

221B Lecture Notes

Many-Body Problems I (Quantum Statistics)

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.

Some of you asked how we understand the dependence on the spatial dimensions d from topology. The point is to consider the *configuration space*, namely the space of (\vec{x}_1, \vec{x}_2)

for two particles, on which the wave function lives. Because we consider two identical particles, the configuration space is modded out by the exchange, R^d/Z_2 . Interchange of two particles correspond to a close loop on this space. The question is if we can consistently associate a phase for a closed loop, and mathematically it is similar to the situation of the Aharonov–Bohm effect.

Because points $\vec{x}_1 = \vec{x}_2$ are fixed points under the Z_2 action, the configuration space is singular; it is an *orbifold* instead of a regular manifold. To avoid the issues with singularities, imagine that they are not allowed to be at the same point due to a hard-core repulsion. Then the configuration space is R^{2d} with a d -dimensional “plane” $\vec{x}_1 = \vec{x}_2$ removed (and modded out by Z_2). If you project this space along the “plane,” it reduces to R^d with the origin removed, $R^d \setminus \{0\}$. It has non-trivial topology, $\pi_{d-1}(R^d \setminus \{0\}) = Z$. If $\pi_1 \neq 0$, it is similar to the situation of the Aharonov–Bohm effect, and a non-trivial phase can be associated with it. This is why “anyon” is possible when $d = 2$. When $\pi_0 \neq 0$, the configuration space is detached into two separate pieces, and extra information (*e.g.*, the discontinuity in the derivative) must be provided to connect the two, and again the boundary condition is arbitrary. On the other hand, $\pi_2 \neq 0$ does not allow any non-trivial loops for interchanging two particles.

2 How Much Smaller is the Hilbert Space?

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.

3 Spin-Statistics Theorem

There is a theorem in relativistic quantum field theory called spin-statistics theorem, proven by Pauli. 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).

4 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.

5 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 , the wave function of two protons must be anti-symmetric under their exchange. A part of the wave function comes from the spin degrees of freedom of two protons. Depending on $S = 0$ (parahydrogen) or $S = 1$ (orthohydrogen) for two proton spins, the spin part of the wave function is either anti-symmetric or symmetric. Everything else being the same between two protons, the anti-symmetry of the $S = 0$ spin wave function must be accompanied by a symmetric 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 keep the minus sign for $S = 0$ case, we need to take l even. On the other hand, for $S = 1$ case, we need to take l odd to keep the wave function anti-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 transi-

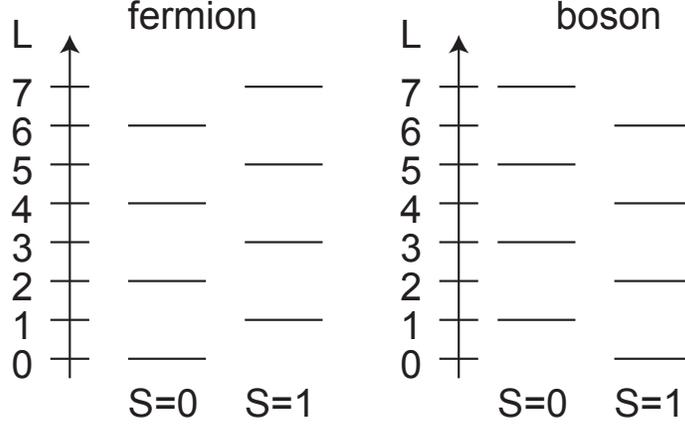


Figure 1: The allowed states for parahydrogen ($S = 0$) and orthohydrogen ($S = 1$) molecules for possible Fermi-Dirac or Bose-Einstein statistics for protons.

tions are most frequent between two nearest states,¹ the $S = 1$ 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 $S = 0$ 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 second spectrum is for $S = 0$, and hence only one spin orientation, but the first one is for $S = 1$, and hence for *three* possible spin orientations. In other words, the lines for the first set of spectrum must be three times stronger than the second set. If protons followed Bose-Einstein statistics instead, the wave function must not change its sign under the interchange of two protons, and hence the $S = 0$ combination should give the first set of spectra while the $S = 1$ the second set, and the relative strengths between two sets reverse.

¹This is actually not the familiar electric dipole (E1) transitions, but rather electric *quadrupole* (E2) transitions that can change the angular momentum by two units.

Correspondingly, the multiplicities of $S = 0$ (singlet) and $S = 1$ (triplet) appears in the calculation of the partition function and hence the specific heat. It was confusing to people like Hund that the observation did not come out as expected. It is because parahydrogen and orthohydrogen behave nearly as independent gas for a long time (like a day). This is so because the weakness of nuclear magnetic moment makes it difficult to cause transitions between para- and orthohydrogen. As a result, two components thermalize within each, but not between each other. See <http://scienceworld.wolfram.com/physics/Ortho-ParaHydrogen.html> for more on the hydrogen molecule.

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.

The situation is actually a little more complicated than what is explained here which completely ignores the electron wave function. For H_2 and N_2 , the electron wave function does not give any signs and the argument above applies unchanged. The ^{14}N nucleus has spin one, and hence the symmetric spin wave function has $S = 0$ and 2 (and hence the multiplicity 6), while the anti-symmetric spin wave function has $S = 1$ (multiplicity 3). The $S = 0, 2$ case has only even J , while $S = 1$ case only odd J . For O_2 , however, the electron wave function produces a sign under the interchange of two nuclei. The most common isotope ^{16}O does not have spin, and hence there is only $S = 0$ (symmetric) spin wave function possible. The nucleus follows the Bose-Einstein statistics. To compensate the sign from the electron wave function, there are only odd J states allowed. See, e.g., <http://tools.ecn.purdue.edu/~me687/MolecularDistHandout.pdf> There are magnetic dipole (M1) transitions among the rotational levels coupled with electron spins. See, e.g., <http://www.iras.ualgary.ca/~volk/oxygen.html>

6 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 $N = 3$,

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

One important word of caution is that multi-particle wave functions are in general *not* given by symmetrized or anti-symmetrized combination of products of single-particle wave functions.

7 Path Integral Formulation

In path integral formulation of quantum mechanics, we calculate the transition amplitudes

$$\langle \vec{x}_f, t_f | \vec{x}_i, t_i \rangle = \int \mathcal{D}\vec{x}(t) e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(t)}. \quad (11)$$

It is important that this transition amplitude contains information about time evolution of an arbitrary state, because

$$\psi(\vec{x}, t) = \langle \vec{x}, t | \psi \rangle = \int d\vec{x}_i \langle \vec{x}, t | \vec{x}_i, t_i \rangle \langle \vec{x}_i, t_i | \psi \rangle = \int d\vec{x}_i \langle \vec{x}, t | \vec{x}_i, t_i \rangle \psi(\vec{x}_i, t_i). \quad (12)$$

The generalization to the N -particle case is just that the Lagrangian contains many particles $L = L(\vec{x}_i(t), \dot{\vec{x}}_i(t))$ and

$$\langle \vec{x}_{1f}, \dots, \vec{x}_{Nf}, t_f | \vec{x}_{1i}, \dots, \vec{x}_{Ni}, t_i \rangle = \int \mathcal{D}\vec{x}_1(t) \dots \mathcal{D}\vec{x}_N(t) e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(t)}. \quad (13)$$

Here, the particle 1 at the initial position \vec{x}_{1i} moves to the final position \vec{x}_{1f} , the particle 2 at the initial position \vec{x}_{2i} to \vec{x}_{2f} , etc, and you sum over all possible paths. Again, the time-evolution is given by integrating over all initial positions for N particles together with the transition amplitude.

When the particles are identical, however, we need to introduce proper (anti-)symmetry of the state. Let us discuss fermions. (The case for bosons can be obtained easily by dropping all minus signs.) Because of the anti-symmetry of the wave function,

$$\Psi(\vec{x}_1, \dots, \vec{x}_i, \dots, \vec{x}_j, \dots, \vec{x}_N) = -\Psi(\vec{x}_1, \dots, \vec{x}_j, \dots, \vec{x}_i, \dots, \vec{x}_N) \quad (14)$$

it is convenient to introduce the anti-symmetrized position bra

$$\langle [\vec{x}_1, \dots, \vec{x}_N] | = \frac{1}{\sqrt{N!}} \sum_{\sigma} (-1)^{\sigma} \langle \vec{x}_{\sigma(1)}, \dots, \vec{x}_{\sigma(N)} |. \quad (15)$$

Here, σ is all possible permutations. The factor $(-1)^{\sigma}$ is $+1$ (-1) for even (odd) permutations. For example, the three-body case is

$$\begin{aligned} \langle [\vec{x}_1, \vec{x}_2, \vec{x}_3] | &= \frac{1}{\sqrt{3!}} (\langle \vec{x}_1, \vec{x}_2, \vec{x}_3 | + \langle \vec{x}_2, \vec{x}_3, \vec{x}_1 | + \langle \vec{x}_3, \vec{x}_1, \vec{x}_2 | \\ &\quad - \langle \vec{x}_3, \vec{x}_2, \vec{x}_1 | - \langle \vec{x}_2, \vec{x}_1, \vec{x}_3 | - \langle \vec{x}_1, \vec{x}_3, \vec{x}_2 |). \end{aligned} \quad (16)$$

Any state given by the form

$$\Psi(\vec{x}_1, \dots, \vec{x}_N) = \langle [\vec{x}_1, \dots, \vec{x}_N] | \Psi \rangle \quad (17)$$

is automatically anti-symmetric under the interchange of two coordinates. In particular, if the state $|\Psi\rangle$ is given in terms of a product of single-particle states $|\Psi\rangle = |\psi_1\rangle |\psi_2\rangle \dots |\psi_N\rangle$, Eq. (17) gives Slater determinant of $\psi_i(\vec{x}_j)$.

Therefore it is useful to consider path integral representation of the transition amplitudes

$$\langle [\vec{x}_{1f}, \dots, \vec{x}_{Nf}], t_f | [\vec{x}_{1i}, \dots, \vec{x}_{Ni}], t_i \rangle. \quad (18)$$

On the other hand, the Lagrangian for identical particles must be invariant under the exchange of particles,

$$\begin{aligned} & L(\vec{x}_1, \dot{x}_1, \dots, \vec{x}_i, \dot{\vec{x}}_i, \dots, \vec{x}_j, \dot{\vec{x}}_j, \dots, \vec{x}_N, \dot{\vec{x}}_N) \\ &= L(\vec{x}_1, \dot{x}_1, \dots, \vec{x}_j, \dot{\vec{x}}_j, \dots, \vec{x}_i, \dot{\vec{x}}_i, \dots, \vec{x}_N, \dot{\vec{x}}_N) \end{aligned} \quad (19)$$

This immediately leads to the identity

$$\begin{aligned} & \langle \vec{x}_{1f}, \dots, \vec{x}_{jf}, \dots, \vec{x}_{kf}, \dots, \vec{x}_{Nf}, t_f | \vec{x}_{1i}, \dots, \vec{x}_{ji}, \dots, \vec{x}_{ki}, \dots, \vec{x}_{Ni}, t_i \rangle \\ &= \langle \vec{x}_{1f}, \dots, \vec{x}_{kf}, \dots, \vec{x}_{jf}, \dots, \vec{x}_{Nf}, t_f | \vec{x}_{1i}, \dots, \vec{x}_{ki}, \dots, \vec{x}_{ji}, \dots, \vec{x}_{Ni}, t_i \rangle \end{aligned} \quad (20)$$

because both all possible path configurations and the associated weight $e^{iS/\hbar}$ are the same for two amplitudes. Using the definition Eq. (15), we find

$$\begin{aligned} & \langle [\vec{x}_{1f}, \dots, \vec{x}_{Nf}], t_f | [\vec{x}_{1i}, \dots, \vec{x}_{Ni}], t_i \rangle \\ &= \frac{1}{N!} \sum_{\sigma} \sum_{\sigma'} \langle \vec{x}_{\sigma(1)f}, \dots, \vec{x}_{\sigma(N)f}, t_f | \vec{x}_{\sigma'(1)i}, \dots, \vec{x}_{\sigma'(N)i}, t_i \rangle \\ &= \sum_{\sigma} \langle \vec{x}_{\sigma(1)f}, \dots, \vec{x}_{\sigma(N)f}, t_f | \vec{x}_{1i}, \dots, \vec{x}_{Ni}, t_i \rangle. \end{aligned} \quad (21)$$

In other words, the path integral sums over all possible paths allowing the positions at the final time slice are interchanged in all possible ways starting from the positions at the initial time slice. For instance, again for the three-body case,

$$\begin{aligned} & \langle [\vec{x}_{1f}, \vec{x}_{2f}, \vec{x}_{3f}], t_f | [\vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}], t_i \rangle \\ &= \langle \vec{x}_{1f}, \vec{x}_{2f}, \vec{x}_{3f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle + \langle \vec{x}_{2f}, \vec{x}_{3f}, \vec{x}_{1f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle \\ &+ \langle \vec{x}_{3f}, \vec{x}_{1f}, \vec{x}_{2f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle - \langle \vec{x}_{3f}, \vec{x}_{2f}, \vec{x}_{1f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle \\ &- \langle \vec{x}_{2f}, \vec{x}_{1f}, \vec{x}_{3f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle - \langle \vec{x}_{1f}, \vec{x}_{3f}, \vec{x}_{2f}, t_f | \vec{x}_{1i}, \vec{x}_{2i}, \vec{x}_{3i}, t_i \rangle. \end{aligned} \quad (22)$$

The graphical representation in Fig. (2) makes it clear that the relative signs are attached according to the number of times pairs are interchanged.

When the spatial dimension is two, the interchange of particles makes the paths intertwined. (In higher dimensions such as three, there is always a way to make them disentangle.) In particular, there is a sense of orientation in the way two paths intertwine. This is what makes anyons possible.

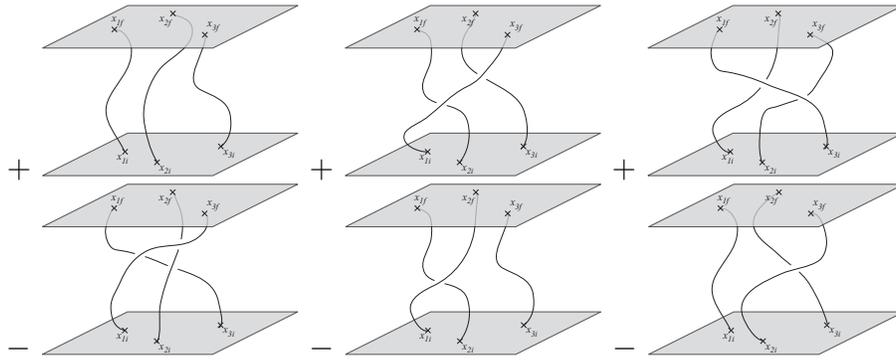


Figure 2: The path integral for three identical fermions.

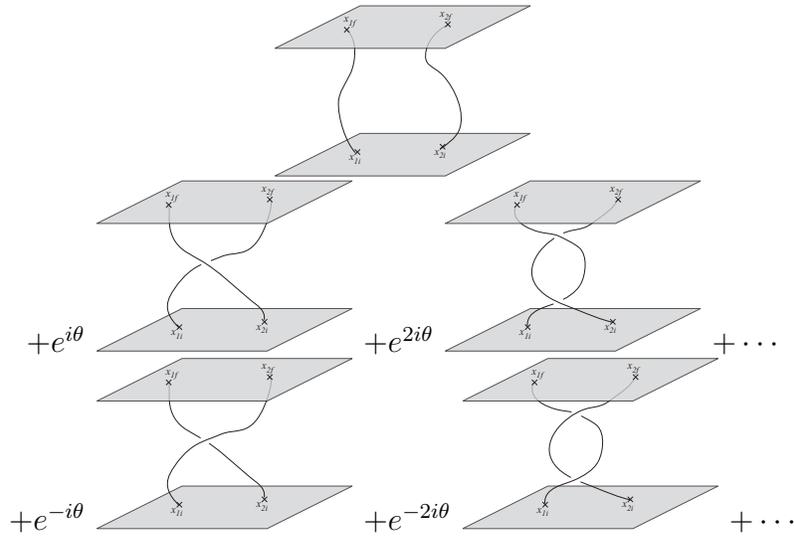


Figure 3: The path integral for two anyons.