

221B Lecture Notes

Many-Body Problems I

1 Quantum Statistics of Identical Particles

If two particles are identical, their exchange must not change physical quantities. Therefore, a wave function $\psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$ of N identical particles should not change the probability density $|\psi|^2$ under exchanging two particles, and hence we need

$$\psi(\vec{x}_1, \dots, \vec{x}_j, \dots, \vec{x}_i, \dots, \vec{x}_N) = e^{i\theta} \psi(\vec{x}_1, \dots, \vec{x}_i, \dots, \vec{x}_j, \dots, \vec{x}_N) \quad (1)$$

where $e^{i\theta}$ is a phase factor. This equation should hold for *any* pairs i, j .

What phase can it be? The requirement is that when you interchange a pair of particles twice, it is the same as not interchanging them. Namely $(e^{i\theta})^2 = 1$, and hence $e^{i\theta} = \pm 1$. The sign $+1$ is for bosons (particles that obey Bose–Einstein statistics) and -1 for fermions (those that obey Fermi–Dirac statistics).

The above argument is actually true only for three spatial dimensions and above. In two dimensions, one can define the orientation in the way you exchange two particles, clockwise or anti-clockwise. Then two clockwise exchanges do not have to give the original wave function. But one clockwise and one anti-clockwise exchange should. (Note that in three dimensions, one can rotate the sheet on which you exchange particles either clockwise or anti-clockwise by 180° to make clockwise and anti-clockwise exchanges the same.) Therefore the phase $e^{i\theta}$ can be anything, and the particles that obey quantum statistics of this sort are called anyons. They appear in the context of Fractional Quantum Hall Effect. In one dimension, two particles cannot go around each other when exchanged. Recall that this is why a delta function potential causes scattering in one-dimension but not above. Therefore, the exchange of particles necessarily involves the scattering phase shift at the same time, and one cannot separate the issue of statistics and interaction. For instance, fermions with self-interactions that produce a phase shift of π are equivalent to bosons with no self-interactions. One can also interpolate between fermions and bosons in terms of phase shifts. Such situations do arise in one-dimensional systems such as polymers and spin chains.

When I studied quantum mechanics, I once had a false impression that all you need to implement statistics is to divide Hilbert space into symmetric

and anti-symmetric parts. Well, it isn't completely wrong, but the point is to find *totally* symmetric and *totally* anti-symmetric wave functions. To see this, let us start with two-body wave functions. Considering two states $|a\rangle$ and $|b\rangle$, there are two possible states for two particles to be in these two states: $|ab\rangle$ and $|ba\rangle$. The first entry refers to the first particle and the second to the second particle. Between these two states, we form symmetric and anti-symmetric combinations:

$$|ab\rangle + |ba\rangle, \quad |ab\rangle - |ba\rangle. \quad (2)$$

The first one qualifies as a wave function for two identical bosons, while the second one for two identical fermions. In addition to these, the states $|aa\rangle$ and $|bb\rangle$ are already symmetric and are allowed for bosons but not for fermions. Therefore, every possible state you can imagine are still used in multi-body wave functions. The situation changes once you go to three particles. When three particles occupy three distinct states $|a\rangle$, $|b\rangle$ and $|c\rangle$, there are six possible states $|abc\rangle$, $|acb\rangle$, $|bca\rangle$, $|bac\rangle$, $|cab\rangle$, $|cba\rangle$. Among them, only combinations

$$|abc\rangle + |acb\rangle + |bca\rangle + |bac\rangle + |cab\rangle + |cba\rangle \quad (3)$$

and

$$|abc\rangle - |acb\rangle + |bca\rangle - |bac\rangle + |cab\rangle - |cba\rangle \quad (4)$$

are allowed for bosons and fermions, respectively, but other four combinations are not. In general, for N particles filling N distinct states, there are $N!$ states to start with, but there is only one totally symmetric state and one totally anti-symmetric state, and the rest of $N! - 2$ states are thrown out. Therefore quantum statistics reduces the size of the Hilbert space quite dramatically.

2 Spin-Statistics Theorem

There is a theorem in relativistic quantum field theory called spin-statistics theorem, proven by Heisenberg. It says that any particle with integer spin, such as photon (spin 1), should obey Bose-Einstein statistics, while any particle with half-odd spin, such as electron (spin 1/2), should obey Fermi-Dirac statistics. I cannot get into the discussion why in this course. The assumptions in this theorem are: (1) Lorentz invariance, (2) causality, and (3) unitarity (*i.e.*, positivity of the norms).

3 Pauli's Exclusion Principle

Pauli set up an ad hoc rule how to fill atomic states with electrons. He claimed that you can put *two* electrons per state. We now know that we can put actually only one electron per state, but there are two possible spin orientations for a given spatial state which effectively reproduces Pauli's rule.

We understand this rule now as a consequence of the anti-symmetrization of the wave function. Because a general fermionic wave function is $|ab\cdots\rangle - |ba\cdots\rangle$ where \cdots part is also anti-symmetrized, setting $a = b$ makes the wave function vanish identically. This is how Pauli's exclusion principle arises in modern quantum mechanics. It is quite remarkable that the definition of "identical particles" immediately lead to only two possibilities (in 3 dimensions) and one of them lead to Pauli's exclusion principle almost trivially.

Therefore, the fact that the electrons obey Pauli's exclusion principle in order to understand atomic spectra tells us that the electron is a fermion.

4 Proton statistics

How do we know that protons obey Fermi-Dirac statistics? We of course know that because of the spin-statistic theorem, but this theorem needed to be established experimentally anyway. We need to know that the proton is a fermion independent of its spin and the spin-statistics theorem.

For that purpose, we consider molecular band spectrum. A molecular band spectrum is what appears in the emission lines from a gas of molecules mostly from vibrational spectra (infrared), but the "lines" appear to be a "band", *i.e.* a thick line. Looking more closely, the thick line actually consists of many many fine lines, which come from rotational deexcitations.

Generally, a diatomic molecule has a rotational spectrum due to the rigid body Hamiltonian

$$H = \frac{\vec{L}^2}{2I} = \frac{\hbar^2 l(l+1)}{2I}. \quad (5)$$

Here it is assumed that the molecule has a dumb-bell shape and can rotate in two possible modes.

In the case of hydrogen molecules H_2 , two atoms are bosons because they consist of two fermions (one electron and one proton). Therefore the total wave function must be symmetric under the exchange of two hydrogen atoms. A part of the wave function comes from the spin degrees of freedom

of two protons. Depending on $S = 0$ or $S = 1$ for two proton spins, the spin part of the wave function is either anti-symmetric or symmetric. Everything else being the same between two hydrogen atoms, the anti-symmetry of the $S = 0$ spin wave function must be compensated by the rotational wave function. Using the relative coordinate $\vec{r} = \vec{x}_1 - \vec{x}_2$ between two protons, the interchange of two protons will flip the sign of $\vec{r} \rightarrow -\vec{r}$. The rotational wave function is nothing but spherical harmonics $Y_l^m(\vec{r})$, which satisfies the property $Y_l^m(-\vec{r}) = (-1)^l Y_l^m(\vec{r})$. Therefore the interchange of two protons would result in a sign factor $(-1)^l$ from the rotational wave function. In order to compensate the unwanted minus sign for $S = 0$ case, we need to take l odd. On the other hand, for $S = 1$ case, we need to take l even to keep the wave function symmetric.

Transitions among rotational levels take place only between the same S , because the nuclear magneton is too small to cause spin flips in the transitions. Therefore rotational spectra appear from transitions among even l states or odd l states, but not among odd and even l 's. Because the transitions are most frequent between two nearest states, the $S = 0$ case causes spectra for $l = 3$ to $l = 1$, $l = 5$ to $l = 3$, and so on, and hence

$$E_\gamma = \frac{\hbar^2}{2I}((2n+1)(2n+2) - (2n-1)2n) = \frac{\hbar^2}{2I}(8n+2) = \frac{\hbar^2}{2I}(10, 18, 26, 34, \dots). \quad (6)$$

On the other hand, the $S = 1$ case causes spectra

$$E_\gamma = \frac{\hbar^2}{2I}((2n+2)(2n+3) - 2n(2n+1)) = \frac{\hbar^2}{2I}(8n+6) = \frac{\hbar^2}{2I}(6, 14, 22, 30, \dots). \quad (7)$$

Having two series of spectra so far does not prove the statistics. But the point is that the first spectrum is for $S = 0$, and hence only one spin orientation, but the second one is for $S = 1$, and hence for *three* possible spin orientations. In other words, the lines for the second set of spectrum must be three times stronger than the first set. If protons followed Bose-Einstein statistics instead, the wave function must change its sign under the interchange of two atoms, and hence the $S = 0$ combination should give the second set of spectra while the $S = 1$ the first set, and the relative strength between two sets reverses.

This method applies in general to any same-nucleus diatomic molecules. In fact, the statistics of nitrogen nuclei ^{14}N was determined to be Bose-Einstein from this type of measurements, and causes a great puzzle. In those

days, people thought that the nuclei consist of protons and electrons, and hence the nitrogen nucleus was believed to be $14p+7e^-$, and hence a fermion. This discrepancy (statistics puzzle), together with a continuous spectrum of nuclear β -decay, let Pauli to speculate the existence of neutrinos.

5 Slater Determinant

Given single particle states, how do we construct a totally anti-symmetric wave function for fermions? Slater answered this question when he was attacking the problem of multi-electron atoms. Calling single particle levels $1, 2, \dots, N$ which N electrons fill, the totally anti-symmetric wave function can be written in terms of a Slater determinant,

$$\psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \psi_1(\vec{x}_1) & \psi_1(\vec{x}_2) & \cdots & \psi_1(\vec{x}_N) \\ \psi_2(\vec{x}_1) & \psi_2(\vec{x}_2) & \cdots & \psi_2(\vec{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(\vec{x}_1) & \psi_N(\vec{x}_2) & \cdots & \psi_N(\vec{x}_N) \end{pmatrix}. \quad (8)$$

Simply because of the properties of a determinant, this automatically gives a totally anti-symmetric wave function.

Here are some examples. When $N = 2$,

$$\psi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2!}} \det \begin{pmatrix} \psi_1(\vec{x}_1) & \psi_1(\vec{x}_2) \\ \psi_2(\vec{x}_1) & \psi_2(\vec{x}_2) \end{pmatrix} = \frac{1}{\sqrt{2}} [\psi_1(\vec{x}_1)\psi_2(\vec{x}_2) - \psi_1(\vec{x}_2)\psi_2(\vec{x}_1)]. \quad (9)$$

For $N = 3$,

$$\begin{aligned} \psi(\vec{x}_1, \vec{x}_2, \vec{x}_3) &= \frac{1}{\sqrt{3!}} \det \begin{pmatrix} \psi_1(\vec{x}_1) & \psi_1(\vec{x}_2) & \psi_1(\vec{x}_3) \\ \psi_2(\vec{x}_1) & \psi_2(\vec{x}_2) & \psi_2(\vec{x}_3) \\ \psi_3(\vec{x}_1) & \psi_3(\vec{x}_2) & \psi_3(\vec{x}_3) \end{pmatrix} \\ &= \frac{1}{\sqrt{6}} [\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\psi_3(\vec{x}_3) + \psi_1(\vec{x}_2)\psi_2(\vec{x}_3)\psi_3(\vec{x}_1) + \psi_1(\vec{x}_3)\psi_2(\vec{x}_1)\psi_3(\vec{x}_2) \\ &\quad - \psi_1(\vec{x}_2)\psi_2(\vec{x}_1)\psi_3(\vec{x}_3) - \psi_1(\vec{x}_3)\psi_2(\vec{x}_2)\psi_3(\vec{x}_1) - \psi_1(\vec{x}_1)\psi_2(\vec{x}_3)\psi_3(\vec{x}_2)] \end{aligned} \quad (10)$$