MANY-BODY QUANTUM FORMALISM

INTRODUCTION

5th LECTURE
FROM THE COURSE
QUANTUM PHYSICS OF LOW DIMENSIONAL STRUCTURES

QPLDS

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QUANTUM ANALYSIS OF QUANTUM OBJECTS

The principle of indistinguishability of quantum particles or just the principle of quantative quantum analysis:

verified experimentally results of quantum calculations should be independent on exchange of symbols used to mark identical objects.

verified experimental results = energy measurements (for example)

Thus, question at the very beginning: How to combine the wave function for the two bodies Ψ_{tot} from the single-body wave-function?

STARTING POINT – SCHRÖDINGER EQUATION

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi_{tot}}{\partial x_1^2}+\frac{\partial^2\Psi_{tot}}{\partial y_1^2}+\frac{\partial^2\Psi_{tot}}{\partial z_1^2}\right)-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi_{tot}}{\partial x_2^2}+\frac{\partial^2\Psi_{tot}}{\partial y_2^2}+\frac{\partial^2\Psi_{tot}}{\partial z_2^2}\right)+V_{tot}\Psi_{tot}=E_{tot}\Psi_{tot}$$

a) Looks like the equation of independent particles (the sum on the left)

b) V_{tot} must be potential energy of the system as a whole, but, if particles are independent, then $V_{tot}=V(x_1,y_1,z_1)+V(x_2,y_2,z_2)$.

c) There exist solutions for the equation with separate single-body terms combined into Ψ_{tot} using <u>multiplication</u>:

$$\boxed{\Psi_{tot}=\Psi(x_1,y_1,z_1)\bullet\Psi(x_2,y_2,z_2)}$$

Simplified, more informative description :

$$\Psi(x_1,y_1,z_1)\Rightarrow\Psi_\alpha(1),$$

where α - the set of quantum numbers (including spin)

by the way: can we measure something from that, at all?

can we $\Psi^*_{tot}\Psi_{tot}=\Psi^*_\alpha(1)\cdot\Psi^*_\beta(2)\Psi_\alpha(1)\cdot\Psi_\beta(2)$?

can we $\Psi^*_{tot}\Psi_{tot}=\Psi^*_\beta(1)\cdot\Psi^*_\alpha(2)\Psi_\beta(1)\cdot\Psi_\alpha(2)$? …

NEITHER

NOR…

Due to principle of <u>indistinguishability</u> we can not measure such densities of probability for the two-body system. Thus, for example:

$$\Psi_\alpha^*(1)\cdot\Psi_\beta^*(2)\Psi_\alpha(1)\cdot\Psi_\beta(2) \underset{2\to 1}{\overset{1\to 2}{\neq}} \Psi_\alpha^*(2)\cdot\Psi_\beta^*(1)\Psi_\alpha(2)\cdot\Psi_\beta(1)$$

However, we can measure:

$$\Psi_{tot}^{(S)*}\Psi_{tot}^{(S)} \underset{2\to 1}{\overset{1\to 2}{=}} \Psi_{tot}^{(S)*}\Psi_{tot}^{(S)} \quad \text{and} \quad \Psi_{tot}^{(A)*}\Psi_{tot}^{(A)} \underset{2\to 1}{\overset{1\to 2}{=}} \Psi_{tot}^{(A)*}\Psi_{tot}^{(A)},$$

where

$$\Psi_{tot}^{(s)} = \frac{\sqrt{2}}{2}[\Psi_\alpha(1)\cdot\Psi_\beta(2)+\Psi_\beta(1)\cdot\Psi_\alpha(2)]$$

and

$$\Psi_{tot}^{(A)} = \frac{\sqrt{2}}{2}[\Psi_\alpha(1)\cdot\Psi_\beta(2)-\Psi_\beta(1)\cdot\Psi_\alpha(2)]$$

Obviously,

$$\Psi_{tot}^{(S)} \underset{2\to 1}{\overset{1\to 2}{=}} \Psi_{tot}^{(S)} \quad \text{and} \quad \Psi_{tot}^{(A)} \underset{2\to 1}{\overset{1\to 2}{=}} -\Psi_{tot}^{(A)}$$

What about 3-body problem?

as $\Psi_{tot}^{(A)} = \frac{1}{\sqrt{2!}} \begin{vmatrix} \Psi_\alpha(1) & \Psi_\alpha(2) \\ \Psi_\beta(1) & \Psi_\beta(2) \end{vmatrix}$

then $\Psi_{tot}^{(A)} = \frac{1}{\sqrt{3!}} \begin{vmatrix} \Psi_\alpha(1) & \Psi_\alpha(2) & \Psi_\alpha(3) \\ \Psi_\beta(1) & \Psi_\beta(2) & \Psi_\beta(3) \\ \Psi_\gamma(1) & \Psi_\gamma(2) & \Psi_\gamma(3) \end{vmatrix}$

Conclusion: in order to describe many-body problem the multiplicative product of single-particle eigen-states should be used

FISHING MANY-BODY QUANTUM FORMALISM

Questions at the beginning:
Why many-body treatment? – it is something related to mesoscopic physics (a very trendy…)

What is a single particle approximation vs. many-body description, at all?

Maybe good idea is to reduce a description of the many-body quantum phenomenon to that of describing a single particle in some effective field contributed by the rest of particles?

What for field operators are used to describe many-body quantum phenomena, at all?

And, what for…?

The Hamiltonian for a system of N non-relativistic particles interacting via two-body forces

$$H = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m}\nabla_i^2\right) + \sum_{i<j} u(\vec{r}_i, \vec{r}_j)$$

(convention: $\sum_{i<j} \equiv \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} \equiv \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ i\neq j}}^{N} \equiv \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}{}'$, thus, there are 0.5 [*N(N-1)*] terms in the potential energy term)

Conclusion: the kinetic energy operator is a simple sum of single-particle operators $-\frac{\hbar^2}{2m}\nabla_i^2$.

In general, including internal degree of freedom (like a spin) the Hamiltonian equals (U below is the sum of kinetic and potential energies)

$$H = \sum_{i=1}^{N} U(\vec{r}_i\, \sigma_i) + \sum_{i<j} u(\vec{r}_i\, \sigma_i, \vec{r}_j\, \sigma_j)$$

Looking for a solution using Schrödinger equation

$$\boxed{H\Phi = E\Phi}$$

Problems… the equation above can not be solved exactly!

Solutions of the problem:

1) solve it approximately,
2) reconsider a <u>new</u> model for the quantum system, however in a style which incorporates the central features of the real objects, for example assume lack of interactions,
3) do not solve it at (try fishing…).

Ad. 2. The new model – the example of the simples model (no interactions for *N* particles):

$$H_0 = \sum_{i=1}^{N} U(\vec{r}_i \sigma_i)$$ - the new reconsidered model Hamiltonian,

$$U(\vec{r}_i \sigma_i)\phi_{l_i} = E_{l_i}\phi_{l_i}$$ - the one-body equation,

or more precisely $U(\vec{r}_i \sigma_i)\phi_{l_i} = E_{l_i}\phi_{l_i}(\vec{r}_i \sigma_i)$, ($l_i$ is a set of quantum numbers for the i^{th} particle,

or less precisely $U(\vec{r}\ \sigma\ )\phi_l\ = E_l\ \phi_l$.

$$\sum_{\sigma} \int \phi_{l_i}^{*} \phi_{l_j} d\vec{r} = \delta_{l_i l_j}$$ - the orthonormality condition,

(integration over spatial components, summation over discrete variables (spins))

or more precisely $\sum_{\sigma}\int \phi^{*}_{l_i}(\vec{r}_i\,\sigma_i)\phi_{l_j}(\vec{r}_j\,\sigma_j)d\vec{r}=\delta_{l_i l_j}$,

or less precisely $\sum_{\sigma}\int \phi^{*}_{l}\phi_{k}\,d\vec{r}=\delta_{lk}$

$H_0\Phi_0 = E_0\Phi_0$ - thus, the new many-body equation,

$\Phi_0 = \prod_{i=1}^{N}\phi_{l_i}$ - the eigen-function for the many-body problem derived from the single-particle description, and

$E_0 = \sum_{i=1}^{N}E_{l_i}$ - the eigen-value for the many-body problem calculated from the single-particle solutions.

What about indistinguishability principle in this example? This problem does not address the problem! Basically it described a single-particle! And the rest in derivations was only “EXPANDED” by subsequent multiplication ! This seems unphysical.

Thus, there is a need for appropriate indistinguishable or distinguishable statistics to describe more realistic many “bodies”…

BOSONS

Particles are identical and many-body waves functions are indistinguishable with respect to the interchange of any two particles (precisely, the interchange of any two coordinates of these particles). Indistinguishable = symmetrical.

Assumptions:

1) There are indeed many particles (not copies of any single particle like in the previous example)
2) Thus, there are many separate sets of quantum numbers describing separate, allowed states of particles. For example, $l_1, l_2, ..., l_N$ is the single-set of quantum numbers.
3) In general, there exists many separate sets of quantum numbers for many-body description. Let's mark an arbitrary set of the numbers by L_i, however for bosons the sets can overlap.

This L_i numerates basically different bosons…?
DIFFERENT BOSONS !?!?!?!?!?!?!?!?!?!

NO!
L_i numerates N single-particle levels!

…more "bosonically" speaking:

For N bosons, ~~**an every boson**~~…, no…

For N bosons there exist N states

BUT

within a given state quantum numbers can repeat
(There is *N* places to be filled in with l_i)

The N-bosons wave function is as follows:

$$\Phi^B(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,...,\vec{r}_N\sigma_N)=\sum_{L_i}^{N}C_{L_i}\Phi^B_{L_i}$$, where

the $\Phi^B_{L_i}$ could be the same as $\Phi_0=\prod_{i=1}^{N}\phi_{l_i}$, as in the previous example, but in general it can be constructed (by multiplications) from repeated single-particle functions ϕ_{l_i} .

FERMIONS

$$\Phi^F(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,...,\vec{r}_N\sigma_N)=\sum_{L_i}^{N}C_{L_i}\Phi^F_{L_i}$$

so easy as B $\rightarrow$ F…, but

for fermions in an arbitrary $\Phi^F_{L_i}$ function the single-particle functions ϕ_{l_i} can not be repeated within expressions.

Remark: the problem of symmetrization can be narrowed to the symmetrization of C's coefficients:

$$C_{L_i}(...n_i....n_j...)=\pm C_{L_i}(...n_j....n_i...)$$

where

$$\begin{cases} + \ for\ bosons \\ - \ for\ fermions \end{cases}$$

DIRAC NOTATION

clumsy	Dirac's
$\phi_{l_i}(\vec{r}_i\,\sigma_i)$ $\phi_l(\vec{r}\,\sigma)$	$<\vec{r}_i\,\sigma_i\,\vert\,l_i>$ or less precisely $<\vec{r}\,\sigma\,\vert\,l>$
$U(\vec{r}_i\,\sigma_i)\phi_{l_i} = E_{l_i}\phi_{l_i}(\vec{r}_i\,\sigma_i)$ $U(\vec{r}\,\sigma\,)\phi_l = E_l\,\phi_l$	$<\vec{r}_i\,\sigma_i\,\vert U\vert\,l_i> = E_{l_i}<\vec{r}_i\,\sigma_i\,\vert\,l_i>$ or less precisely $<\vec{r}\,\sigma\,\vert U\vert\,l> = E_l<\vec{r}\,\sigma\,\vert\,l>$ or without denoting the <u>coordinate representation</u> $\vert U\vert\,l> = E_l\,\vert\,l>$
$\sum_\sigma\int\phi_l^*\phi_k^* d\vec{r} = \delta_{lk}$	$\sum_\sigma\int<l\,\vert\,\vec{r}\,\sigma><\vec{r}\,\sigma\,\vert\,k>d\vec{r} = \delta_{lk}$ or simply $<l\,\vert\,k> = \delta_{lk}$
$\sum_\sigma\int\phi_l^*(\vec{r}\,\sigma)U(\vec{r}\,\sigma)\phi_k(\vec{r}\,\sigma)d\vec{r}$ Matrix element of a one-body operator "between" two single-particle wave-functions	$<l\,\vert U\vert\,k>$
$\sum_{\sigma_1}\sum_{\sigma_2}\int\phi_i^*(\vec{r}_1\,\sigma_1)\phi_j^*(\vec{r}_2\,\sigma_2)U(\vec{r}_1\,\sigma_1,\vec{r}_2\,\sigma_2,)\phi_l\,(\vec{r}_1\,\sigma_1)\phi_k\,(\vec{r}_2\,\sigma_2)d\vec{r}_1 d\vec{r}_2$ Matrix element of a two-body operator "between" two single-particle wave-functions: $<ij\,\vert U\vert\,lk>$	

A state vector:

$$| l >\equiv \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$ - this is something expressed in a matrix formalism,

$< | l >\equiv \phi$ is the wave-function in a given representation, thus:

$$< | l >\equiv \phi = \begin{bmatrix} \xi_1 & \xi_2 & \xi_3 & \xi_4 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$