Lecture 4 - Relativistic Correction of Schrödinger's Equation 02/09/16

For a non-degenerate $|E_0\rangle$,

$E^{(1)} = \langle E_0 | V | E_0 \rangle$

└ first-order perturbation just the expectation value

$$E^{(2)} = \sum_i \frac{|\langle i | V | E_0 \rangle|^2}{E_0 - E_i}$$

— where the second-order energy correction is always negative (repels the levels)

For a degenerate energy E_0, you must diagonalize V (find the eigenvalues and eigenvectors) truncated to the degenerate subspace.

degenerate subspace: $\{|m\rangle\}$

with orthogonal complement $\{|i\rangle\}$

first-order perturbation: The secular equation

$$\sum_{m'} \underbrace{\langle m | V | m' \rangle}_{\text{V truncated to the m-subspace}} \langle m' | \Psi \rangle = E^{(1)} \langle m | \Psi \rangle$$

ex: Homework Hamiltonian

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

degenerate subspace $|m\rangle$:

$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \longleftrightarrow E_0 = 0$ — both vectors have the same energy (span the degenerate subspace)

orthogonal complement $|i\rangle$:

$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \longleftrightarrow E_0 = 1$

Second Order Secular Equation

If $E^{(1)}$ is degenerate, then to find $E^{(2)}$ we must diagonalize the second-order secular equation

find the eigenstates of:

$$\sum_i \frac{\langle m | V | i \rangle \langle i | V | m \rangle}{E_0 - E_i}$$

where the eigenvalues of this operator are the potential perturbation values for $E^{(2)}$

mathematical note:

for σ_z, eigenvalues $= \pm 1$

└ Pauli matrices; σ_x, σ_y as well

$\underbrace{A = a\mathbb{1} + \vec{b}\cdot\vec{\sigma}}$

most general Hermitian 2×2 matrix

choose $\vec{b} = |\vec{b}|\hat{z}$ such that

$A = a\mathbb{1} + |\vec{b}|\sigma_z$

$\therefore$ Eigenvalues are $a \pm |\vec{b}|$

*for a 2×2 Hermitian matrix, you can find the eigenvalues by inspection by writing the operator as a scalar plus a vector dotted into a Pauli matrix

Relativistic Corrections

Let's talk about relativity for a minute...

The Schrödinger equation is NOT Lorentz invariant.

• in relativistic conditions, you're determining the potential for an infinitely large momentum

→ consequently, there's a chance the particle could be anywhere in the Universe

ex: The Free Particle ($\hbar = 1$)

$$\overbrace{i\partial_t}^{\text{one time derivative}}\psi = \frac{-1}{2m}\underbrace{\nabla^2}_{\text{two space derivatives}}\psi \text{ is not Lorentz invariant}$$

→ add a time derivative or remove a space derivative to make invariant

Dirac proposed that we may remove a space derivative so that this becomes Lorentz invariant and yields the relativistic form of $E = p^2/2m$

in Special Relativity, we have instead $E^2 = p^2c^2 + m^2c^4$

$i\partial_t\psi = \mathcal{H}\psi$

$= (\alpha^i p_i c + \beta mc^2)\psi$ *where both α & β commute with p

└ just some unknown operator that is linear in momentum

For non-zero p, how do we obtain $E^2 = p^2c^2 + m^2c^4$?

→ What does $E^2 = p^2c^2 + m^2c^4$ imply about the operators α^i and β?

→

($c=1$ now)

Assume: $\psi = e^{-iEt} e^{i\vec{p}\cdot\vec{x}} \psi_0$

$\psi_0 = \psi(x=0, t=0)$ a constant vector in some as yet undetermined Hilbert space $\mathcal{H}_{other}$ → such that the full physical Hilbert space may be expressed as

p acts non-trivially here & they commute

$$\mathcal{H}_{phys} = \mathcal{H}_{space} \otimes \mathcal{H}_{other}$$

α, β act non-trivially here

$i\partial_t \psi = E\psi$

$$(i\partial_t)^2 \psi = E^2 \psi = \mathcal{H}^2 \psi$$
$$= (\alpha^i p_i + \beta m)(\alpha^j p_j + \beta m)\psi$$
$$= [\alpha^i \alpha^j p_i p_j + \underbrace{(\alpha^i \beta + \beta \alpha^i)}_{\text{this term must} = 0} m p_i + \beta^2 m^2]\psi$$

$p_i \mid p_j$ interchangable here

to match the E^2 equation:

- $\beta^2 = 1$
- $\alpha^i \beta + \beta \alpha^i = 0$ (α^i and β anti-commute)
- $\alpha^i \alpha^j + \alpha^j \alpha^i = 2\delta^{ij}$ ← Kronecker delta

*Note: this relation also holds for Pauli matrices

$$\sigma^i \sigma^j + \sigma^j \sigma^i = 2\delta^{ij}$$

$$\sigma^x \sigma^y + \sigma^y \sigma^x = 0; \quad \sigma^x \sigma^x + \sigma^x \sigma^x = 2I_2$$

$\rightarrow \alpha^i = \sigma^x \otimes \sigma^i$

tensor product space

$\beta = \sigma^z \otimes I_2$

$\beta^2 = I_2 \otimes I_2 = I_4$

$$\sigma^i \sigma^j = (\sigma^x)^2 \otimes \sigma^i \sigma^j$$
$$= \underbrace{I_2 \otimes \sigma^i \sigma^j}_{}$$

a four-dimensional vector space

Check:

$$\alpha^i \beta + \beta \alpha^i = (\sigma^x \otimes \sigma^i)(\sigma^z \otimes I_2) + (\sigma^z \otimes I_2)(\sigma^x \otimes \sigma^i)$$
$$= \sigma^x \sigma^z \otimes \sigma^i + \sigma^z \sigma^x \otimes \sigma^i$$
$$= 0 \checkmark$$

→

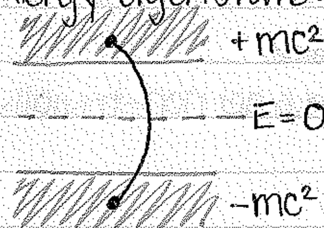
$$\beta = \sigma^z \otimes I_2 \longleftrightarrow \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

$$\alpha^i = \sigma^x \otimes \sigma^i \longleftrightarrow \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}$$

for the lowest energy eigenstate: $\vec{p} = 0$

$\beta m \Psi = E \Psi$

$E = \pm mc^2$



A wavefunction can't just predict matter, it must also predict antimatter.