Lecture

Rotations for spin $\frac{1}{2}$ particles

$$\vec{S} = \frac{\hbar}{2} \vec{s}$$

$$\vec{S} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(independent traceless 2x2 Hermitian matrices)

$$\sigma_i \sigma_j = \delta_{ij} \mathbf{I} + i \frac{3}{2} \epsilon_{ijk} \sigma_k .$$

$$R_2(\phi) = e^{-\frac{i}{\hbar} \vec{S}_z \phi} = e^{-\frac{i}{\hbar} \left( \vec{x} \sigma_z \right) \phi} = e^{-\frac{i}{\hbar} \sigma_z \phi}$$

$$= \sum_{n=0}^{\infty} \frac{(-i \sigma_z \phi)^n}{n!} = \sum_{n=0}^{\infty} \frac{(-i \sigma_z \phi)^{2n+1}}{(2n+1)!}$$

Use $\sigma_z^2 = \mathbf{I}$

$$= \sum_{n=0}^{\infty} \frac{(-i \sigma_z \phi)^{2n}}{(2n)!} = \sum_{n=0}^{\infty} \frac{(-i \sigma_z \phi)^{2n}}{(2n)!} \frac{1}{2^{2n}} \frac{2^{2n+1}}{(2n+1)!}$$

If we set $\phi = 2\pi$:

$$\sin \left( \frac{2\pi}{2} \right) = \sin \pi = 0$$

$$\cos \left( \frac{2\pi}{2} \right) = \cos \pi = -1$$

$$R_2(2\pi) = -\mathbf{I}$$
1. $\langle \psi | \phi \rangle$ is all initial and final spin $\frac{1}{2}$ particles are rotated by $2\pi$: $\langle \psi | \phi \rangle = \langle \psi' | \phi' \rangle = \langle \psi | \phi \rangle (-1)^{+1}$

2. 2 Beams of Neutrons

one goes through a magnetic field

$$\frac{dS^z}{dt} = \frac{i}{\hbar} \left[ H, S^z \right]$$

$$H = -\frac{eq}{2m} \mathbf{B} \cdot \mathbf{S}$$

$$\frac{dS^x}{dt} = \frac{i}{\hbar} \left( -\frac{eq}{2m} \mathbf{B} \right) \mathbf{S} \cdot \mathbf{S}$$

while in the field the spin rotates about the $z$ axis with frequency $\omega = \frac{eqB}{2m}$, the amount of rotation can be controlled by how long one particle is in the field.
For a particulate moving in the z direction with the spin polarized in the x direction when the beams are recombined

\[ \langle \uparrow | (1 + \cos \omega t) + \downarrow \sin \omega t \rangle \uparrow | (1 + \cos \omega t) + \downarrow \sin \omega t \rangle \]

\[(1 + \cos \omega t)^2 + \sin^2 \omega t = 2 + 2 \cos \omega t \]

up to normalization this will vanish when \( \omega t = \pi \) - this happens by rotating through by \( 2\pi \).

\[ \text{Variational Methods} \]

Assume \( H \) has a complete set of eigenvectors with eigenvalues bounded from below

\[ H | \psi_n \rangle = E_n | \psi_n \rangle \]

\[ E_1 \leq E_2 \leq E_3 \ldots \]

(we choose to label the states as above)

Let \( | \psi \rangle \) be any normalizable vector, we use completeness of the eigenvectors of \( H \) to write

\[ | \psi \rangle = \sum_{n=1}^{\infty} | \psi_n \rangle \langle \psi_n | \psi \rangle = \sum_{n=1}^{\infty} C_n | \psi_n \rangle \]

where

\[ \sum_{n=1}^{\infty} |C_n|^2 = \sum_{n=1}^{\infty} \langle \psi_n | \psi_n \rangle \langle \psi_n | \psi \rangle = \langle \psi | \psi \rangle = 1 \]
Consider

\[ \langle \chi | H | \chi \rangle = \sum_{n=1}^{N} \langle \psi_{n} | H | \psi_{n} \rangle \langle \psi_{n} | \chi \rangle \langle \chi | \psi_{n} \rangle \]

\[ = \sum_{n=1}^{N} E_{n} |\langle \psi_{n} | \chi \rangle|^{2} \]

\[ \geq \sum_{n=1}^{N} E_{0} |\langle \psi_{n} | \chi \rangle|^{2} \]

\[ = E_{0} \sum_{n=1}^{N} |\langle \psi_{n} | \chi \rangle|^{2} \]

\[ = E_{0} \]

This shows that no matter how we choose the vector \( |\chi\rangle \), as long as it is normalized, that

\[ \langle \chi | H | \chi \rangle \geq E_{0} \]

In order for there to be equal we must have

\[ \sum_{n=1}^{N} E_{n} |\langle \psi_{n} | \chi \rangle|^{2} = \sum_{n=1}^{N} E_{0} |\langle \psi_{n} | \chi \rangle|^{2} - \]

\[ = \sum_{n=1}^{N} (E_{n} - E_{0}) |\langle \psi_{n} | \chi \rangle|^{2} \]
since each term in the sum is a product of non-negative quantities

1. If $|\psi_n(\mathbf{k})|^2 \neq 0 \Rightarrow E_n = E_0$

2. $E_n = E_0$ for some $n$ just means that the ground state is degenerate and $|\psi\rangle$ is a linear combination of states with energy $E_0$

Putting these together we get:

\[
\begin{align*}
\langle \chi | H | \chi \rangle & = E_0 \\
\langle \chi | H | \chi \rangle & = E_0 \Rightarrow \\
|\chi\rangle & \text{ is an eigenstate of } H \text{ with energy } E_0
\end{align*}
\]

This is a very powerful method. If we choose to have a class of functions parameterized by parameters $\mathbf{z} = (z_1, \ldots, z_N)$
\[ \langle \psi(\vec{a}) | H | \psi(\vec{a}) \rangle \geq E_0. \]

The left side is an ordinary function of the \( N \) parameters \( a_1, \ldots, a_N \). It has a minimum (which is \( = E_0 \)).

If we minimize this function, then \( E(\vec{a}) \) gets closer to \( E_0 \) and \( \psi(\vec{a}) \) gets closer to \( \psi_0 \).

To minimize this,

\[
\frac{\partial}{\partial a_i} \frac{\langle \psi(\vec{a}) | H | \psi(\vec{a}) \rangle}{\langle \psi(\vec{a}) | \psi(\vec{a}) \rangle} = 0 \quad i=1 \ldots N
\]

This gives \( N \) equations to find points \( \vec{a}^* \) that are extrem values of

\[
F(\vec{a}) = \frac{\langle \psi(\vec{a}) | H | \psi(\vec{a}) \rangle}{\langle \psi(\vec{a}) | \psi(\vec{a}) \rangle}.
\]
To find a minimum

\[ F(\bar{a}^* + s\bar{a}) = F(\bar{a}^*) + \frac{1}{2} \sum \frac{\partial^2 F}{\partial a_i \partial a_j}(\bar{a}^*) s a_i s a_j > 0 \]

The condition for this is that the \( N \times N \) matrix

\[ \frac{\partial^2 F}{\partial a_i \partial a_j}(\bar{a}^*) = F_{ij} \]

has only positive eigenvalues.

To see this note

\[ U_{ij} F_{jk} U_{kj} = \lambda_i \delta_{ie} \quad \lambda_i > 0 \]

\[ \sum F_{ij} s a_i s a_j = (U_{in} \lambda_n U_{nq}^*) s a_i s a_j \]

\[ \sum (U_{nq}^{\times} a_{nq}) \lambda_n (U_{rs} s a_s) \rightarrow \]

\[ \sum \lambda_r (\sum U_{rq} s a_q)^2 \lambda_r > 0 \]

In general, this only gives a local minimum.
consider the case of the hydrogen ground state \((l=0)\)

\[
H = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - \frac{e^2}{4\pi \epsilon r}
\]

This is the Hamiltonian for the reduced wave function

\[
\psi(r) = r R_n(r)
\]

Try

\[
\lambda(x) = N(x) re^{-\alpha x}
\]

as an trial wave function

If we normalize this,

\[
1 = \int_0^\infty r e^{-2\alpha x} dr = N^2 \left(-\frac{1}{2} \frac{d}{dx}\right)^2 \int_0^\infty e^{-2\alpha x} dr
\]

\[
= N(x)^2 \left(-\frac{1}{2} \frac{d}{dx}\right)^2 \frac{1}{2\alpha} = N(x)^3 \left(-\frac{1}{2} \frac{d}{dx}\right) \left(\frac{1}{4\alpha^2}\right)
\]

\[
= N^2 \left(\frac{1}{4\alpha^3}\right)
\]

\[
N(x) = 2\alpha^{3/2}
\]

\[
\lambda(x) = 2\alpha^{3/2} r e^{-\alpha x}
\]
\[
\frac{d^2}{dr^2} X = 2 \alpha^{3/2} \frac{d}{dr} \left( e^{-\alpha r} - \alpha r e^{-\alpha r} \right) \\
= 2 \alpha^{3/2} \left( -2 \alpha + \alpha^2 r \right) e^{-\alpha r}
\]

\[
\langle \gamma(\alpha) \chi | \chi(\alpha) \rangle =
\]

\[
4 \alpha^3 \int_0^\infty dr \left[ -\frac{\hbar^2}{2m} (-2 \alpha + \alpha^2 r) r - \frac{e^3}{4\pi} r \right] e^{-2\alpha r} =
\]

\[
4 \alpha^3 \left[ \left( \frac{\hbar^2 \alpha}{m} - \frac{e^3}{4\pi} \right) \int_0^\infty e^{-2\alpha r} - \frac{\hbar^2}{2m} \alpha^2 \int_0^\infty e^{-2\alpha r} \right]
\]

\[
(-\frac{1}{\alpha} \frac{d}{d\alpha}) \left( \frac{\hbar^2}{2m} \right) \left( \frac{1}{\alpha} \frac{d}{d\alpha} \right)
\]

\[
\frac{1}{4} \alpha^3
\]

\[
\text{= } \left[ \frac{\hbar^2 \alpha}{m} - \frac{e^3}{4\pi} \right]
\]

\[
\left[ \frac{\hbar^2 \alpha}{2m} - \frac{e^3}{4\pi} \right]
\]

\[
\frac{d}{d\alpha} \left[ \frac{\hbar^2 \alpha}{2m} - \frac{e^3}{4\pi} \right] = 0 \quad \frac{\hbar^2 \alpha}{m} - \frac{e^3}{4\pi} = \nu
\]

\[
\alpha = \frac{me^3}{4\pi \hbar^2}
\]

Using this in

\[
\langle \chi | M | \chi \rangle = \frac{\hbar^2}{2m} \left( \frac{m^2 e^4}{4\pi^2 \hbar^4} \right) - \frac{e^3}{4\pi} \left( \frac{me^3}{4\pi \hbar^2} \right)
\]

\[
- \frac{m}{2\hbar^2} \left( \frac{e^3}{4\pi} \right)^2
\]
This is the exact ground state energy which means

\[ 2\alpha^{3/2}e^{-\alpha r} = R_{10} \]

\[ \alpha = \frac{mE}{4\pi\hbar^2} \]

is the exact radial wave function

Let \( |\chi_n\rangle \) be a finite 'set of orthogonal vectors.

Consider the trial function

\[ |\Psi(\alpha)\rangle = \sum_{n=1}^{N} C_{n} |\chi_n\rangle \alpha^n \sqrt{\sum_{n=1}^{N}|C_n|^2} \]

This is the general sum of a normalized vector in the subspace spanned by the vector \( |\chi_n\rangle \)
Application to linear algebra

Assume $H|\psi_n\rangle = E_n|\psi_n\rangle$ exact order the exact eigenvalues so

$E_1 \leq E_2 \leq E_3 \ldots$

Pick an arbitrary set of orthonormal vectors $(N)$

$|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle$

$\langle \psi_i | \psi_j \rangle = \delta_{ij}$

Consider the projected eigenvalue problem

$\Pi_N = \sum_{k=1}^{N} |\psi_k\rangle \langle \psi_k |$

$\Pi_N - \Pi_N \Pi_N |\chi\rangle = \tilde{E} \Pi_N |\chi\rangle$

by this equation I mean

$\sum_{k, l, r=1}^{N} \langle \psi_r | H | \psi_l \rangle \langle \psi_l | \psi_k \rangle = \tilde{E} \sum_{k, l=1}^{N} \langle \psi_l | H | \psi_k \rangle$

multiply by $\langle \chi |$ on both sides

$\sum_{k=1}^{N} \langle \psi_k | H | \psi_l \rangle \langle \psi_l | \psi_k \rangle = \tilde{E} \langle \chi | \psi_k \rangle$

or

$\sum_{k=1}^{N} \left( \tilde{E} \delta_{nk} - \langle \psi_k | H | \psi_l \rangle \right) \langle \psi_l | \chi \rangle = 0$
This has non-zero solutions when the determinant of the matrix vanishes. The determinant is a degree $N$ polynomial in $\hat{E}$.

Because $H$ is Hermitian, it has $N$ real roots $\hat{E}_n$ for $n = 1, \ldots, N$ and $N$ orthonormal eigenvectors $|\phi(n)\rangle$.

As in the case of the exact eigenvalues, we number them as:

$$\hat{E}_1 < \hat{E}_2 < \hat{E}_3 < \ldots < \hat{E}_N$$

we know by the variational principle that

$$E_1 \leq \hat{E}_1$$

Consider the linear combination

$$c_1 |\phi(1)\rangle + c_2 |\phi(2)\rangle \equiv |\psi\rangle$$

we can choose the coefficients so the linear combination is $\perp$ to $|\phi(1)\rangle$

$$c_1 <\psi|\phi(1)\rangle + c_2 <\psi|\phi(2)\rangle = 0 \equiv 1$$

$$c_2 = -c_1 \frac{<\psi|\phi(1)\rangle}{<\psi|\phi(2)\rangle}$$

we choose the remaining coefficient so this is normalized to 1.
Consider
\[ \langle \chi | H | \chi \rangle = \sum_{n=1}^{\infty} \langle \chi | \psi(n) \rangle E_n \langle \psi(n) | \chi \rangle \]

since \[ \langle \chi | \psi(1) \rangle = 0 \]

\[ \langle \chi | H | \chi \rangle = \sum_{n=2}^{\infty} K \langle \chi | \psi(n) \rangle |^2 (E_2 + (E_n - E_2) \]

because of the way that we order eigenvalues \[ E_n - E_2 \geq 0 \]

\[ = \sum_{n=2}^{\infty} K \langle \chi | \psi(n) \rangle |^2 E_2 \]

\[ = \sum_{n=2}^{\infty} K \langle \chi | \psi(n) \rangle |^2 E_2 \] (since \[ \langle \chi | \psi(1) \rangle = 0 \])

\[ = E_2 \]

\[ \therefore \langle \chi | H | \chi \rangle \geq E_2 \]

but
\[ \langle \chi | H | \chi \rangle = 2 (C_1 \langle \chi | \chi_1 \rangle + C_2 \langle \chi | \chi_2 \rangle ) \cdot (C_1 \langle \chi | \chi_1 \rangle + C_2 \langle \chi | \chi_2 \rangle ) \]

\[ = |C_1|^2 \tilde{E}_1 + |C_2|^2 \tilde{E}_2 \]

since \[ \tilde{E}_2 \geq \tilde{E}_1 \]

\[ = |C_1|^2 (\tilde{E}_1 - \tilde{E}_2 + \tilde{E}_2) + |C_2|^2 \tilde{E}_2 \]

\[ = \tilde{E}_2 + |C_1|^2 (\tilde{E}_1 - \tilde{E}_2) \]

\[ \leq 0 \]

\[ \langle \chi | H | \chi \rangle \leq \tilde{E}_2 \]

\[ \tilde{E}_2 \geq \langle \chi | H | \chi \rangle \geq E_2. \]
we can proceed by induction

\[ c_1 |\psi_1\rangle + c_2 |\psi_2\rangle + c_3 |\psi_3\rangle = |\chi\rangle \]

and choose \( c_1, c_2, c_3 \) so they are

1 to \( |\psi_1\rangle \) and \( |\psi_2\rangle \) and

normalized to 1 the same

method gives

\[ \tilde{E}_3 \equiv |\langle \chi | H | \chi \rangle| \equiv E_3 \]

This means that by choosing

a basis and truncating to

a finite dimensional subspace

the \( k \) lowest eigenvector of

the projected bound is a variational

bound on the \( k \) lowest vector

of the exact eigenvalue problem

\[ E_k \leq \tilde{E}_k \]

It is also possible to show

that if \( E_k = \tilde{E}_k \) then the

\( |\chi\rangle \) is the exact solution.