Week ⓪

PHY 304 Quantum Mechanics-II
Instructor: Sebastian Wüster, IISER Bhopal, 2022

These notes are provided for the students of the class above only. There is no guarantee for correctness, please contact me if you spot a mistake.

6 Mathematical interlude II

6.1 Administrative affairs

(i) Office: drop me an email to arrange a skype call
Lecture times: Mon 10-10:55 am, Wed, Fri 9 am - 9:55 am (Slot E)
place: AB1A1 and Studio AIR
Office hours: Wed 14:30-16:30.
Phone: 1213
Email: sebastian@iiserb.ac.in
webpage: http://home.iiserb.ac.in/~sebastian/teaching.html

(ii) Literature:

- D. J. Griffiths, *Introduction to Quantum Mechanics* [GR] **the** textbook
- R. Shankar, *Principles of Quantum Mechanics*, [SH]
- J. J. Sakurai, *Modern Quantum Mechanics* [SA]

The course will mainly follow GR and SH. Where stray topics are taken from elsewhere I will try to indicate this.

(iii) Lectures and tutorials

- I am arranging lecture notes into "week" segments, based on similar content. While most of those segments should indeed take a week for us to work through, this will not be true for all and they may take less or more often more time.

- One of the weekly sessions will alternate between tutorial and TA-class in studio AIR as you are used to (A) In one week we shall have a flipped classroom tutorial. In these we will do little tasks to understand the material more deeply. You will have to have gone through the lecture notes *prior* to the flipped classroom session. (B) The following week we shall do a TA-class/assignment class in which you present the solutions of assignments to each other. This semester we will require everyone to present at least once, otherwise your final assignment score will be halved. We also require everyone, when asked, to be able to present solutions that carry their name. Either of these sessions are also implicitly Q&A sessions where you should ask your mates, the TAs and myself any questions you may have.

(iv) Assessment: *Note: The weightages and numbers will be added once the senate guidelines for the next semester are out*

- **2 scheduled Quizzes: 15%** There will be two quizzes lasting 1-1.5 hours.

- **Assignments: 20%** There will be about five to seven assignments handed out with a two week deadline each. I expect you to form teams of 4-6 students and stick in these teams for the semester. Hand in only one solution per team. The TA is instructed to give full marks for *any serious attempt* at a given question of the assignment, even if the result is wrong. This is to discourage copying and encourage doing it yourself. However, the TA is asked to deduct marks for messy presentation and blatant copying from anywhere. The same teams will be used in tutorials, see below. Submit your final assignment solution via email to the TA. All has to be integrated in a single file, e.g. pdf. This may be a good opportunity to learn LaTex and nicely typeset your solution, but handwritten and good-quality scanned/photographed is fine too. *See also notes above about TA class.*

- **Numerics component of assignments:** Moderns science almost always necessitates the heavy use of computers. Most assignments will contain a numerics component, to be done using matlab and/or mathematica. Please make the campus license version downloadable from the CC webpage available on at least one computer in your team. You shall also need VPN access to the campus network for the matlab license. For each assignment, I will provide a template code package that you have to only minorly edit. See notes on numerics assignments online. No prior experience of either programming or matlab should be required, but if you read some online notes regarding introduction to matlab in the first weeks, that might allow you to have more fun with this part of the assignments.

- **TA class and tutorial attendance: 5%** These will be compulsory. When attendance is less than 60% the marks for this component are 0, and for more than 90% they are 100. In between they are as per fractional attendance.

- **Mid-sem exam: 30%, Final exam: 30%** The exams will try to test understanding of the essential *physics* concepts taught, not maths. For guidance regarding what are the most important concepts look at the quizzes, assignments and tutorials. All exams will be designed to give a significant advantage to those students that solved all tutorials and assignments by *themselves* within their team.

6.2 Course Outline

PART 2 (PHY304)

6) **Mathematical Interlude II:** $\sim$ 2 weeks
- Motivation, Symmetries and conservation laws

7) **Approximation methods for time-independent problems:** $\sim$ 4 weeks
- Time independent perturbation theory, variational method, WKB approximation

8) **Quantum scattering theory:** $\sim$ 2 weeks
- Born approximation, partial wave decomposition

9) **Quantum dynamics:** ~ 3 weeks
   - Time dependent perturbation theory, Fermi's golden rule, adiabatic theorem

10) **Advanced topics:** ~ 2 weeks
   - Basic Gauge theory, Charged particle in an electromagnetic field, Relativistic quantum mechanics

Contents

6.3 Math content

Some good news: Most of possibly new math to do with quantum mechanics, you already encountered in QM-I. You can treat part II as an extensive exercise in that regard. We will mention some links to group theory in passing in the next week, but those will be bonus material only.

6.4 Motivation

- In PHY303 QM-I we have now covered most of the essential basics of non-relativistic quantum mechanics. So why do we need QM-II? It turns out that we unfortunately also covered pretty much all major examples where a closed analytical solution is possible. I have already acquainted you with the idea to simply solve some problems that are too hard for analytics on the computer, but that typically only works for small problems, few dimensions, few particles etc. Also, even if the computer can solve it for us, it cannot understand it for us.

- Hence for almost all practical problems, we require a powerful set of approximation methods, which are subject of the present course. Their main purpose is not to just solve complex problems, but to gain physical understanding that cannot be gained without them. The methods are logically grouped into (i) time-independent ones, that help us find eigenstates of the TISE (1.62) for cases that are more complicated than those for which we can find a direct solution, and (ii) time-dependent ones, that help us find solutions of the TDSE (1.2) for cases with time-dependent Hamiltonian, that we have essentially not yet looked at, at all.

- Some directions where we shall need approximations: We looked at the particle in a square well, plane wave, harmonic oscillator, spin etc. But what if there are multiple particles of these types, all coupled to each other?

- The main time-independent problems of practical interest are to find the ground-state of a complex system, for example in material science. We want to then be able to understand complex systems based on similar more straightforward systems, see example 45 below.

- However whenever we want to talk about excited states, effective Hamiltonians actually become naturally time-dependent, because without that the system cannot actually reach the excited state. See also example 46 below.

- We had seen in week 3, that interesting things happen when matter-waves hit a potential obstacle, such as the finite square barrier. I had already alerted you to the fact that these

things becomes much more involved in 3D, since there are now many more directions into which the matter-wave can be scattered. Since quantum mechanical scattering experiments are a major tool for unravelling fundamental physics, most notably in atomic, molecular, nuclear and particle physics, we will go through the basics of that in one section of this course.

Example 45, Infinite square well potential with a bump: Revisit the online app http://www.falstad.com/qm1d/ . Select the infinite square well, small mass and narrow barrier, to get wider energy spacing. Then select "Mouse=Edit function", and draw a small pump into the potential energy $V(x)$, see figure below right. Effectively we are adding $V(x) = V_{\text{box}} + V_{\text{bump}}$, where V_{box} is from Eq. (2.10) and V_{bump} is the potential we have just drawn.
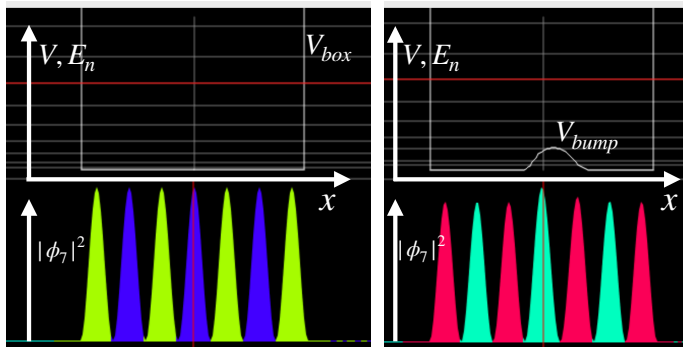
left: (left) Usual probability density in eigenstate $|\phi_7|^2$ (ignore color) and energy E_7 (red line), see Eq. (2.18). (right) Probability density and energies in new eigenstate of potential including V_{bump}.
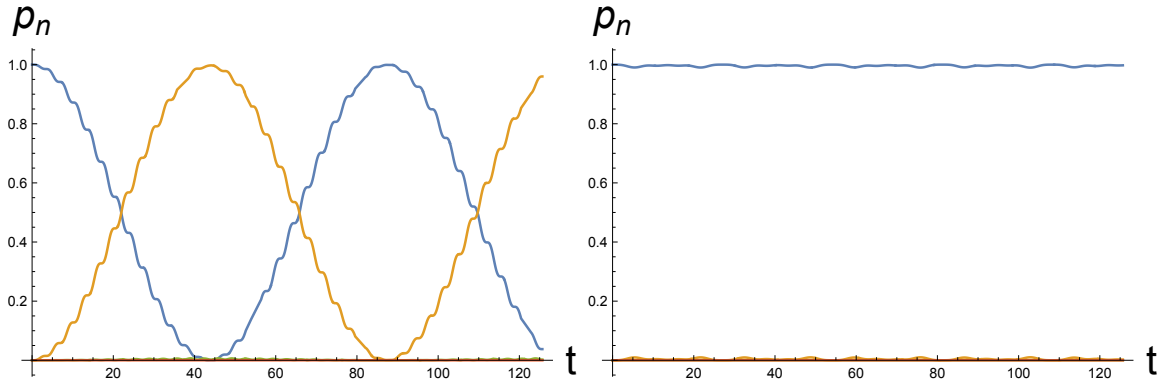
What we see is that the eigenstates and eigenenergies do change, but not much, and the statechanges only happens in the region where V_{bump} is nonzero. Presumably the small change has to do with the fact that $V_{\text{bump}} \ll E_7$, so it seems logical that it does not affect the state too badly. How can we understand this analytically?

Example 46, Driven quantum dot: Review Assignment5 (QM-I) Q2(c). We had looked at a particle (e.g. electron) in an infinite square well e.g. quantum dot potential) subject to a periodically varying external force (e.g. from the electric field of a laser), with Hamiltonian

$$\hat{H}(t) = \frac{\hat{p}}{2m} + V(\hat{x}) + F_0 \hat{x} \sin(\omega_0 t). \tag{6.1}$$

In the earlier question, you had set up the matrix representation of the explicitly time-dependent Hamiltonian (see section 3.3) and solved the ensuring TDSE (3.30) on a computer. We initialize the wavefunction in the ground state $\Psi(x, t = 0) = \phi_1(x)$, from Eq. (2.18). For slightly more extreme (dimensionless) parameters than taken in the assignment solution ($\hbar = m = 1$, $a = 4$, $F_0 = 0.05$), we find the results below:

6.5 Revision of QM-I

Before we embark on the program suggested above, we will spend the first week re-viewing the key points of QM-I. In particular also the last weeks (10,11,12) are really important and exciting and traditionally might have received less of your attention last semester than warranted. To help you get you up to speed after the break, please work through the following guide:

(a) **Mathematics** This is a physics course, but we must use the language of mathematics. In QM-I you have learnt or deepened the concepts of: Function vector spaces aka Hilbertspaces (section 1.5.4), eigenvalue problems of matrices (Eq. (1.15)) and operators (Eq. (1.23)), Hermitian operators (Eq. (1.24), section 3.4), unitary operators (section 1.5.3, section 3.9), commutators (Eq. (2.45), Eq. (3.41)), operators as matrices (section 3.3). *If when reading this list, you do not feel reasonably familiar with any keyword, please revisit the relevant section.*

(b) **Basic structure of quantum mechanics** Instead of a well defined position and momentum as in classical mechanics, the quantum mechanical particle is described by a wave function $\Psi(x,t) \in \mathbb{C}$. Answer the following questions as a self-check: What is the interpretation/meaning of this wavefunction?_____(section 1.4, section 3.6). Why is it complex and what do complex numbers tell us?_____ (section 1.6.4). What is the value of $\int dx |\Psi(x,t)|^2$ and why?_____ (section 1.6.1, section 1.5.2). What is the importance of a global complex phase $\Psi(x,t) \to e^{i\varphi}\Psi(x,t)$ with $\varphi \in \mathbb{R}$?_____(section 1.6.1). Which equation governs how the wavefunction changes in time ?_____(section 1.4). What is

the meaning of stationary state and how do we find those?_____ (section 1.6.5).
If you could answer all those questions, just proceed. If not, please revisit the links in brackets.

(c) **Measurements in quantum mechanics** How do we find the probability of a measurement of any observable?_____(section 3.6). Why do we need operators in quantum mechanics?_____ (section 1.6.2, section 3.6). What happens to the quantum state while we find a certain measurement result?_____ (section 1.4, section 3.6). How to we find the mean of a large number of measurements?_____(section 1.5.2, section 1.6.2). How do we find the uncertainty or standard deviation of a large number of measurements?_____ (section 1.6.2 ,section 3.7).

(d) **Solutions of the TISE and why we need them** For what do we need the TISE? _____(section 1.6.5, section 3.6). In which cases and how can we also find time-dependent information (time-evolution) from the TISE?_____(section 1.6.5). Which nice properties do solutions of the TISE have?_____(section 1.6.5, section 3.4). List a few practical aspects needed to solve the TISE, how many different methods do you know?_____(weeks 3-5, section 3.3). What is the meaning of degeneracy? _____(section 3.4.1).

(e) **Solutions of the TDSE and why we need them** Why do we need the TDSE in addition to the TISE?_____(section 3.6). How many methods to solve the TDSE do you know?_____(section 1.6.5, Assigment 3(QM-I), section 3.3). List a few physical phenomena for which knowing the TISE is not enough_____(section 6.4).

(f) **Uncertainty relations** What is the basic mathematical origin of uncertainty relations in quantum mechanics? List an intuitive and a formal reason. _____(Phy106 weeks5/6, section 1.6.3, section 3.7). Which uncertainty relations do you know?_____(section 1.6.3, section 3.7, section 3.8.1) What is the relation between uncertainty relations and operators sharing eigenfunctions? _____(section 3.8) What is special with the energy-time uncertainty relation, and why do we have to be careful using it?_____(section 3.8.1)

(g) **Quantum effects** List at least six quantum mechanical phenomena that are in an essential way different from behaviour in classical mechanics. _____(*Hint:* section 2.2.1, section 2.2.4, section 1.4, section 3.6).

(h) **Algebraic solutions to quantum problems** With which trick can you often avoid finding all the eigenstates and energies from the TISE, and instead use the action of operators onto states directly? _____(section 2.3.1, section 4.4)

(i) **Angular momentum** How is angular momentum dealt with in quantum mechanics? _____(section 4.1.2) Which different types of angular momentum do you know? _____(section 4.1.2, section 4.3, section 4.7.1) Which links between angular momentum and particle motion do you know from classical mechanics and how are they preserved in quantum mechanics? _____(example 33, example 35) How do we add angular momenta of two particles ? _____(section 4.8)

(j) **Many-Partices or dimensions** What changes in the math when you move from a single particle to many particles? or from one dimension to many dimensions? _____(section 4.1, section 5) How can we often tackle those complications to resort back to our easier 1D solutions? _____(section 1.6.5, section 4.1.1) Explain the concept of indistinguishable

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particles in quantum mechanics?_____(section 5.1) What is the fundamental consequence of this principle? _____(Eq. (5.4)) Which classification of particles does it lead to?_____(section 5.1)

What is entanglement and why is it interesting?_____(section 5.2)

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6.6   Symmetries and conservation laws

You know what conservation laws are from classical mechanics and QM-I (e.g. Eq. (3.53)). From classical mechanics you also know that these can be traced back to <u>symmetries</u> of the (classical) Hamiltonian (i.e. symmetries of "the problem"), using <u>Noether's theorem</u>. Now that both courses are complete, let us see briefly how symmetry principles lead to conservation laws in quantum mechanics, exactly as they do in classical mechanics. Essentially you think of the contents of this section as the quantum mechanical version of Noether's theorem.

First let us remind ourselves what a symmetry of a system means:

Example 47, Continous and discrete spatial symmetries: A symmetry of a system is a coordinate transformation that leaves the system unchanged.
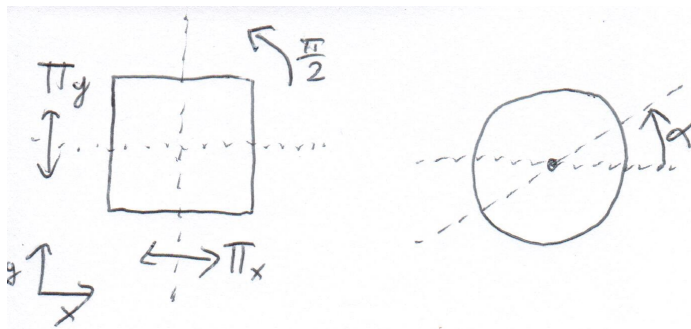
left: (left) For example the square shape has a discrete rotational symmetry: We can rotate the square (or the coordinate system)s by $\varphi = n\pi/2$ with integer n and you would not be able to tell the difference. It also has two mirror symmetries: flipping the x direction and flipping the y direction.

(right) In contrast, the circle has a continuous rotational symmetry. You can rotate it by any angle φ and would not be able to tell the difference.

- The above should remind you of what you intuitively know. If you want to make it more formal, the shapes are defined by a sub-set of coordinates, e.g. $\{-a < x < a$ and $-a < y < a\}$. Now e.g. the mirror symmetry Π_x implies that this set of coordinates is <u>unchanged</u> under the coordinate transformation $x \leftrightarrow x' = -x$, $y' = y$.

Through the next few sections, we will look at several important symmetry operations, and how they affect a quantum state (wavefunction) and an operator. The main objective will be to define "symmetry of a quantum mechanical system = symmetry of the Hamiltonian operator".

6.6.1 Translations

We want to translate a wavefunction in space, i.e. move it without changing its shape.
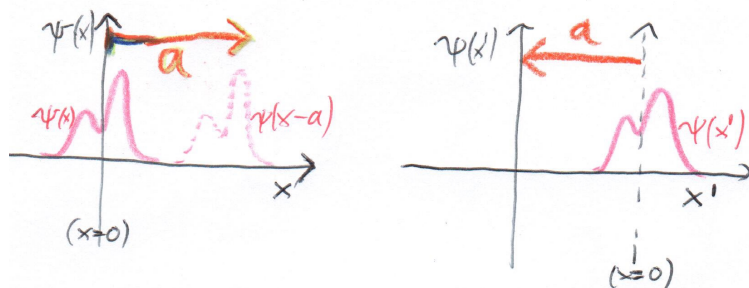
left: This is illustrated on the left. There is two viewpoints to shifting the function. In the <u>active</u> transformation, we keep our coordinate system unchanged and write a function $\Psi(x - a)$ instead of $\Psi(x)$, which is shifted by a <u>to the right</u>.

In the <u>passive</u> transformation, we redefined our coordinate $x' = x - a$, and then write the original function $\Psi(x')$ in terms of the new coordinate.

For performing the shift that we define the

Translation operator $\hat{T}(a)$ that shifts a wavefunction $\Psi(x)$ by a to the right.

$$\hat{T}(a)\Psi(x) = \tilde{\Psi}(x) = \Psi(x - a). \tag{6.2}$$

It turns out we can write

$$\hat{T}(a) = e^{-i\frac{a}{\hbar}\hat{p}} \tag{6.3}$$

We thus say the momentum operator $\hat{p}$ is the <u>generator of translations</u>.

- Proof: We use the Taylor expansion of $\Psi(x - a)$ around the point x

$$\Psi(x - a) = \sum_{n=0}^{\infty} \frac{(-a)^n}{n!} \frac{d}{dx} \psi(x) \tag{6.4}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-ia}{\hbar} \hat{p} \right)^n \psi(x) = e^{-i\frac{a}{\hbar}\hat{p}} \psi(x). \tag{6.5}$$

- The translation operator is unitary $\hat{T}(a)^{-1} = \hat{T}(-a) = \hat{T}^{\dagger}$.

We had seen in section 3.9 that we can choose to work with time-evolving states and time-independent operators as well as the reverse, since the only thing that matters in the end is the time evolution of expectation values. The same approach can be taken for translations. We defined a <u>translated operator</u> $\hat{\tilde{O}}$ as one that has the same expectation value in the untranslated state $|\Psi\rangle$, as the original operator $\hat{O}$ in the translated state $|\tilde{\Psi}\rangle$:

$$\langle \Psi |\hat{\tilde{O}}| \Psi \rangle = \langle \tilde{\Psi} |\hat{O}| \tilde{\Psi} \rangle = \langle \Psi |\hat{T}^{\dagger}(a)\hat{O}\hat{T}(a)| \Psi \rangle. \tag{6.6}$$

For the second equality we have used Eq. (6.2) and Eq. (3.23) [newly added]. From Eq. (6.6) we can now infer the form of a

Shifted operator

$$\hat{\tilde{O}} = \hat{T}^\dagger(a)\hat{O}\hat{T}(a). \tag{6.7}$$

Example 48, Shifted position operator: Let us test what shifted operator means, by shifting the position operator $\hat{x}$. We can do this in two different ways. The first one is described in Griffith example 6.1, using (6.2) and a test function. The second one, uses Assignment 6, Q2.

According to (6.7), we have

$$\hat{\tilde{x}} = \hat{T}^\dagger(a)\hat{x}\hat{T}(a) \overset{Eq. \ (6.3)}{=} e^{i\frac{a}{\hbar}\hat{p}}\hat{x}e^{-i\frac{a}{\hbar}\hat{p}} = \cdots \tag{6.8}$$

In Assignment 6, you had shown that $e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}} = \hat{B} + \lambda[\hat{A}, \hat{B}]$ for two operators $\hat{A}$ and $\hat{B}$ that commute with their commutator. Using $\hat{A} = \hat{p}$, $\hat{B} = \hat{x}$ and $\lambda = \frac{ia}{\hbar}$, this matches (6.8). Also, since $[\hat{x}, \hat{p}] = i\hbar$ is just a number, the operators clearly satisfy the requirement to commute with their commutator. Thus we can write

$$\cdots = \hat{x} + \frac{ia}{\hbar}\underbrace{[\hat{p}, \hat{x}]}_{=-i\hbar} = \hat{x} + a. \tag{6.9}$$

This agrees with what you find with Griffith' method. We essentially just re-express the position coordinate in the shifted coordinate system shown in the figure at the beginning of section 6.6.1.

We are now finally in the position to define

Translational symmetries of a quantum system We say the system is invariant under a translation by a, if its Hamiltonian is invariant:

$$\hat{\tilde{H}} = \hat{T}^\dagger(a)\hat{H}\hat{T}(a) \overset{!}{=} \hat{H}. \tag{6.10}$$

Since $\hat{T}^\dagger(a) = \hat{T}^{-1}$ we can rewrite this as

$$[\hat{H}, \hat{T}(a)] = 0, \tag{6.11}$$

i.e. the Hamiltonian commutes with the translation (symmetry) operator.

- If we write the Hamiltonian as $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, we can show easily that $\hat{\tilde{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x} + a)$. For the potential we use Eq. (6.9) and to see that the momentum does not shift we can use (6.3) (exercise).

- A system thus has a translation symmetry, if its potential energy does.

Let's look at two different important cases:

Some systems are invariant under <u>any translation</u> a, which implies that the potential vanishes or is constant. In particular that implies that they are invariant under any infinitesimally small translation, with a infinitesimally small. In that case we can expand (6.3) to $\hat{T}(a) = e^{-i\frac{a}{\hbar}\hat{p}} \approx 1 - i\frac{a}{\hbar}\hat{p}$, which means that (6.11) becomes equivalent to $[\hat{H}, \hat{p}] = 0$. But from Eq. (3.53) we know that this implies also the <u>conservation of momentum</u>. We thus have shown that

> **Translation invariant Hamiltonians imply momentum conservation**

- This is essentially the same statement that you get in classical mechanics using Noether's theorem for a continuous translational symmetry.

- In quantum mechanics we might be tempted to distinguish two (seemingly) different statements of "conservation of an observable $\hat{O}$": (i) We could demand that the <u>expectation value does not change</u>. This is guaranteed from $[\hat{H}, \hat{O}] = 0$ using Eq. (3.53). (ii) We could demand that the <u>probability p_k of every possible measurement outcome o_k does not change</u>. In fact this is <u>also</u> guaranteed by $[\hat{H}, \hat{O}] = 0$. *Proof:* The probability to measure o_k in the quantum state $|\Psi(t)\rangle$ is given by

$$p_k = |\langle \varphi_k | \Psi(t) \rangle|^2, \tag{6.12}$$

where $|\varphi_k\rangle$ is the eigenstate of $\hat{O}$ with eigenvalue o_k (see postulate III in section 3.6). According to Eq. (1.70) we can write the time-dependent state as $|\Psi(t)\rangle = \sum_n c_n(0)e^{-iE_nt/\hbar}|\phi_n\rangle$, where $|\phi_n\rangle$ is an eigenstate of the Hamiltonian. However since $[\hat{H}, \hat{O}] = 0$, according to Eq. (3.48) these have shared eigenfunctions, so we can identify $|\phi_n\rangle = |\varphi_n\rangle$, such that

$$p_k = |\langle \varphi_k | \Psi(t) \rangle|^2 = \left| \langle \varphi_k | \sum_n c_n(0)e^{-iE_nt/\hbar} | \varphi_n \rangle \right|^2 = \left| \sum_n c_n(0)e^{-iE_nt/\hbar} \underbrace{\langle \varphi_k | \varphi_n \rangle}_{\delta_{nk}} \right|^2$$

$$= |c_k(0)e^{-iE_kt/\hbar}|^2 = |c_k(0)|^2, \tag{6.13}$$

which hence also does not change in time.

Suppose the potential has a discrete translational symmetry, which means that $V(x+a) = V(x)$ is true for <u>some special choice of a</u>, but not for all a. Let's call this $a = d$. An example would be $V(x) = V_0 \cos^2(\pi x/d)$, see also figure in example 49 below. We know from (6.11) that in this case $[\hat{H}, \hat{T}(d)] = 0$ and we know from section 3.8 that we can thus choose all eigenfunctions $\phi(x)$ of the Hamiltonian, such that they are simultaneously eigenfunctions of the translation operator:

$$\hat{H}\phi(x) = E\phi(x), \qquad \text{and} \qquad \hat{T}(d)\phi(x) = \lambda\phi(x), \tag{6.14}$$

for some λ. From (6.2) we can write $\hat{T}(d)\phi(x) = \phi(x-a) = \lambda\phi(x)$. Since $\hat{T}(d)$ is unitary, its eigenvalues fulfill $|\lambda|^2 = 1$ (exercise, assignment), hence they can be written as $\lambda = e^{i\varphi}$ for real φ,

thus

$$\phi(x - a) = e^{i\varphi}\phi(x). \tag{6.15}$$

It turns our this is equivalent to

Bloch's theorem The eigenstates $\phi(x)$ of a particle in a potential $V(x + d) = V(x)$ with periodicity d take the form

$$\phi_q(x) = e^{iqx}u(x), \tag{6.16}$$

where $u(x) = u(x - d)$ is a periodic function, with the same period as the potential. q is called the crystal momentum.

- Proof: It is clear that Eq. (6.15) follows from Eq. (6.16). In the other direction, let us write $\phi(x) = e^{iqx}u(x)$ for unknown $u(x)$, which is clearly possible. Then $u(x - d) = \phi(x - d)e^{-iq(x-d)} \overset{Eq. (6.15)}{=} e^{i(\varphi+qd)}\phi(x)e^{-iqx}$ which is equal to $u(x)$ if we set $\varphi = -qd$. q is called the crystal momentum.

Example 49, Electrons in a crystal lattice: The simplest model of electrons in a solid material are non-interacting electrons that feel a periodic potential due to the crystal ions in the material.
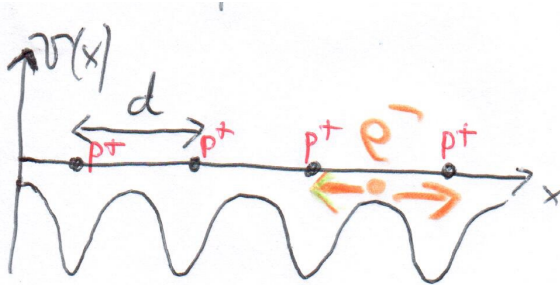

left: An electron (orange dot), moving in the periodic potential $V(x)$ (black) created by the screened solid-crystal ions p^+ (black ●), which are periodically arranged with period d. We can thus use Bloch's theorem Eq. (6.16) to find electronic states $u(x)$ which we now need to find only over one period $x \in [0, d]$ of the lattice.

To find actual energies we still have to solve TISE in terms of $u(x)$. What we find in this case is a bandstructure: Energies $E_n(q)$ cover certain ranges of energies as a function of q (bands) with certain other ranges of energies forbidden (gaps). This is in contrast to the free particle in section 2.1, where you find a matching q to generate every energy $E(q) = \hbar^2 q^2/(2m)$.

6.6.2 Parity

Besides the discrete translation we just saw, other discrete symmetries we had already seen earlier are mirror symmetries.
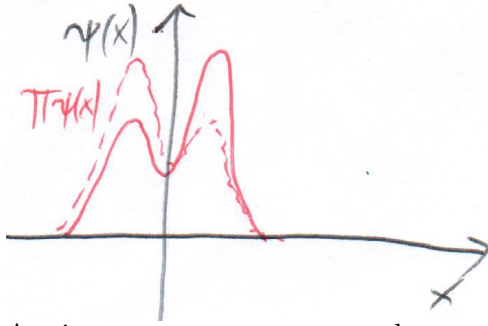
left: The parity operation just mirrors the function at the origin, see Eq. (6.17). Here we show an example of a function $\Psi(x)$ (solid) that is not parity symmetric. Hence its mirror image $\Psi(-x)$ (dashed) looks different.

A mirror symmetry corresponds to an inversion of space, which we formalize using the

Parity transformation operator $\hat{\Pi}$ which acts on a wavefunction Ψ as

$$\hat{\Pi}\Psi(x) = \tilde{\Psi}(x) = \Psi(-x). \qquad \text{(1D)}$$

$$\hat{\Pi}\Psi(\mathbf{r}) = \tilde{\Psi}(\mathbf{r}) = \Psi(-\mathbf{r}). \qquad \text{(3D)} \qquad\qquad (6.17)$$

- The parity operator is Hermitian (exercise) and its own inverse $\hat{\Pi} = \hat{\Pi}^{-1}$. Similar to Eq. (6.7), an operator transforms as $\hat{\tilde{O}} = \hat{\Pi}\hat{O}\hat{\Pi}$ under parity.

- E.g. using the position space representation of Eq. (6.6) (integration for the scalar product), you can then show that the position and momentum operators transform as $\hat{\Pi}\hat{\mathbf{r}}\hat{\Pi} = -\mathbf{r}$ and $\hat{\Pi}\hat{\mathbf{p}}\hat{\Pi} = -\hat{\mathbf{p}}$.

- If a Hamiltonian has an inversion symmetry, which means $\hat{\Pi}\hat{H}\hat{\Pi} = \hat{H}$, we again know that its eigenfunctions are also eigenfunctions of the parity operator. This is typically the case if the potential is symmetric $V(\mathbf{r}) = V(-\mathbf{r})$. Eigenfunctions of the parity operator are the odd and even functions, with eigenvalues (-1) and (+1) respectively. Together we see the result of Assignment 3 Q1b in QM-I, in a more elegant way.

- Using Eq. (3.53) you can show that the parity of a wavefunction is conserved if the Hamiltonian has an inversion symmetry (exercise). This means that a symmetric wavefunction will remain symmetric as time goes on, and an anti-symmetric one will remain anti-symmetric.

- In 3D there are a few more mirror symmetries, the complete inversion symmetry of space used above: $\hat{\Pi}\hat{\mathbf{r}}\hat{\Pi} = -\mathbf{r}$, or separate inversions of only some of the cartesian axes (i.e. $x \to -x$ without changing y and z).

- An important example of a parity symmetric Hamiltonian is the Hydrogen Hamiltonian (4.72). We thus know from the discussion above, that all Hydrogen wavefunctions (4.91) must have a definite symmetry under the parity operation. You can verify $\phi_{n\ell m}(\mathbf{r}) = (-1)^{\ell}\phi_{n\ell m}(-\mathbf{r})$.

Example 50, Dipole selection rules: You already were told in PHY106 (weeks 7+10) that Hydrogen atoms can make transition between different electronic states $\phi_{n\ell m}$ as in Eq. (4.91) if they interact with light. In a preview of PHY402 "Atomic and Molecular physics", these transitions are mainly governed by matrix elements of the electric dipole operator of the atom $\hat{\mathbf{d}} = -e\hat{\mathbf{r}}$. [a] Transitions are possible if

$$\mathcal{M} = \langle \phi_{n'\ell'm'} | (-e\hat{\mathbf{r}}) | \phi_{n\ell m} \rangle \neq 0. \tag{6.18}$$

By smartly inserting $\mathbb{1} = \hat{\Pi}\hat{\Pi}$ at two places we can show

$$\mathcal{M} = \langle \phi_{n'\ell'm'} | \hat{\Pi} \underbrace{\hat{\Pi}(-e\hat{\mathbf{r}})\hat{\Pi}}_{=e\hat{\mathbf{r}}} \underbrace{\hat{\Pi}| \phi_{n\ell m} \rangle}_{=(-1)^{\ell}| \phi_{n\ell m} \rangle} = \langle \phi_{n'\ell'm'} | (-1)^{\ell'}(e\hat{\mathbf{r}})(-1)^{\ell} | \phi_{n\ell m} \rangle = \mathcal{M}(-1)^{\ell+\ell'+1}. \tag{6.19}$$

This only allows $\mathcal{M} \neq 0$ if $\ell + \ell' + 1$ is even, hence $\ell \neq \ell'$: Transition are only possible (likely) between states of different parity (different ℓ). In PHY402 you will learn the stronger rule $|\ell - \ell'| = 1$.

An even simpler result is found for $n = n'$, $\ell = \ell'$ $m = m'$, in which case $\mathcal{M}$ is the expectation value of the electric dipole (i.e. the permanent electric dipole in the state $| \phi_{n\ell m} \rangle$. It vanishes due to (6.19), hence Hydrogenic states do not have a permanent dipole moment (see also tutorial 6(QM-I), Stage3)

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[a]It is the electric field of the light that has the dominant effect. Since atoms are neutral, the highest order interaction is with the electric dipole.

6.6.3 Rotations

In higher dimensions (2D, 3D), we have an additionally coordinate transformation to translations and inversions, called "rotations". This is sketched below for a coordinate rotation in 2D:
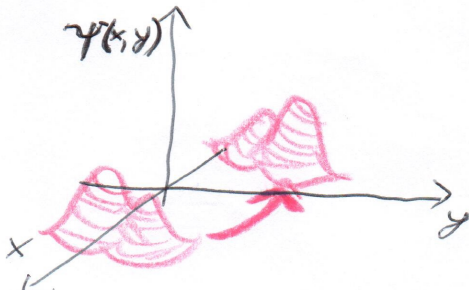
left: We draw an original function of two variables $\Psi(x,y)$ (left mountain), and then the same function at rotated coordinates $\Psi(x',y')$ (right mountain). This is easiest expressed in polar coordinates $\Psi(r,\varphi) \to \Psi(r,\varphi-\alpha)$, but we could rotate the cartesian coordinates as well.

We follow the same approach as in section 6.6.1 to formalise transformations under rotations of wavefunctions. We define the

> **Rotation operator** for a rotation about the z-axis by an angle α as
>
> $$\hat{R}_z(\alpha)\Psi(r,\theta,\varphi) = \Psi(r,\theta,\varphi-\alpha) \qquad (6.20)$$
>
> This time we can write it as
>
> $$\hat{R}_z(\alpha) = e^{-i\frac{\alpha}{\hbar}\hat{L}_z} \qquad (6.21)$$
>
> We thus say the angular momentum operator $\hat{L}_z$ is the <u>generator of rotations about the z-axis</u>.

- The reasoning behind Eq. (6.21) is similar to that for Eq. (6.3) (exercise).

- More generally we find that rotation around an arbitrary axis $\mathbf{n}$ changes the wavefunction by

$$\hat{R}_\mathbf{n}(\alpha) = e^{-i\frac{\alpha}{\hbar}\mathbf{n}\cdot\hat{\mathbf{L}}}, \qquad (6.22)$$

  thus the angular momentum operator $\hat{\mathbf{L}}$ is the generator of rotations.

- Using the same argumentation as in section 6.6.1, we now see that a Hamiltonian is rotationally symmetric $\hat{R}_\mathbf{n}(\alpha)^\dagger \hat{H}\hat{R}_\mathbf{n}(\alpha) = \hat{H}$, if $\hat{H}$ commutes with $\hat{\mathbf{L}}$, and according to Eq. (3.53) in that case angular momentum is conserved. This is again the same result that we obtain in classical mechanics, based on Noether's theorem for continuous rotational symmetries.

6.6.4 Time translations

We had already seen in section 3.9, that for cases with a time-independent Hamiltonian (that means the system is "translation invariant in time"), the operator that maps a wavefunction from time t_0 to time $t_0 + t$ is the <u>time evolution operator</u> (see Eq. (3.60))

$$\hat{U}(t,0) = e^{-i\frac{\hat{H}}{\hbar}t}. \qquad (6.23)$$

If we compare this with Eq. (6.3) and Eq. (6.21), it makes sense to call the Hamiltonian the <u>generator of time translations</u>. Similarly again to classical mechanics, we can show using Eq. (3.53) that energy is conserved, if the Hamiltonian is not explicitly time dependent, which means the system is time translation invariant.

6.6.5 Symmetries and Degeneracy

We had discussed degeneracy in section 3.4.1. Very often, degeneracy in the spectrum of a Hamiltonian $\hat{H}$ can be traced back to its symmetries. Specifically

> **Symmetries that lead to degeneracy** If a Hamiltonian has at least two non-commuting symmetries, its spectrum must contain degenerate states.

- Proof: Let $\hat{Q}$ and $\hat{\Lambda}$ be the generators of the symmetry (e.g. like the momentum operator for translations in section 6.6.1). We had seen that them generating a symmetry implies $[\hat{H}, \hat{Q}] = 0$ and $[\hat{H}, \hat{\Lambda}] = 0$, but we assume $[\hat{Q}, \hat{\Lambda}] \neq 0$. Let's pick an eigenstate $|\phi_n\rangle$ of the energy $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$, then

$$\hat{H}\left[\hat{Q}|\phi_n\rangle\right] = \hat{Q}\underbrace{\hat{H}|\phi_n\rangle}_{E_n|\phi_n\rangle} = E_n\left[\hat{Q}|\phi_n\rangle\right]. \tag{6.24}$$

Thus $\hat{Q}|\phi_n\rangle$ is <u>also</u> an eigenstate of $\hat{H}$ with eigenvalue E_n (and we can show the same thing for $\hat{\Lambda}|\phi_n\rangle$). We have <u>not yet</u> show that the eigenvalue E_n is degenerate, since all three states, $|\phi_n\rangle$, $\hat{Q}|\phi_n\rangle$ and $\hat{\Lambda}|\phi_n\rangle$ might be <u>the same state</u>. Recall from section 1.6.1 that "same state" still allows the wavefunctions to differ by a complex global phase. However if $\hat{Q}|\phi_n\rangle \sim |\phi_n\rangle$ and $\hat{\Lambda}|\phi_n\rangle \sim |\phi_n\rangle$ then $|\phi_n\rangle$ also was an eigenfunction of $\hat{Q}$ and of $\hat{\Lambda}$. If this is true for all n, then $\hat{Q}$ and $\hat{\Lambda}$ share a set of eigenfunctions, in which case we know from section 3.8 that $[\hat{Q}, \hat{\Lambda}] = 0$, which contradicts our assumption. Hence there has to be at least one $|\phi_n\rangle$ for which either $\hat{Q}|\phi_n\rangle \not\propto |\phi_n\rangle$ or $\hat{\Lambda}|\phi_n\rangle \not\propto |\phi_n\rangle$ or both, and thus there is a degeneracy.

Example 51, Single symmetry: Consider the 1D harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$, see section 2.3. The Hamiltonian is symmetric under parity $\hat{\Pi}$, see section 6.6.2, which means $[\hat{H}, \hat{\Pi}]$. However there is <u>no second symmetry</u>. Hence all eigenfunctions of $\hat{H}$ are simultaneous eigenfunctions of $\hat{\Pi}$, which means they are either symmetric or anti-symmetric, compare Eq. (2.64). But this means that $\hat{\Pi}|\phi_n\rangle$ is always <u>the same state</u> as $|\phi_n\rangle$ and there is no degeneracy. Hence the words " at least two" above are very important.

Example 52, Multiple symmetries: Consider the isotropic 2D harmonic oscillator

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2). \tag{6.25}$$

This has many more symmetries: $\hat{\Pi}_x$ ($x \leftrightarrow -x$), $\hat{\Pi}_y$ ($y \leftrightarrow -y$), $\hat{\Pi}$ ($\mathbf{r} \leftrightarrow -\mathbf{r}$) and rotations $\hat{R}_z(\alpha)$ about any angle α, see section 6.6.3. We had found the eigenstates in section 4.1.1 (just remove the z dimension there), and found an energy $E_{n_x,n_y} = \hbar\omega(n_x + n_y + 1)$. Thus most states are degenerate (e.g. $n_x = 1$, $n_y = 0$ has the same energy as $n_x = 0$, $n_y = 1$.

6.7   Classical foundations of quantum mechanics [BONUS]

Now that (most of) you have also completed the course in classical mechanics (PHY303), it might be interesting to briefly look at the deep links between the formalisms in both cases. These were crucial for the development of quantum mechanics and can still help its deeper understanding, while there is not usually enough time in a modern syllabus to look at them in the depth they deserve.

I compiled a very brief summary of the links in the [notes on classical mechanics](#) (week 11, section 4.6.).