

# Week 12

PHY 303 Quantum Mechanics

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## 5 Two particle quantum mechanics

We had already taken a first glimpse at how to handle more than one particle in quantum mechanics in section 4.1.3 and section 4.6.1. Let us explore this a bit more, to introduce some of the most fundamental and far reaching implications.

We had already given a generic Hamiltonian for two non-interacting particles in (4.28). When there are no interactions, we can again make a product Ansatz in the two particle wavefunction (5.2), writing

$$\psi(\mathbf{r}_a, \mathbf{r}_b) = \phi(\mathbf{r}_a)\eta(\mathbf{r}_b), \quad (5.1)$$

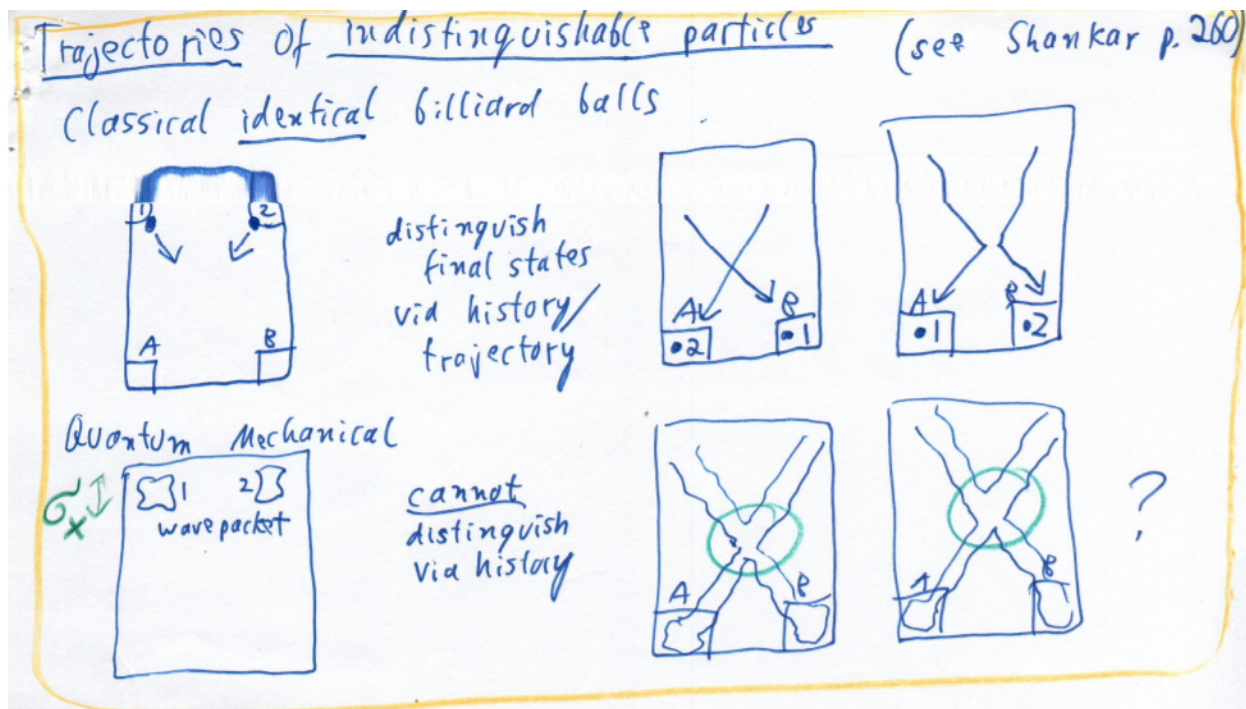
perform separation of variables on the TISE that follows from the Hamiltonian (4.28) and reach two independent TISEs:

$$\begin{aligned} \left[ -\frac{\hbar^2}{2m_a} \Delta_{\mathbf{r}_a} + V(\mathbf{r}_a) \right] \phi(\mathbf{r}_a) &= E_a \phi(\mathbf{r}_a), \\ \left[ -\frac{\hbar^2}{2m_b} \Delta_{\mathbf{r}_b} + V(\mathbf{r}_b) \right] \eta(\mathbf{r}_b) &= E_b \eta(\mathbf{r}_b). \end{aligned} \quad (5.2)$$

Suppose each Hamiltonian has quantised eigenstates  $\phi_n(\mathbf{r}_a)$ ,  $\eta_m(\mathbf{r}_b)$ , a joint solution could be  $\Psi_{nm}(\mathbf{r}_a, \mathbf{r}_b) = \phi_n(\mathbf{r}_a)\eta_m(\mathbf{r}_b)$ , which we would reasonably interpret as corresponding to “particle a is in state  $n$  and particle b is in state  $m$ ”. However this idea runs into some fundamental trouble:

### 5.1 Indistinguishable particles

How would you distinguish two identical fundamental particles? I.e. two electrons in the same spin state? The answer is you cannot, since there is no additional label you can flag it with. In classical mechanics, you could in principle distinguish even fully identical objects  $a$  and  $b$  via their position history  $\mathbf{r}_a(t)$  and  $\mathbf{r}_b(t)$ , but due to the HUP (1.46) this does not work in quantum mechanics, see diagram below:



- We conclude that a statement like “particle a is in state  $n$  and particle b is in state  $m$ ” does not make sense for indistinguishable particles.
- All we could hope to say is “there is some particle in state  $n$  and another one in state  $m$ ”.
- This implies that mathematically, the wavefunction  $\psi(\mathbf{r}_a, \mathbf{r}_b)$  must be equivalent to  $\psi(\mathbf{r}_b, \mathbf{r}_a)$ .
- In practice, we can often also deal with “distinguishable” particles in quantum mechanics, even if they are the same type of particle, as long as they never get too close to each other<sup>14</sup>.

Since the overall phase or sign of a wave-function does not matter (see section 1.6.1), “being equivalent” still allows for a change in the complex phase. We thus demand  $\psi(\mathbf{r}_a, \mathbf{r}_b) = e^{i\varphi}\psi(\mathbf{r}_b, \mathbf{r}_a)$ . Swapping the position again then gives  $\dots = (e^{i\varphi})^2\psi(\mathbf{r}_a, \mathbf{r}_b)$ . How we are back where we started, hence we need  $(e^{i\varphi})^2 = 1$ , which is true for  $\varphi = 0, \pi$ . We have thus shown the

### Indistinguishable particle exchange symmetry

$$\psi(\mathbf{r}_a, \mathbf{r}_b) = \pm\psi(\mathbf{r}_b, \mathbf{r}_a). \quad (5.3)$$

The two-particle wavefunction for two indistinguishable particles must be symmetric or anti-symmetric under exchange of those two particles.

<sup>14</sup>Meaning their wavefunctions never overlap

**Example 43, (Anti-)symmetrized wavefunctions:** Let us reconsider the state we had seen earlier  $\Psi_{nm}(\mathbf{r}_a, \mathbf{r}_b) = \phi_n(\mathbf{r}_a)\eta_m(\mathbf{r}_b)$ . Since particles are indistinguishable  $m_a = m_b$  in (5.2) and  $\phi_n$  and  $\eta_m$  really label the same set of eigenfunctions of a TISE. Let us thus use the label  $\phi$  only:  $\Psi_{nm}(\mathbf{r}_a, \mathbf{r}_b) = \phi_n(\mathbf{r}_a)\phi_m(\mathbf{r}_b)$ . We can fix the symmetrisation issues by writing

$$\tilde{\Psi}_{nm}(\mathbf{r}_a, \mathbf{r}_b) = \frac{1}{\sqrt{2}} (\phi_n(\mathbf{r}_a)\phi_m(\mathbf{r}_b) \pm \phi_m(\mathbf{r}_a)\phi_n(\mathbf{r}_b)), \quad (5.4)$$

either way this now satisfies (5.3), but the meaning has changed from “particle a is in state  $n$  and particle b is in state  $m$ ” to “there is some particle in state  $n$  and another one in state  $m$ ” as required.

We also know which are which:

**Bosons and Fermions** Particles with integer spin  $s = 0, 1, 2$  are called Bosons. They are the ones which have a symmetric many-body wavefunction, i.e.  $\oplus$  in (5.3). Particles with half-integer spin  $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$  are called Fermions. They are the ones which have an anti-symmetric many-body wavefunction, i.e.  $\ominus$  in (5.3).

- You can show this later in relativistic quantum mechanics, where the link between wavefunction symmetry and spin quantum number arises from the requirement to form a Lorentz invariant Hamiltonian where events outside the light-cone cannot affect each other. This is called spin-statistics theorem.
- Fundamental Fermions are all the matter particles, electrons, quarks and their higher generation counterparts as well as neutrinos. You can deduce from repeated applications of (4.126) that the combinations of an odd number of Fermions is a Fermion, while the combination of an even number of Fermions is a Boson. Thus also neutrons and protons are Fermions, since they contain three quarks. Then in turn, neutral atoms with an odd number of neutrons are also Fermions.
- Fundamental Bosons are all the force carriers photons, gluons, W and Z Bosons and the Higgs Boson. Composite Bosons are e.g. pions,  $\pi^{0,\pm}$ , which are bound states of a quark and an anti-quark. With the same argumentation as above, also neutral atoms with an even number of neutrons are Bosons.
- The most important difference between a Fermionic and a Bosonic wavefunction is at  $\mathbf{r}_a = \mathbf{r}_b = \mathbf{r}$ , i.e. when the particles try to be at the same place. For Bosons this is fine, for Fermions (5.3) gives you  $|\psi(\mathbf{r}, \mathbf{r})|^2 = 0$ , i.e. there is zero probability for two Fermions to ever be in the same place.

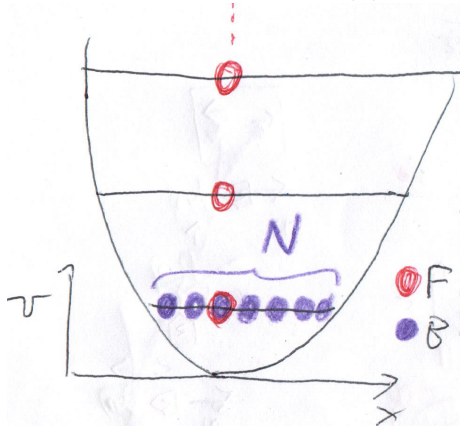
The perhaps most important consequence of the above is the

**Pauli exclusion principle** Two indistinguishable Fermions cannot occupy the same single particle quantum state  $\phi_0$ .

- Both particles in the same state would be described by  $\psi(r_a, r_b) = \phi_0(r_a)\phi_0(r_b)$ , but that wavefunction is not correctly anti-symmetric. We would have to write  $\psi(r_a, r_b) = [\phi_0(r_a)\phi_0(r_b) - \phi_0(r_b)\phi_0(r_a)]/\sqrt{2} = 0$  in an attempt to anti-symmetrize this to fulfill (5.3), but clearly this vanishes. Note that the tag “indistinguishable Fermions” only applies to particles in identical spin-states (otherwise you can distinguish them via the spin state).
- Pauli’s exclusion principle and the Hydrogen states from section 4.6 are nearly enough to understand the periodic table of elements. The same calculations as in section 4.6 gives us the solutions for a single electron seeing a nuclear charge of  $+Ze$  instead of  $+e$ , where  $Z$  is the number of protons in the nucleus. You just have to replace  $e^2 \rightarrow Ze^2$  in all our solutions. Ignoring electron-electron interactions in a first step, you can then find all the eigenstates for heavier atoms using techniques as for Eq. (5.2) and the Pauli principle. The latter forces us to fill two electrons only, into each Hydrogen-like state. The primary way that electron-electron interactions show up, is through the concept of screening: The two electrons in e.g. the  $|1s\rangle$  state of Lithium are much closer to the nucleus than the valence electron inserted into  $|2s\rangle$ . As a result they screen the nucleus for the valence electron, which thus sees an “effective nuclear charge”  $Z_{\text{eff}} \approx 1$  instead of  $Z = 3$ . This explains the periodic recurrences of e.g. ionisation energies. For (much) more details we refer to PHY402 “Atomic and molecular physics”, where you will discuss multi-electron atoms.

For Bosons, there is no problem in occupying the same quantum state. This allows for example a

**Example 44, Bose-Einstein condensate:** Consider  $N$  non-interacting Bosonic atoms in a 1D harmonic oscillator potential as shown below. Using the same statement as for (5.2) for those  $N$  atoms we find just one TISE such as Eq. (2.42) in section 2.3 for *each* of those atoms. The absolute ground-state thus clearly is  $\psi(x_1, x_2, \dots, x_N) = \phi_0(x_1)\phi_0(x_2) \dots \phi_0(x_N)$ , with SHO ground-state  $\phi_0(x)$  from Eq. (2.64).



**left:** Thus all  $N$  atoms are in the same single particle state  $\phi_0$ . The resultant many-particle state  $\psi$  describes what is called a Bose-Einstein condensate. In contrast Fermionic atoms would fill oscillator quantum states one by one, see on the left. See more on this in PHY435 “quantum many body physics of degenerate gases”.

The two different variants of many body wavefunctions give rise to fascinating and useful behaviour, that you can explore further in courses on super-conductivity (involving a Bose-Einstein condensate of cooper pairs), superfluidity, neutron stars (stabilised by the Pauli principle applied to neutrons) etc.

## 5.2 Entanglement

Let us in this section consider quantum systems that have two *distinguishable parts*, labelled  $a$  and  $b$ . We can then classify quantum-states into two classes.

**Entangled and separable states** We call a quantum state  $\psi(\mathbf{r}_a, \mathbf{r}_b)$  for two particles  $a$  and  $b$  separable, if it can be written as a product of a state for particle  $a$  and particle  $b$ , e.g.

$$\psi(\mathbf{r}_a, \mathbf{r}_b) = \phi_a(\mathbf{r}_a)\phi_b(\mathbf{r}_b). \quad (5.5)$$

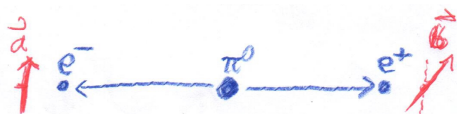
We call it entangled, if it cannot be written as a product, e.g.

$$\psi(\mathbf{r}_a, \mathbf{r}_b) = \frac{1}{\sqrt{2}} [\phi_a(\mathbf{r}_a)\phi_b(\mathbf{r}_b) - \phi_b(\mathbf{r}_a)\phi_a(\mathbf{r}_b)]. \quad (5.6)$$

- The easiest system in terms of which to think about entanglement, is a spin-1/2 object. In terms of the triplet and singlet states in (4.125), which are entangled and which are separable? (exercise).
- Entanglement is typically created through interactions of parts  $a$  and  $b$ .

Entangled states have some intriguing properties, which are best highlighted when considering the

**EPR paradox** Here EPR stands for Einstein-Podolsky-Rosen, who invented the paradox (in a slightly different guise) to show that quantum mechanics cannot simultaneously be real, local and complete.



**left:** A neutral pion  $\pi^0$  can decay into an electron  $e^-$  and a positron  $e^+$ . Since the pion has spin  $s = 0$ , angular momentum conservation requires the two decay products to be in the spin-singlet state of Eq. (4.125):  $|\psi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ . In this state, neither electron nor proton has a well defined spin: A measurement of either will give  $\uparrow$  or  $\downarrow$  with 50% probability, on both particles (see postulate III in section 3.6).

However after we measured e.g.  $\uparrow$  on the first particle, the state collapses according to postulate IV in section 3.6. In this case this means that  $|\psi\rangle \rightarrow |\uparrow\downarrow\rangle$ . Now we know the spin of the first and the second particle, so a measurement on the first seems to have affected the second. This argument applies even if the second particle is e.g. light-years away, causing EPR to conclude that something was “missing” in the quantum mechanical description of reality. There could be some “hidden variables” that explain the apparent weirdness.

The so-called paradox was ultimately resolved by

**Bell's theorem** Bell considered a more complicated version of the above, where spin is not measured only along the  $z$ -axis, but along two arbitrary axes in space  $\mathbf{a}$  and  $\mathbf{b}$ . Let's stick to just the  $z$  and  $x$  axes for the moment. Using our results Eq. (4.114), you can see that you can write the entangled state from example 5.2 also as  $|\psi\rangle = (|\leftarrow\rangle|\rightarrow\rangle - |\rightarrow\rangle|\leftarrow\rangle)/\sqrt{2}$ . So now if you randomly measure the spin along the  $x$  or  $z$  direction on one particle, the other one will always point opposite regardless of choice of measurement. How did it even “know” which axis we were going to measure?

Bell looked at the correlations  $P(\mathbf{a}, \mathbf{b}) = \langle \psi | (\mathbf{a} \cdot \hat{\mathbf{S}}_a)(\mathbf{b} \cdot \hat{\mathbf{S}}_b) | \psi \rangle$  and showed that the quantum mechanical result  $P(\mathbf{a}, \mathbf{b}) = -\mathbf{a} \cdot \mathbf{b}$  cannot be ever explained by a local hidden variable theory, who have to satisfy an inequality (Bell's inequality) that is violated by the quantum mechanical result. The quantum mechanical prediction was confirmed by many experiments since (first by Alain Aspect 1982, using entangled photons).

- The proof of Bell's theorem is not that hard, and can be found in Griffith, chapter 12. We refer to that also for more details on what is meant by locality, and by “hidden variable theories”.
- Ultimately this is just another instance, where we have to abandon concepts from our everyday intuition in quantum mechanics. In quantum mechanics, it is simply impossible to individually, locally, describe two objects after they have interacted. In the example above, the interaction happens during the pion decay. Instead we have to describe them with a (usually entangled) two-body wavefunction such as (5.2), that ultimately is a highly non-local object once the two particles have moved far apart from each other.
- The experimental demonstration of quantum mechanical violations of Bell's inequality essentially solve the dispute between “realist” and “orthodox” interpretations mentioned in section 1.4 (and discussed much more in Griffith), in favor of the orthodox interpretation. Ascribing the particle(s) a pre-existing state prior to measurements would again require the use of some hidden variables.
- Bell's theorem also implies that entanglement is a stronger feature than classical correlations (since classical correlations are exactly what would be used in a hidden variable theory). It comes as no surprise then, that it is also the key resource based on which “quantum computers” can do tasks that classical computers cannot do in reasonable time.

This section again was more intended as an appetiser, you would get the main course on entanglement in courses on quantum information, quantum optics or entanglement itself.

The End