenstates dependent on the small perturbation V which takes us from the unperturbed to the perturbed Hamiltonian:

$$\mathcal{H} = \mathcal{H}^{(0)} + \lambda V$$

Where λ is a parameter that renders the perturbation small.

We then expand the eigenvectors and eigenvalues of \mathcal{H} as a power series in λ :

$$\left|\phi_{n}\right\rangle = \sum_{i=0}^{\infty} \lambda^{i} \left|i\right\rangle_{n} = \left|0\right\rangle_{n} + \lambda \left|1\right\rangle_{n} + \lambda^{2} \left|2\right\rangle_{n} + \dots$$

$$E_n = \sum_{i=0}^{\infty} \lambda^i E_{ni} = E_{n0} + \lambda E_{n1} + \lambda^2 E_{n2}...$$

Such that (for $\lambda = 0$):

$$\mathcal{H} |\phi_n\rangle = \mathcal{H}^{(0)} |0\rangle_n = E_{n0} |0\rangle_n$$

Where $|0\rangle_n$ is the eigenfunction and E_{n0} is the eigenvalue for the analytically solvable Hamiltonian $\mathcal{H}^{(0)}$.

7.1.1 General Idea

Subbing this into the eigenvalue equation for \mathcal{H} yields:

$$\mathcal{H} |\phi_n\rangle = E_n |\phi_n\rangle$$

$$\left(\mathcal{H}^{(0)} + \lambda V\right) \left(|0\rangle_n + \lambda |1\rangle_n + \lambda^2 |2\rangle_n + \ldots\right) = \left(E_{n0} + \lambda E_{n1} + \lambda^2 E_{n2} \ldots\right) \left(|0\rangle_n + \lambda |1\rangle_n + \lambda^2 |2\rangle_n + \ldots\right)$$

We will now drop the n subscript for clarity. Comparing coefficients of λ^n yields:

$$\mathcal{H}^{(0)} |0\rangle = E_0 |0\rangle$$

$$\mathcal{H}^{(0)} |1\rangle + V |0\rangle = E_0 |1\rangle + E_1 |0\rangle$$

$$\mathcal{H}^{(0)} |2\rangle + V |1\rangle = E_0 |2\rangle + E_1 |1\rangle + E_2 |2\rangle$$

$$\vdots$$

7.1.2 First Order

Rearranging the second equation above (coefficients of λ^1) yields:

$$\mathcal{H}^{(0)}|1\rangle - E_0|1\rangle = E_1|0\rangle - V|0\rangle$$

Taking the inner product of this equation with $\langle 0|$ yields:

zero by orthonormality
$$\underbrace{\langle 0 | \, \mathcal{H}^{(0)} \, | 1 \rangle}_{\text{zero by hermitian } \mathcal{H}^{(0)}} - \underbrace{E_0 \, \langle 0 | 1 \rangle}_{\text{unity by orthonormality}} = E_1 \underbrace{\langle 0 | 0 \rangle}_{\text{unity by orthonormality}} - \langle 0 | \, V \, | 0 \rangle$$

$$0 = E_1 - \langle 0 | V | 0 \rangle$$
$$E_1 = \langle 0 | V | 0 \rangle$$

Which gives us a simple equation for the first order energy correction to a system energy eigenvalue:

$$E_n \approx E_{n0} + E_{n1}$$

This can then be reinserted into the original equation to solve for the first order correction to the system eigenstate $|1\rangle$.

7.1.3 Second Order

Basically difficult and kinda pointless to learn. The short answer is that each correction depends on the ones before it, so first you do the first order correction, sub those into the second order equation, and then smash it with maths until it breaks.

In general, when chugging through the maths, the second order correction depends on all the unperturbed eigenstates $|0\rangle_n$ and their energy eigenvalues. For this reason, second order corrections are often mathematically (and I mean this in it's most metaphorical sense) all fucked up. FILL THIS IN

7.1.4 Trivia

- The first order correction frequently disappears due to symmetries. We must resort to the second order correction to get any meaningful answer. For this reason we call these perturbations 'difficult' and 'boring'.
- The second order correction can conceptually be understood as what happens on the 'second' time step. So the eigenstate can evolve into any other state, then back to itself in the interval. If this doesn't make sense, just do what the mathematicians do: don't worry about it and focus on the algebra.

•

7.1.5 Degenerate Eigenvalues

DO THIS TOO

7.2 The Variational Principle

The variational principle states that the expectation value of the Hamiltonian evaluated on any arbitrary state is greater than or equal to the ground state energy of the system.

7.2.1 Proof

Proving this is straightforward. For a Hamiltonian $\hat{\mathcal{H}}$ there exists a complete set of orthonormal eigenstates $\{|\phi_n\rangle\}$ with energies $\{E_n\}$ such that $E_0 < E_1 < E_2 < \dots$ Computing the expectation value for an arbitrary state $|\chi\rangle$ yields:

$$\left\langle \hat{\mathcal{H}} \right\rangle_{\chi} = \frac{\left\langle \chi \right| \hat{\mathcal{H}} \left| \chi \right\rangle}{\left\langle \chi \right| \chi \right\rangle}$$

Using the expansion principle:

$$|\chi\rangle = \sum_{i=0}^{\infty} c_i |\phi_i\rangle$$

$$\begin{split} \left< \hat{\mathcal{H}} \right>_{\chi} &= \frac{\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} c_{j}^{*} c_{i} \left< \phi_{j} \right| \hat{\mathcal{H}} \left| \phi_{i} \right>}{\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} c_{j}^{*} c_{i} \left< \phi_{j} \right| \hat{\mathcal{H}} \left| \phi_{i} \right>} \\ &= \frac{\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} c_{j}^{*} c_{i} E_{i} \left< \phi_{j} \right| \phi_{i} \right>}{\sum_{i=0}^{\infty} |c_{i}|^{2}} \\ &= \frac{\sum_{i=0}^{\infty} |c_{i}|^{2} E_{i}}{\sum_{i=0}^{\infty} |c_{i}|^{2}} \\ \left< \hat{\mathcal{H}} \right>_{\chi} - E_{0} &= \frac{\sum_{i=0}^{\infty} |c_{i}|^{2} (E_{i} - E_{0})}{\sum_{i=0}^{\infty} |c_{i}|^{2}} \end{split}$$

Since every term on the RHS is non-negative:

$$\left\langle \hat{\mathcal{H}} \right\rangle_{\chi} - E_0 \geqslant 0$$

And thus:

$$\left\langle \hat{\mathcal{H}} \right\rangle_{\chi} \geqslant E_0$$

Proving the variational principle.

7.3 Pauli Exclusion Principle

FILL THIS IN

7.4 THE REST OF THE STUFF?!