Symmetry restrictions on Ψ. Example of parity invariance.

QM of Identical Particles ✓ Ref. Davydov, Ch. IX; Sakurai, Ch. 6

1) When we solve the Schrödinger problem: $\mathcal{H}\psi_n = E_n\psi_n$, we generate a large class of eigenfcns $\{\psi_n\}$ which satisfy orthogonality $[\int dx\, \psi_m^* \psi_n = \delta_{mn}]$, obey closure $[\sum_n \psi_n^*(x)\psi_n(x') = \delta(x-x')]$, and can be used as a complete set for general states of the system $[\Psi(x) = \sum_n a_n \psi_n(x)]$. Even so, the eigenfcns $\psi_n(x)$ -- emergent as solutions to $\mathcal{H}\psi_n = E_n\psi_n$ -- may not be individually in a form suitable for representing eigenstates of the system. The ψ_n may have to be adjusted to meet other conditions (beyond $\mathcal{H}\psi_n = E_n\psi_n$) required by the system symmetries.

An example is the wavefcn symmetry required by parity invariance. Suppose the system Hamiltonian is invariant under reflection of position cds: $\mathcal{H}(-x) = \mathcal{H}(x)$.

So// $\underline{\mathcal{H}(x)\psi(x) = E\,\psi(x)}$ ✓ original S. Eqtn $\rightarrow \mathcal{H}(-x)\psi(-x) = E\,\psi(-x)$ ✓ reflected S. Eqtn

but// $\mathcal{H}(-x) = \mathcal{H}(x)$, so reflected eqtn: $\underline{\mathcal{H}(x)\psi(-x) = E\psi(-x)}$.

and// $\psi(-x)$ & $\psi(x)$ satisfy the same Schrödinger Eqtn: $\mathcal{H}\psi = E\psi$. **(1)**

So// $\psi(-x) = c\,\psi(x)$, $c = \text{cnst}$; $\psi(x) = c\,\psi(-x) = c^2\psi(x) \Rightarrow c^2 = 1$.

and// $c = \pm 1 \Rightarrow \boxed{\psi(-x) = (\pm)\psi(x)}$ ✓ $\binom{\text{even}}{\text{odd}}$ parity, when: $\mathcal{H}(-x) = \mathcal{H}(x)$.

When $\mathcal{H}$ has this symmetry, the only ψ's which can be used to represent an eigenstate of the system must have even or odd reflection symmetry. This distinction makes little difference until the (degenerate) state is perturbed by some $V(x)$:

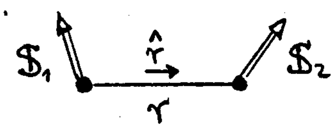
$$\text{pert}^{\underline{b}}\text{n } V(x) \Rightarrow E \begin{cases} E_+ = E + \langle\psi(x)|V(x)|\psi(x)\rangle, & \text{for even parity component,} \\ E_- = E + \langle\psi(-x)|V(x)|\psi(-x)\rangle, & \text{for odd parity} \quad '' \quad ; \end{cases} \qquad (2)$$

(by 1st order pert$^{\underline{b}}$n theory). The E_- perturbation is $\langle\psi(x)|V(-x)|\psi(x)\rangle$, and so the energy difference is: $\underline{\Delta E = (E_+ - E_-) = \langle\psi(x)|V(x) - V(-x)|\psi(x)\rangle}$. This ΔE is generally nonzero, and gives a physical basis for distinguishing between even & odd ψ's.

Examples of multi-particle systems with exchange symmetry.

2) We shall now study some symmetry restrictions on Ψ which follow from the QM treatment of n "identical particles". The prototype QM system here is an n-electron atom, where the electrons are bound to the nucleus and interact with (mainly repel) each other; the electrons are identical in the sense that if an electron in the k^{th} orbital is exchanged with an electron in the l^{th} orbital, the atom remains totally unchanged -- the electrons are indistinguishable.

Another, simpler example of a QM system with exchange symmetry is that of two identical spins interacting via a dipole-dipole coupling...



dipole moments: $\mu_i = g_i \mu_0 \mathbb{S}_i$, $i = 1 \& 2$;

$$\left.\begin{array}{c}\text{dipole-dipole}\\ \text{coupling}\end{array}\right\} \mathcal{H}(1,2) = g_1 g_2 \frac{\mu_0^2}{r^3}\left[(\mathbb{S}_1 \cdot \mathbb{S}_2) - 3(\mathbb{S}_1 \cdot \hat{r})(\mathbb{S}_2 \cdot \hat{r})\right]. \tag{3}$$

The spins are labelled as though we knew that the "first" particle is at position 1, while the "second" particle is at position 2. But since the particles are identical, we should not be able to distinguish this ordering from that where the "first" particle is at position 2, and the "second" at position 1 -- i.e. from an ordering where the particles have exchanged places. The new ordering is governed by

$$\rightarrow \mathcal{H}(2,1) = g_2 g_1 \frac{\mu_0^2}{r^3}\left[(\mathbb{S}_2 \cdot \mathbb{S}_1) - 3(\mathbb{S}_2 \cdot \hat{r})(\mathbb{S}_1 \cdot \hat{r})\right] = \mathcal{H}(1,2). \tag{4}$$

Under the exchange, r is invariant $\hat{r} \rightarrow (-)\hat{r}$, and only the labelling of the $\mathbb{S}_i$ changes. The exchange invariance of the system is realized by the fact that $\mathcal{H}(2,1) = \mathcal{H}(1,2)$... both orderings will have the same energies, etc. In turn, the exchange symmetry for $\mathcal{H}$ will restrict the choice of eigenfcns.

We will return to this simple spin-spin system in a while (and actually write down the eigenfcns, etc). But now we do a more general analysis to assess the effects of exchange symmetry.

Exchange invariance of $\mathcal{H}$ ⇒ system Ψ must be even or odd under exchange.

3) For an n-particle Hamiltonian $\mathcal{H}(1\ldots k\ldots l\ldots n)$, where "k" represents all the coordinates [e.g. position $\mathbf{r}_k$, & momentum $\mathbf{p}_k$, spin $\mathbf{S}_k$, etc.] necessary to specify the k^{th} particle, we can show quite generally that an exchange symmetry for $\mathcal{H}$ requires that the system eigenfcns $\Psi(1\ldots k\ldots l\ldots n)$ are either <u>even</u> or <u>odd</u> under the same exchange. That is...

if// $\mathcal{H}(1\ldots l\ldots k\ldots n) = \mathcal{H}(1\ldots k\ldots l\ldots n)$ ← $\mathcal{H}$ is invariant under exchange of k^{th} & l^{th} particle;

then// $\Psi(1\ldots l\ldots k\ldots n) = \pm\Psi(1\ldots k\ldots l\ldots n)$ ← system wavefcn Ψ must be <u>even</u> or <u>odd</u> under $k \leftrightarrow l$. (5)

Proof is simple:

① $\mathcal{H}(1\ldots k\ldots l\ldots n)\Psi(1\ldots k\ldots l\ldots n) = E\Psi(1\ldots k\ldots l\ldots n)$ ← original S. Eqtn.

② $\underbrace{\mathcal{H}(1\ldots l\ldots k\ldots n)}_{\text{equals } \downarrow}\Psi(1\ldots l\ldots k\ldots n) = E\Psi(1\ldots l\ldots k\ldots n)$ ← $k \leftrightarrow l$ exchanged

③ $\mathcal{H}(1\ldots k\ldots l\ldots n)\Psi(1\ldots l\ldots k\ldots n) = E\Psi(1\ldots l\ldots k\ldots n)$ ← $\mathcal{H}$ symmetry used

Compare ① & ③: $\Psi(1\ldots l\ldots k\ldots n)$ & $\Psi(1\ldots k\ldots l\ldots n)$ obey <u>same</u> S. Eqtn, so...

$\Psi(1\ldots l\ldots k\ldots n) = A\,\Psi(1\ldots k\ldots l\ldots n)$, $A = \text{cnst}$

Exchange $k \leftrightarrow l$ again to show $A^2 = 1$, or $A = \pm 1$.

So// $$\underline{\underline{\Psi(1\ldots l\ldots k\ldots n) = \pm\Psi(1\ldots k\ldots l\ldots n)}}$$ ← Ψ is <u>even</u> or <u>odd</u> under $k \leftrightarrow l$. **QED** (6)

More formally, we could have proceeded as follows:

Let $\mathcal{E}_{kl}$ be an operator which exchanges all cds of k^{th} & l^{th} particles.

So, e.g.: $\mathcal{E}_{kl}\Psi(1\ldots k\ldots l\ldots n) = \Psi(1\ldots l\ldots k\ldots n)$.

(1) Show eigenvalues of $\mathcal{E}_{kl}$ are just ± 1, as in Eq.(6) above.

(2) Show $\mathcal{E}_{kl}$ is a linear, Hermitian operator.

(3) Show $[\mathcal{H}, \mathcal{E}_{kl}] = 0$, for the n-particle Ham^n $\mathcal{H}(1\ldots k\ldots l\ldots n)$.

Then system wavefcns Ψ are simultaneously eigenfcns of $\mathcal{H}$ <u>and</u> $\mathcal{E}_{kl}$. (7)