8.044 Statistical Physics I
Spring 2008

Wavefunctions, One Particle

Hamiltonian $\widehat{\mathcal{H}}(\widehat{\vec{r}}, \widehat{\vec{p}}, \widehat{\vec{s}})$

Wavefunction $\psi_n(\vec{r}, \vec{s})$

$\vec{r}$ and $\vec{s}$ are the variables.

n is a state index and could have several parts.

For an e^- in hydrogen $\psi = \psi_{n,l,m_l,m_s}(\vec{r}, \vec{s})$

$$\widehat{\mathcal{H}}(\widehat{\vec{r}}, \widehat{\vec{p}}, \widehat{\vec{s}})\, \psi_n(\vec{r}, \vec{s}) = E_n\, \psi_n(\vec{r}, \vec{s})$$

$\psi_n(\vec{r},\vec{s})$ often factors into space and spin parts.

$$\psi_n(\vec{r},\vec{s}) = \psi_{n'}^{\text{space}}(\vec{r})\,\psi_{n''}^{\text{spin}}(\vec{s})$$

$\psi_n^{\text{space}}(x) \propto e^{-\alpha x^2/2} H_n(\sqrt{\alpha}\,x)$ H.O. in 1 dimension

$\psi_n^{\text{space}}(\vec{r}) \propto e^{i\vec{k}\cdot\vec{r}}$ free particle in 3 dimensions

$\psi_{n''}^{\text{spin}}(\vec{s})$

Spin is an angular momentum so for a given value of the magnitude S there are $2S + 1$ values of m_S.

For the case of $S = 1/2$ the eigenfunctions of the z component of $\vec{s}$ are $\phi_{1/2}(\vec{s})$ and $\phi_{-1/2}(\vec{s})$

$$\widehat{S}_z \, \phi_{1/2}(\vec{s}) \; = \; \frac{\hbar}{2} \phi_{1/2}(\vec{s})$$

$$\widehat{S}_z \, \phi_{-1/2}(\vec{s}) \; = \; -\frac{\hbar}{2} \phi_{-1/2}(\vec{s})$$

$\psi^{\text{spin}}_{n''}(\vec{s})$ is not necessarily an eigenfunction of $\widehat{S}_z$. For example one might have

$$\psi^{\text{spin}}_{n''}(\vec{s}) = \frac{1}{\sqrt{2}}\,\phi_{1/2}(\vec{s}) + \frac{1}{\sqrt{2}}\,\phi_{-1/2}(\vec{s})$$

In some cases $\psi_n(\vec{r}, \vec{s})$ may not factor into space and spin parts. For example one may find

$$\psi_n(x, \vec{s}) = f(x)\,\phi_{1/2}(\vec{s}) + g(x)\,\phi_{-1/2}(\vec{s})$$

Many Distinguishable Particles, Same Potential, No Interaction

Lump space and spin variables together

$\vec{r}_1, \vec{s}_1 \rightarrow 1 \quad \vec{r}_2, \vec{s}_2 \rightarrow 2$ etc.

$$\widehat{\mathcal{H}}(1, 2, \cdots N) = \widehat{\mathcal{H}}_0(1) + \widehat{\mathcal{H}}_0(2) + \cdots \widehat{\mathcal{H}}_0(N)$$

In this expression the single particle Hamltonians all have the same functional form but each has arguments for a different particle.

The same set of single particle energy eigenstates is available to every particle, but each may be in a different one of them. The energy eigenfunctions of the system can be represented as products of the single particle energy eigenfunctions.

$$\psi_{\{n\}}(1,2,\cdots N) = \psi_{n_1}(1)\psi_{n_2}(2)\cdots\psi_{n_N}(N)$$

$\{n\} \equiv \{n_1, n_2, \cdots n_N\}$. There are N #s, but each n_i could have an infinite range.

$$\widehat{\mathcal{H}}(1,2,\cdots N)\,\psi_{\{n\}}(1,2,\cdots N) = E_{\{n\}}\,\psi_{\{n\}}(1,2,\cdots N)$$

Many Distinguishable Particles, Same Potential, Pairwise Interaction

$$\hat{\mathcal{H}}(1, 2, \cdots N) = \sum_{i=1}^{N} \hat{\mathcal{H}}_0(i) + \frac{1}{2} \sum_{i \neq j} \hat{\mathcal{H}}_{\text{int}}(i, j)$$

The $\psi_{\{n\}}(1, 2, \cdots N)$ are no longer energy eigenfunctions; however, they could form a very useful basis set for the expansion of the true energy eigenfunctins.

Indistinguishable Particles

$$\hat{P}_{ij}\, f(\cdots i \cdots j \cdots) \equiv f(\cdots j \cdots i \cdots)$$

$(\hat{P}_{ij})^2 = \hat{I} \quad \Rightarrow \quad$ eigenvalues of $\hat{P}_{ij}$ are $+1, -1$

It is possible to construct many-particle wavefunctions which are symmetric or anti-symmetric under this interchange of two particles.

$$\hat{P}_{ij}\, \psi^{(+)} = \psi^{(+)} \qquad\qquad \hat{P}_{ij}\, \psi^{(-)} = -\,\psi^{(-)}$$

Identical $\Rightarrow$ no physical operation distinguishes between particle i and particle j. Mathematically, this means that for all physical operators $\hat{\mathcal{O}}$

$$[\hat{\mathcal{O}}, \hat{P}_{ij}] = 0$$

$\Rightarrow$ eigenfunctions of $\hat{\mathcal{O}}$ must also be eigenfunctions of $\hat{P}_{ij}$.

$\Rightarrow$ energy eigenfunctions ψ_E must be either $\psi_E^{(+)}$ or $\psi_E^{(-)}$.

$\Rightarrow$ states differing only by the interchange of the spatial and spin coordinates of two particles are the <u>same</u> state.

Relativistic quantum mechanics requires

$$\text{integer spin} \leftrightarrow \psi_E{}^{(+)} \qquad [\text{Bosons}]$$

$$\text{half-integer spin} \leftrightarrow \psi_E{}^{(-)} \qquad [\text{Fermions}]$$