Part III Catch-Up Workshop: Quantum Mechanics

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In this workshop we will catch up on the major lessons of QM before you get started with the Part III theoretical physics courses. We will do this by means of working through a series of examples. These are designed to refresh knowledge that may have been lost or gone rusty. You will not find anything here beyond standard QM material – it is however presented in a way that is meant to maximize the applicability to Part III (mainly QFT) and may differ from the way you learnt it in your previous QM courses.

The topics we will touch are roughly

- Hilbert Space, Observables, etc.
- Dirac (Bra-Ket) Notation, Schrödinger & Heisenberg Picture
- Probabilities & Measurement
- Harmonic Oscillator, Spin Algebra, Ladder Operators
- Perturbation Techniques
- ...

Furthermore, you are encouraged to bring any questions or specific problems about QM to the lecture, so we can talk about those in detail.

Please get in touch regarding comments and suggestions, or if you find errors in this script, at kafr2@cam.ac.uk. The current version can be found at www.damtp.cam.ac.uk/user/kafr2/.
Units & Notation

Since most formulas and expressions in QM and QFT have loads of c’s and ℏ’s, it is very convenient to work in a unit system such that \( c = ℏ = 1 \). In other words, we measure all physical quantities in relation to the fundamental constants \( c, ℏ \), etc, and appropriate combinations thereof. This is called natural units. At the level of our formulas, you can imagine we rescaled all coordinates, parameters, functions, etc. by a combination of the natural constants (in the fashion of a coordinate change) to obtain new, unit-free coordinates, parameters, functions. This is sometimes called “nondimensionalization”.

We sometimes use \( \vec{\nabla} \) (read nabla) to mean the the following. For a function: \((\vec{\nabla} f)_i = \partial_{x_i} f\), the components of the gradient \( d f \). For a vector(field) \( \vec{v}(x) \) we write its divergence as \( \vec{\nabla} \cdot \vec{v} \) and (in 3d) its curl as \( \vec{\nabla} \times \vec{v} \).

Recommended Material

- Griffiths, *Introduction to Quantum Mechanics* (!)
- Dirac, *The Principles of Quantum Mechanics*
- Weinberg, *Lectures on Quantum Mechanics*
- First two chapters of *arxiv:0810.0344* (!)
- PQM lecture notes by Ron Horgan, www.damtp.cam.ac.uk/user/rrh
- Past PQM example sheets, www.damtp.cam.ac.uk/user/examples (!)
- for QFT: Nair, *QFT – A Modern Perspective* (!)

1 Principles

The central equation in QM is of course the Schrödinger equation

\[
  i\hbar \partial_t \Psi(t, x) = \left( -\frac{\hbar^2}{2m} \partial_x^2 + V(x) \right) \Psi(t, x) \tag{1}
\]

describing the time evolution of the function \( \psi(t, x) \) in terms of a PDE. It involves the potential energy \( V(x)\psi(t, x) \) and the kinetic energy \( -\frac{\hbar^2}{2m} \partial_x^2 \psi(t, x) \). The sum of potential and kinetic energy is called the Hamiltonian, and is already in classical mechanics responsible for the time evolution of a system. Recall that \( H(x, p) = \frac{p^2}{2m} + V(x) \) and the equations of motion for any quantity \( f(x, p) \) is

\[
  \frac{d}{dt} f = \{ H, f \} = \frac{\partial H}{\partial p} \frac{\partial f}{\partial x} - \frac{\partial H}{\partial x} \frac{\partial f}{\partial p} , \tag{2}
\]
using the Poisson bracket \{·, ·\} between the two functions \(H\) and \(f\). In words we can say that the Hamiltonian function \(H\) generates time evolution by acting on (other functions) via the Poisson bracket \(\{H, ·\}\). So in particular we get
\[
\dot{x} = \frac{p}{m}, \quad \dot{p} = -\nabla V(x),
\]
(3)
describing a classical trajectory \(γ(t) = (x(t), p(t))\) in phase space. Note that, given two solutions \(γ_1(t)\) and \(γ_2(t)\), the sum \(γ_1 + γ_2\) is not necessarily also a solution of the equations of motion. In fact, this can generically only be the case if the system eq. (3) is linear, i.e. the potential is at most quadratic.

Of course we know from Schrödinger’s experiments with his cat that if two states of a system are physical, i.e. they solve the fundamental equation of motion of nature, then so is any linear combination of the two. Say the fundamental eqm of nature is given by some differential operator \(L\) acting on a function \(f\) describing the current state of a system:
\[L(f) = 0.\]
The previous comments imply that \(L\) must be a linear operator and hence its solution space be a vector space! By now we are of course already talking about the Schrödinger equation (1) with the operator given by
\[
L = -i\hbar \frac{∂}{∂t} + \frac{1}{2m}(i\hbar \frac{∂}{∂x})^2 + V(x).
\]
(4)
We also know that the functions \(ψ(t, x)\) on which this operator acts have a very special interpretation: their mod-square \(ρ(t, x) = |ψ(t, x)|^2\) is a probability distribution on configuration space. They encode with which probability the system is in which state. For this last sentence to make sense, the total probability on configuration space needs to be unity, or at the very least finite, so that we can renormalise \(ψ\) if need be
\[
\int d^4x ρ(t, x) \equiv \int d^4x |ψ(t, x)|^2 < ∞.
\]
(5)

It will turn out to be very rewarding to take seriously that the solutions of eq. (1) have the analytic structure of a Hilbert space. Let’s recall the definition: A Hilbert space \(H\) is a complex vector space with an inner product \(\langle ψ|ξ⟩\) between vectors, which satisfies

1. \(\langle ψ|ξ⟩ = ⟨ξ|ψ⟩^*\)
2. \(⟨ψ|α_1ξ_1 + α_2ξ_2⟩ = α_1⟨ψ|ξ_1⟩ + α_2⟨ψ|ξ_2⟩\), with \(α_{1,2} ∈ \mathbb{C}\)
3. \(|ψ|^2 = ⟨ψ|ψ⟩ ≥ 0\) and \(⟨ψ|ψ⟩ = 0\) iff \(|ψ⟩ = 0\)

\(^1\)We loosen the condition of unit total probability so that the solution space remains a vector space. This has to be taken into account later.
Clearly these conditions are very sensible and may seem nearly too obvious to even mention. You will however soon encounter very important physical theories which violate some of these conditions, and dealing with this issue will take a good deal of work.

Anyway, in QM, the two relevant examples are the familiar $\mathbb{C}^n$, and the space of complex functions with the inner product

$$\langle \psi | \xi \rangle = \int d^d x \, \psi^*(x) \xi(x) . \quad (6)$$

The latter example is infinite dimensional, and we think of every function $\psi(x)$ as a “vector” in this infinite dimensional space. The passage from a finite to infinite dimensional vector space can roughly be thought of as making the index $i$ of a vector $\psi_i$ continuous, so the component form together a function $\psi(x)$. However, since there are infinitely many coordinates, we have to include a new requirement: for a vector to be sensible, it better have a finite length, i.e. $\langle \psi | \psi \rangle \leq \infty$, which we recognize as eq. (5).

From your linear algebra course you should be familiar with the concept of a basis and a change of basis. In short, a vector is independent of a basis, but the components which we use to describe the vector are not. A basis is specified by a (complete) set of basis vectors, and the components of any vector in that basis are simply the projection of the vector on the basis elements. The components of a vector in two different bases are related by a matrix, whose entries are the inner products of basis elements. In the case of complex functions, you should be familiar with the two most common bases: the position space and momentum space basis. The components of a vector $|\psi\rangle$ are given by

$$\psi(x) = \langle x | \psi \rangle \quad \text{and} \quad \tilde{\psi}(p) = \langle p | \psi \rangle \quad (7)$$

in the respective bases. We put the tilde over the Fourier transform of $\psi$ to emphasize that it is a different function, though related, to $\psi$. Since we claimed that the set of basis elements for position space $\langle x \rangle$ and momentum space $\langle p \rangle$ form a basis, they had better satisfy the completeness relation:

$$\int d^d x \, |x\rangle \langle x| = \mathbb{1} \quad \text{and} \quad \int d^d p \, |p\rangle \langle p| = \mathbb{1} . \quad (8)$$

Finally, if $\psi(x)$ and $\tilde{\psi}(p)$ are the components of the same vector, just in expressed in different bases, then there should be a basis change relating the two. Indeed, using eq. (8), we find

$$\tilde{\psi}(p) = \langle p | \psi \rangle = \langle p | \mathbb{1} | \psi \rangle = \int d^d x \, \langle p | x \rangle \langle x | \psi \rangle = \int d^d x \, \langle p | x \rangle \, \psi(x) , \quad (9)$$

which we recognize as the Fourier transform of $\psi(x)$ given that the matrix elements of the change of basis are $\langle p | x \rangle \propto e^{ipx}$. So, taking the Fourier of a function corresponds simply to a basis change in this Hilbert space.
Q 1.1 Use the canonical commutation relation $[\hat{x}, \hat{p}] = i$ to show that

$$e^{ia\hat{p}} \hat{x} e^{-ia\hat{p}} = \hat{x} + a$$

and hence

$$e^{-ia\hat{p}} |x\rangle = |x + a\rangle .$$

From this deduce that $\langle p|x\rangle \propto e^{-ipx}$ and finally fix the normalization by unitarity.

Observables

While the state of a physical system is represented by a vector in a Hilbert space, the possible observables, i.e. measurable quantities, are represented by operators (think infinitely large matrices). When the system is in a given state $\psi$, the average value of an observable $O$, represented by the operator $\hat{O}$, is defined as

$$O(\psi) \equiv \langle \hat{O} \rangle \psi := \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle}$$

If this quantity is supposed to be measurable in the real world, it had better be a real number. Setting the imaginary part of $O(\psi)$ to zero leads us to the requirement $\hat{O} = \hat{O}^\dagger$, i.e. that the operator representing an observable be hermitian, or self-adjoint.

Hermitian operators acting on a Hilbert space have a few properties that are very handy for calculations, and also crucial for their interpretation with respect to the real world. As soon as we know that an operator is hermitian, we know that

- its eigenvectors $|\psi_i\rangle$ form a complete basis, $I = \sum_i |\psi_i\rangle\langle \psi_i|$, 
- its eigenvectors (eigenspaces) are mutually orthogonal $\langle \psi_i | \psi_j \rangle = \delta_{ij}$, 
- its eigenvalues $\lambda_i$ are real.

Q 1.2 Prove the second and third property of hermitian operators above.

The most fundamental observable of a system is of course its total energy, represented by the hermitian operator $\hat{H}$, the Hamiltonian. Further observables are the average location, momentum, spin, etc, as all those quantities are represented by hermitian operators. Nonetheless, there are also many important non-hermitian operators and in general there is no bound to what (useful) operators one might imagine.

Often it is convenient to define an operator in terms of its spectral decomposition, that is, it’s eigenvectors and eigenvalues. E.g. the position operator $\hat{x}$ is defined in the position basis as

$$\hat{x} = \int d^dx x |x\rangle\langle x| .$$
These spectral decompositions are very useful in explicit computations. Finding the matrix elements of an operator in a given basis works just as in usual linear algebra, with the difference that the indices on a matrix have now turned into continuous parameters. Hence, the matrix elements are functions (or rather distributions) of two variables, e.g. $O(x,y) = \langle x|O|y\rangle$.

**Q 1.3** Write the basis independent vectors $|\psi\rangle$, $\hat{x}|\psi\rangle$, $\hat{p}|\psi\rangle$, as well as the operators $\hat{x}$, $\hat{p}$, in position basis and in momentum basis.

Note that in a given basis, we can understand the “matrix elements” of an operator as an integral kernel $(O\psi)(x) = \int dxdy O(x,y)\psi(y)$.

**Q 1.4** What are $\rho(\vec{x}) := \langle \psi|\delta(3)(\hat{x} - \vec{x})|\psi\rangle$ and $\vec{J}(\vec{x}) := \frac{1}{2m}(\hat{p}, \delta(3)(\hat{x} - \vec{x}))|\psi\rangle$ in terms of the position space wave function $\psi(x)$? Can you write $\vec{\nabla} \cdot \vec{J}(x)$ in a similar way?

Another way of defining an operator is to declare how it acts on a complete set of basis vectors. Again for the position operator, we can define it in terms of its action on the position space basis, $\hat{x}|x\rangle = x|x\rangle$. Naturally, the definition in terms of its spectrum is a special case of this.

**Q 1.5** Show that the operator $\hat{p}$, defined by its action in position space as $\psi(x) \rightarrow i\partial_x \psi(x)$, is hermitian by showing that $\langle \psi|\hat{p}|\xi\rangle = (\langle \xi|\hat{p}|\psi\rangle)^*$ is true in the position space basis.

Incidentally, we can now use the basis independent notation in our Hilbert space, which is also known as **Dirac notation**, to write the Schrödinger equation (1) very compactly as

$$i\partial_t |\psi\rangle = \hat{H}|\psi\rangle,$$

where $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$.

**Q* 1.6** Recall that in 3d a particle with charge $e$ in an electro-magnetic field follows the Hamiltonian $H(x,p) = \frac{1}{2m}(\hat{p} - e\hat{A}(x))^2$, where the em-potential $\vec{A}$ determines the magnetic field $\vec{B} = \vec{\nabla} \times \vec{A}$ and the electric field $\vec{E} = -\partial_t \vec{A}$.

a) Derive/verify the classical eom $\vec{F} \equiv m\ddot{\vec{x}} = e(\vec{E} + \dot{\vec{x}} \times \vec{B})$.

b) What is the velocity (i.e. tangent vector) along the path of the particle $\dot{\vec{x}}$? Denote it $\vec{p}_A \equiv m\vec{v}$. Calculate the Poisson bracket $\{ (p_A)_i, (p_A)_j \}$.

c) What is the quantum Hamiltonian in terms of $\hat{p}$ and $A(\hat{x})$? Is there a normal ordering ambiguity in promoting the functions to operators? (Hint: remember the Coulomb gauge fixing condition $\vec{\nabla} \cdot \vec{A} = 0$.)

d) Going to canonical quantization ($[x^i, p_j] = i\delta^i_j$), what is the position space representation for $\vec{p}_A$? Show that the commutator becomes $[(p_A)_i, (p_A)_j] = \epsilon_{ijk} B_k$. 

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This is the first instance of a gauge theory, which will become very important in QFT and GR and you will learn a lot about it over the next terms. The non-vanishing of the commutator \([\{p_A\}_i, (p_A)_j]\) indicates that the particle moves in a \textit{curved space}. In this example the curvature does not reside in (position-)space, but rather in an “internal” space. See e.g. Nair or Nakahara for more.

**Probabilities**

Given that we can calculate the \textit{expectation value} of an observable in a state \(\psi\) using eq. (12), it is natural to ask what the outcome of a single measurement will be. The probabilistic nature of QM says that this question is ill-posed. We can only sensibly ask for the probability to measure some value. Recall that the expectation value is in general a sum over all possible outcomes, weighted by their probability. Inserting the spectral decomposition of the operator \(\hat{A}\) in terms of its eigenvalues \(a_i\) and (orthonormal) eigenvectors \(|i\rangle\) yields

\[
\sum_i \lambda_i p(\lambda_i) = \langle \hat{A} \rangle_{\psi} = \sum_i a_i |\langle i | \psi \rangle|^2 / \| \psi \|^2 .
\]

We recognize that the probability to measure a given eigenvalue \(a_i\) is given by the

\[
p(a_i) = |\langle i | \psi \rangle|^2 / \| \psi \|^2 = \langle \langle i | \psi \rangle \times \langle i | \psi \rangle \rangle_{\psi} \equiv \langle P_A(i) \rangle_{\psi}
\]

where we defined the \textit{projection operator} on the \(i^{th}\) eigenstate of \(\hat{A}\).

**Q 1.7** Check that \(P_a(i)\) is indeed a projection operator (i.e. \(P^2 = P\)) and observable (i.e. \(P^\dagger = P\)). Construct the projection operator projecting on two states \(P_A\{\{i,j\}\}\), then on an arbitrary subset of the spectrum of \(\hat{A}\).

If we want to compute the probability to find an eigenvalue within a certain range of the spectrum, we likewise take the expectation value of the projection operator onto that part of the spectrum.

**Q 1.8** a) Show that \(\langle \psi | \psi \rangle\) is constant in time using eq. (14) (with general \(H\)) and the product rule for differentiation. What property of \(\hat{H}\) is crucial?

b) Using the Dirac notation form for \(\vec{\nabla} \cdot \vec{j}\), evaluate \(\partial_t \rho + \vec{\nabla} \cdot \vec{j}\) using the \textit{Schrödinger equation} (14) with a Hamiltonian \(\hat{H} = \frac{1}{2m} \hat{p}^2 + V(\hat{x})\). What is the interpretation for \(\rho, \vec{j}\) and the differential equation they satisfy?

c) What is the relation between a) and b)?

d) What happens if the Hamiltonian is not hermitian? What is the interpretation for this?
Now that we know the probability for each possible outcome of a measurement, we can go ahead and actually perform it. A crucial property of (the Copenhagen interpretation of) QM is that measurements cause the wave function to collapse. Given we measure an observable $\hat{A}$, and find a value $a_i$ (corresponding to the $i^{th}$ eigenvalue of $\hat{A}$). The measurement will cause the wave function to become

$$|\psi\rangle \rightarrow P_A(i)|\psi\rangle = |i\rangle \langle i|\psi\rangle.$$  

(17)

This is an instant projection. It represents a non-continuous, non-unitary evolution. (There exist other interpretations of QM which avoid the wave function collapse, see e.g. de-coherence.) Note that before and after the measurement the time evolution is given by the Schrödinger equation.

Let’s examine what this means for two consecutive measurements of the same observable $\hat{A}$:

**Q 1.9**

a) What is the probability to find a system in state $a_j$ at time $T > 0$ if it was in state $a_i$ at time 0? (Hint: What is $\psi(t)$ for $T > t > 0$?)

b) What if the eigenvector associated with $a_i$ is an energy eigenstate?

c) What is the probability to measure the eigenvalue $a_j$ at time $t$ if we prepare the system to be in the state for eigenvalue $a_i$ at time 0? (Hint 1: What is $|\psi(t)\rangle$ for $t > t_1$?)

**Q* 1.10** Use the result from the last question to compute the probability for a free particle, $\hat{H} = \frac{p^2}{2m}$, to be at position 0 at time 0, and then be measured at position $x$ at time $t$. (You may have to go to imaginary time $t \rightarrow -it_E$ to compute an integral and go back to real time $t_E \rightarrow it$.)

**Uncertainty**

An immediate consequence of the representation of observables by operators (again, think matrices) is that observables no longer necessarily commute. E.g. the commutator between the position and momentum operator is

$$[\hat{x}, \hat{p}] = i\hbar$$  

(18)

and is important enough to carry the name canonical commutation relation. (It is called canonical because it follows from the classical mechanics by replacing the Poisson bracket by the commutator, $\{x, p\}_PB = 1 \rightarrow [\hat{x}, \hat{p}] = i\hbar$, which is an adhoc, yet canonical, procedure.)

**Q 1.11** Using the position basis expressions for $\hat{x}, \hat{p}$, find the position space expression for the commutator $[\hat{p}, f(\hat{x})]$, for a function $f$, by letting it act on an arbitrary vector. Compare this with what you get without choosing a basis, by writing $f$ as a Taylor expansion.
The effect of this is that the uncertainty in different observables become correlated, even if they were classically uncorrelated. Recall that the uncertainty (variance) for the value of an observable $\hat{A}$ is given by
\[
\sigma_A^2(\psi) := \langle (\hat{A} - \langle \hat{A} \rangle_\psi)^2 \rangle_\psi = \langle \hat{A}_0^2 \rangle_\psi,
\]
(19)
where for convenience we introduced the shorthand $\hat{A}_0 = \hat{A} - \mathbb{I} \langle \hat{A} \rangle_\psi$. The interpretation of this uncertainty is that some properties of the system simply do not have an exact value, but are smeared out over an interval $\sigma_A$ around the average, depending on the state.

**Q 1.12** Show that the uncertainty of the observable $\hat{A}$ in the state $\psi$ satisfies $\sigma_A^2(\psi) \geq 0$, with $\sigma_A^2(\psi) = 0$ iff $\psi$ is an eigenvector of $\hat{A}$.

Now, it follows from the positivity of the norm ($\| \cdot \| \geq 0$) that the product of the uncertainties of two observables is obeys
\[
\sigma_A^2(\psi) \sigma_B^2(\psi) \geq \left( \frac{1}{2} \langle \{\hat{A}_0, \hat{B}_0\} \rangle_\psi \right)^2 + \left( \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle_\psi \right)^2,
\]
(20)
the Schrödinger uncertainty relation. Note that the symmetric part $\{\hat{A}_0, \hat{B}_0\}$, is in direct analogy with the classical version of this relation. The quantum contribution comes from the commutator $[A, B]$, and has no classical analogue. This becomes particularly interesting when $\hat{A}$ and $\hat{B}$ are conjugate variables, so that the commutator is $i\hbar$. Then we can write a weaker, but more practical bound
\[
\sigma_A(\psi) \sigma_p(\psi) \geq \hbar/2,
\]
(21)
where the rhs is now independent of the state $\psi$.

**Q 1.13** Show eq. (20) by considering the function $f(\lambda) = \langle |\hat{A}_0 + \lambda \hat{B}_0|^2 \rangle_\psi$ and its minimum, for $\lambda \in \mathbb{C}$.

**Transformations & Unitarity**

Many computation become much easier if we choose a good basis for the Hilbert space. The basis independence of the result is guaranteed if we only allow basis changes that preserve the norm $\| \cdot \|$. This amounts to the requirement of unitarity of the operator $U$ implementing the basis change
\[
U^\dagger U = \mathbb{I},
\]
(22)
Unitary operators on our Hilbert space are the analogue of orthogonal matrices for $\mathbb{R}^n$.  

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[1] In particular, it doesn’t mean that we are not able, technologically or otherwise, to measure the precise value – the system just does not have a fixed value for $\hat{A}$. The right picture is that of a wave: it simply does not make sense to ask for its “location” to higher accuracy than its wavelength.
Now, the Schrödinger equation (14) says that the evolution of a physical system is given by the operator

\[ \hat{U}(t) = \exp(-i t \hat{H}) , \] (23)

which hence carries the name evolution operator.

\textbf{Q 1.14}  
\begin{enumerate}
\item[(a)] Check that \(|\psi(t)\rangle = U(t)|\psi_0\rangle\) solves the Schrödinger equation (14).
\item[(b)] Check that the evolution operator is unitary if \(\hat{H}\) is hermitian.
\item[(c)] Check that the evolution operator for shifting by a time \(t_1 + t_2\) can be obtained by first translating by \(t_1\) and then by \(t_2\).
\end{enumerate}

In other words, the action of \(U(t)\) acting on states generates a shift in time.

There is in general a close relationship between unitary operators and transformations. Firstly note that for every hermitian operator \(\hat{A}\) there is a unitary operator \(\hat{U}_A = \exp(i \hat{A})\). Physically, the relation is that \(\hat{U}_A\) generates a shift in the observable conjugate to \(A\). For example for position \(\hat{x}\) and momentum \(\hat{p}\):

\textbf{Q 1.15}  
\begin{enumerate}
\item[(a)] Show that the operator \(\hat{U}_p(a) = \exp(i a \hat{p})\) indeed generates a shift of the observable \(\hat{x}\) by the amount \(a\) in the sense that \(\hat{U}_p(a)|x\rangle = |x + a\rangle\) as well as \(\exp(-i a[\hat{p}, \cdot])f(\hat{x}) = \hat{U}_p(a)^\dagger f(\hat{x}) \hat{U}_p(a) = f(\hat{x} + a)\). (Tip: you can e.g. show that the operator relations hold when acting on a complete set of basis vectors, and hence (since linear) on all of the Hilbert space.)
\end{enumerate}

As you observed earlier, the operator \(\hat{U}_A\) is unitary if \(A\) is hermitian, i.e. observable.

This is again in analogy with classical mechanics, where every observable (function on phase space), generates a canonical transformation on the phase space via the Poisson bracket,

\[ (x, p) \rightarrow \exp(-a \{f, \cdot\})(x, p) . \] (24)

Remember that canonical transformations are coordinate changes, which preserve the symplectic structure. This fits in place nicely with the statement that unitary operators effect basis changes on Hilbert space. (If you want to learn more about this perspective on quantum mechanics you should look up geometric quantization, e.g. in chp 20 of Nair’s “modern perspective on QFT”, which in any case is highly recommendable for learning QFT!)
Heisenberg Picture

Going further along the lines of the previous paragraph, we could ask for the time evolution of observables directly. Using the Schrödinger equation (14) we find

$$\frac{d}{dt}\langle \hat{O} \rangle_\psi = i\langle [\hat{H}, \hat{O}] \rangle_\psi ,$$

(25)

where the time dependence sits purely with the state $|\psi(t)\rangle$ and $\mathcal{O}$ can be any (product of) operator(s). It is not hard to see that you get the same answer if instead of using the Schrödinger equation, you used the Heisenberg equation

$$\frac{d}{dt}\hat{O} = i[\hat{H}, \hat{O}]$$

(26)

for the time dependence of an operator, while the state is now fixed in time.

Q 1.16 Check that both a) (14) with $\frac{d}{dt}\hat{O} = 0$ and b) eq. (26) with $\frac{d}{dt}|\psi\rangle = 0$ lead to the right equation of motion for expectation values eq. (25).

It is not difficult to see that the solution of the Heisenberg equation is given by

$$\hat{O}(t) = U(t)\dagger\hat{O}(0)U(t) ,$$

(27)

which could of course be obtained directly by inspection of the matrix element $\langle \psi|\mathcal{O}|\psi\rangle$, and stripping the time evolution operator off the state, onto the operator.

In summary, note that the time evolution either affects the state of the system and the operators are constant

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle , \quad \mathcal{O}(t) = \mathcal{O}(0)$$

(28)

or vice versa

$$|\psi(t)\rangle = |\psi(0)\rangle , \quad \mathcal{O}(t) = U(t)\dagger\mathcal{O}(0)U(t) .$$

(29)

Since these two formulations describe the same physics, in fact the difference between them is completely unobservable, they are merely different pictures of the same underlying principle. They carry the names Schrödinger and Heisenberg picture respectively.

Q 1.17 Using $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$, determine the commutation relation $[\hat{x}, \hat{p}]$ from the requirement that the operators $\hat{x}$ and $\hat{p}$ fulfil an equation analogous to the classical eom eq. (3). Note the close similarity to the classical computation involving the Poisson bracket.
Tensor Product & Identical particles

When combining two physical systems, represented by Hilbert spaces $H_1, H_2$ and Hamiltonians $\hat{H}_1, \hat{H}_2$, we get a system with Hilbert space

$$\mathcal{H} = H_1 \otimes H_2,$$

(30)

the tensor product of the individual spaces, and a Hamiltonian

$$\hat{H} = \hat{H}_1 \otimes \mathbb{I} + \mathbb{I} \otimes \hat{H}_2.$$

(31)

If the bases of the Hilbert spaces $H_{1,2}$ were $|i_{1,2}\rangle$, then the basis elements of the tensor product are $|i_1, i_2\rangle = |i_1\rangle \otimes |i_2\rangle$. A general element of the combined Hilbert space can be expressed as a linear combination of these:

$$|\phi\rangle = \sum_{i_1, i_2} c_{i_1, i_2} |i_1\rangle \otimes |i_2\rangle,$$

(32)

where the $c_{i,j}$ are some coefficients. Clearly, the number of basis elements and hence the dimension of the combined Hilbert space is $\dim \mathcal{H} = \dim H_1 \cdot \dim H_2$. (The generalization to combining several physical systems follows analogously.)

Q 1.18 What is the dimension of the state space for a spin-$\frac{1}{2}$ particle? What is the dimension of the state space for $N$ spin-$\frac{1}{2}$ particles?

For the purpose of calculations you can think of the several states and operators living in different worlds; they behave within their Hilbert spaces as you are used to, e.g.

$$\left( A \otimes \hat{B} \right) (|\psi\rangle \otimes |\xi\rangle) = \left( A|\psi\rangle \right) \otimes \left( \hat{B}|\xi\rangle \right)$$

(33)

and

$$\left( \langle \psi | \otimes \langle \xi | \right) \left( |\psi'\rangle \otimes |\xi'\rangle \right) = \langle \psi | \psi' \rangle \langle \xi | \xi' \rangle$$

(34)

In particular the energy of a state $|\psi\rangle \otimes |\xi\rangle$ is given by

$$\left( \hat{H}_1 \otimes \mathbb{I} + \mathbb{I} \otimes \hat{H}_2 \right) (|\psi\rangle \otimes |\xi\rangle) = (E_1(|\psi\rangle) + E_2(|\xi\rangle)) (|\psi\rangle \otimes |\xi\rangle)$$

(35)

if $\psi$ and $\xi$ are eigenstates of $\hat{H}_{1,2}$ respectively. Often the trivially acting part is omitted, so we abbreviate $\hat{H}_1 \otimes \mathbb{I} + \mathbb{I} \otimes \hat{H}_2$ as simply $\hat{H}_1 + \hat{H}_2$ and use the index to remind us which subspace the operator acts on.

It is crucial to observe that not every state in the combined system is a product of two individual states – rather, it is generally a superposition of such combined states. This leads to the phenomenon known as entanglement, but we won’t dwell on this further.
A very important special case of a combining systems occurs when the constituents describe the same type of particle, e.g. $\mathcal{H}_1 \simeq \mathcal{H}_2$ and $\hat{H}_1 = \hat{H}_2$. Then we find a new requirement that any state has to fulfil. Consider the operator $S$, called \textit{swap operator}, which we define by its action on the basis elements as

$$S : \mathcal{H}_1 \otimes \mathcal{H}_2 \rightarrow \mathcal{H}_1 \otimes \mathcal{H}_2$$

$$S (|i_1\rangle \otimes |i_2\rangle) \mapsto e^{i\alpha} |i_2\rangle \otimes |i_1\rangle ,$$

where $\alpha$ is some phase ($|\alpha| = 1$), understood as part of the definition of $S$. Recall that two states $|\psi_1\rangle$ and $|\psi_2\rangle$ are \textit{equivalent}, i.e. the same physical state, if they differ only by a phase, $|\psi_2\rangle = \alpha|\psi_1\rangle$. (This ambiguity may seem innocuous, but has very far reaching and delicate consequences.) Hence we included an arbitrary phase $\alpha$ in the definition of $S$, in order not to lose generality.

Now, generically,\(^3\) experiments find that in nature two possibilities are realized: $\alpha = 1$ and $\alpha = -1$. Note that in both cases $S^2 = \mathbb{I}$. Furthermore, particles with integer spin (Bosons) are found to have $\alpha = 1$ while particles with half-integer spin (Fermions) have $\alpha = -1$.

So if we are combining identical bosons, the product state has to satisfy

$$S|\psi\rangle = |\psi\rangle$$

while for Fermions it has to satisfy

$$S|\psi\rangle = -|\psi\rangle .$$

In other words, the combined state space is just the (anti-)symmetric part of the tensor product. They are spanned by the (anti-)symmetric combinations of basis vectors

$$|i, j\rangle = |i\rangle|j\rangle + |j\rangle|i\rangle \quad \text{for } i \leq j$$

and

$$|i, j\rangle = |i\rangle|j\rangle - |j\rangle|i\rangle \quad \text{for } i < j$$

respectively. E.g. a two-fermion system can never be in a state $|\psi\rangle \otimes |\psi\rangle$, which is the famous Pauli exclusion principle.

Note that this phase $\alpha = \pm 1$ has important consequences for the thermodynamic properties of the full system and is hence hardly just a technicality.

**Ladder Operators**

Ladder operators are one of the many avatars of complex methods in physics. Let’s start by writing the classical Hamiltonian for the harmonic oscillator

\(^3\)Using QFT one can in fact prove that this has to be the case, if their interactions are to make sense. Particles for which $\alpha$ is not $\pm 1$, called \textit{anyons}, are possible in 2d and can be realized in condensed matter lab experiments.
not using two real coordinates $x, p$, but instead one complex coordinate

$$z = x \sqrt{\frac{m\omega}{2}} + p \frac{i}{\sqrt{2m\omega}}, \quad \bar{z} = z^*,$$

in terms of which the Hamiltonian becomes

$$H(p, x) \rightarrow H(z) = \omega z \bar{z} = \omega |z|^2.$$  (42)

To quantize we promote these variables to operators ($z \rightarrow a$, $\bar{z} \rightarrow a^\dagger$) and write the Hamiltonian as the symmetric product

$$\hat{H} = \frac{\omega}{2} \{a, a^\dagger\} \equiv \frac{\omega}{2} (aa^\dagger + a^\dagger a)$$  (43)

using the anti-commutator $\{A, B\} \equiv [A, B]_+ = AB + BA$.

Q 1.19 Show that $\langle \psi | \hat{H} | \psi \rangle \geq 0$ for any state $| \psi \rangle$ by using the property $\| \cdot \|^2 \geq 0$ of Hilbert spaces (and $\omega > 0$).

Q 1.20 Write the operators $a, a^\dagger$ in position space and compute their anti-commutator $\{a, a^\dagger\}$. Do you recognize the result? Also compute their commutator $[a, a^\dagger]$ basis independent, using the canonical commutation relation eq. (18).

Q 1.21 Show $\langle \psi | \hat{H} | \psi \rangle > 0$ for any state $| \psi \rangle$ by refining your answer to Q 1.19.

Q 1.22 Show that $a, a^\dagger$ act on eigenstates of $\hat{H}$ by shifting their eigenvalue by $\pm 1$. Since the spectrum of $\hat{H}$ is bounded from below, argue that there must be a state which is annihilated by $a$.

In a general system, the state which is annihilated by (all) lowering operators, is defined to be the vacuum and given the symbol $|0\rangle$ or $|\Omega\rangle$. Note that this is not the zero element of the Hilbert space, i.e. not $\vec{0}$. It is some non-trivial vector, and often a great deal of effort goes just into figuring out what exactly the vacuum of a theory is.

Q 1.23 a) Use the commutation relation $[a, a^\dagger]$ to calculate the norm of the states $|n\rangle = c_n (a^\dagger)^n |0\rangle$. Calculate the overlap $\langle n | m \rangle$. Finally choose $c_n$ such that $\langle n | n \rangle = 1$ and write down $\langle n | m \rangle$ in terms of the normalized states.

b) Show that you can realize the commutation relation for $a, a^\dagger$ via $a \rightarrow \partial a^\dagger$, by showing $a^n f(a^\dagger) |0\rangle = f^{(n)}(a^\dagger) |0\rangle$ for any polynomial $f$.

c) Repeat a) by realising the commutation relation as in b).

Q 1.24 Consider the coherent state $|\lambda\rangle = \exp(\lambda a^\dagger) |0\rangle$ for some $\lambda \in \mathbb{C}$. Show that it is an eigenstate of the annihilation operator $a$. Calculate the overlap $\langle \lambda | \rangle$, e.g. by realising the $a, a^\dagger$ commutation relation via $a \rightarrow \partial a^\dagger$. Calculate the average energy $\langle H \rangle \lambda := \langle \lambda | H | \lambda \rangle / \langle \lambda | \lambda \rangle$. 14
2 Spin

Spin is an abstract dynamical property of particles and can be thought of in analogy to the the familiar angular momentum. Though tempting, it is not correct to think of a particle spinning around itself like a top. The analogy is however very deep, which is captured in the statement that the spin and angular momentum obey the same *algebra*. Recall that the $i$th component of the angular momentum operator is defined as

$$\hat{L}_i = (\hat{x} \times \hat{p})_i = \epsilon_{ijk} \hat{x}_j \hat{p}_j,$$

from which we can verify the commutation relations (angular momentum algebra)

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k$$

(45)

Note that the definition of $\hat{L}_i$ in terms of position and momentum gives it a natural interpretation as the quantum operator associated to classical angular momentum $\vec{L} = \vec{x} \times \vec{p}$.

Q 2.1 *When promoting the classical angular momentum to an operator, is there a normal ordering ambiguity in the definition? Use the canonical commutation relation to verify eq. (45).*

As we mentioned before, an observable (hermitian operator) generates transformations on states. In order to get a feel for what this operator does:

Q* 2.2 *Calculate the action of $\exp(i \vec{\alpha} \cdot \vec{L})$ on a scalar function $f(\vec{x})$. (Hint 1: go to a basis for $\mathbb{R}^3$ in which $\vec{\alpha}$ looks simple. Hint 2: you should find that $f(\vec{x}) \to f(R(\vec{\alpha}) \vec{x})$, where $R(\vec{\alpha})$ is the rotation matrix around the vector $\vec{\alpha}$.)*

We now create a new set of operators, $\hat{S}_i$, called spin operators and declare they obey the same commutation relations as the angular momentum operators eq. (45), i.e.

$$[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk} \hat{S}_k$$

(46)

for the components of the spin vector $(\hat{S})_i = \hat{S}_i$. So far, this is an abstract algebra. If we want to describe an actual physical system and calculate its properties, we’ll have to choose an appropriate *representation* for this algebra.

Q 2.3 *Verify that $\hat{S}_i = \frac{1}{2} \sigma_i$, where the three matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices, satisfies eq. (46).*
Q 2.4 Calculate the value of the spin $s$ for this representation using the relation

$$S^2 \equiv \vec{S} \cdot \vec{S} = s(s+1) \mathbb{1}.$$  \hspace{1cm} (48)

What is the Hilbert space that this operators act on? Write down a basis and a generic element of it.

Having a spin-$\frac{1}{2}$ representation and the corresponding space of physical states at hand, we go on to define the Hamiltonian operator. Let’s couple the spin to an constant external magnetic field $\vec{B}$ by taking

$$H = \vec{S} \cdot \vec{B} = \sum_i \hat{S}_i B_i,$$  \hspace{1cm} (49)

where $\vec{B}$ is some constant vector. For convenience, let’s rotate our measuring apparatus such that its z-axis is parallel to the magnetic field, in other words, take $\vec{B} = b \hat{e}_z$.

Q 2.5 Find the (normalized) eigenvectors and eigenvalues of the Hamiltonian eq. (49) and denote them by $|\pm\rangle$ and $E_{\pm}$ respectively. Given a state $|\psi\rangle = c_1 |+\rangle + c_2 |--\rangle$ at time zero, what is $|\psi(t)\rangle$? I.e., calculate the time evolution operator $U(t) = \exp(-itH)$ for eq. (49) and apply it to the vector $v = (c_1, c_2)^T$.

Note that we can guarantee the state to be normalized if we set $c_1 = \sin(\vartheta/2)$ and $c_2 = \cos(\vartheta/2) e^{i\varphi}$.

Q 2.6 What are the value ranges for $\vartheta, \varphi$ so that all physical states are parametrized? Given this parametrization what is the state space of the spin-$\frac{1}{2}$ system? Can you express $|\psi(t)\rangle$ in this form and what are $\vartheta(t)$ and $\varphi(t)$?

Q 2.7 Calculate the average spin $\vec{S}(t) = \langle \vec{S} \rangle_{\psi(t)}$ in the state $\psi(t)$. (Hint: Look at $S_z$ and $\vec{S}_\perp = (S_x, S_y)$ separately, and express $\vec{S}_\perp(t) = R(t)\vec{S}_\perp(0)$ using a time dependent rotation matrix $R$.)

Observe the rotation of the spin expectation value around the axis of the magnetic field, called precession. Given the nice behaviour of the expectation value, we can go further and ask how the operator itself evolves (in the Heisenberg picture)

Q 2.8 Calculate the time evolution of the operator $\vec{S}$ given by eq. (26). (Hint 1: you can e.g. use the spin algebra to turn the Heisenberg equation into a linear coupled ODE. Hint 2: separate $\vec{S}$ into $S_z$ and $S_\perp$ as above.)

Q* 2.9 Repeat Q 2.5 without making the simplification $\vec{B} = b \hat{e}_z$. If you choose the right basis for the Hilbert space, this exercise requires nearly no additional computation.
Q* 2.10 Compute the matrix exponential \( \exp(i \vec{a} \cdot \vec{\sigma}) \) for any vector \( \vec{a} \). In addition to the algebra eq. (46), you'll need to use that \( \{\sigma_i, \sigma_j\} = 2\delta_{ij} \).

3 Perturbation Theory

There are not many quantum systems that admit an exact analytic solution (finding the eigenstates and their energies), so in general a more widely applicable method for extracting the physics from a Hamiltonian is needed. One way is to split the Hamiltonian \( H \) in question into a part that we can solve, \( H_0 \), and treat the remainder as a perturbation.

\[
H = H_0 + H_I \quad (50)
\]

Of course this split is arbitrary, but typically \( H_0 \) will describe a particle with either no, or quadratic potential. For this to be useful, there needs to be some sense in which the contribution from \( H_I \) is much smaller than that from \( H_0 \), so we expand the quantities of interest in a series.

In QFT you will be mainly concerned with calculating transition amplitudes. Recall from Q 1.9 that the probability to measure a particle in state \( |i\rangle \) at time 0 and then in state \( |j\rangle \) at time \( t \) is

\[
P_{i \rightarrow j}(t) = | \langle i | \exp(-it\hat{H}) | j \rangle |^2 \quad (51)
\]

where \( |i\rangle \) are the normalized eigenvectors of some observable, e.g. position eigenstates, momentum eigenstates or energy eigenstates.

To make use of the split into a known Hamiltonian and a perturbation we need to use the operator identity

\[
\exp(A + \epsilon B) = e^A + \epsilon \int_0^1 ds \ e^{(1-s)A} \ B \ e^{sA} + \mathcal{O}(\epsilon^2) \quad (52)
\]

or equivalently

\[
\exp(-it(H_0 + \epsilon H_I)) = e^{-itH_0} + \epsilon \int_0^t dt' \ e^{-i(t-t')H_0} \ H_I \ e^{-it'H_0} + \mathcal{O}(\epsilon^2) \quad (53)
\]

A mnemonic for this is that the perturbation \( H_I \) is inserted at every possible point along the interval of evolution \([0,t]\), dressed by evolution under the free \( H_0 \) before and after.

Q 3.1 Show the above relation e.g. by expanding both sides in their Taylor expansions and counting powers of \( A \) and \( B \). (Tip: You may need the binomial coefficient.)

This expansion is particularly useful if the states of interest are eigenstates of the unperturbed system \( H_0 \).
Q 3.2 When $|i\rangle, |j\rangle$ are energy eigenstates of $H_0$ with different energy, insert eq. (53) into the transition amplitude and find the leading correction, expressed in terms of the matrix element $\langle i|H_I|j\rangle$. (Assume $\langle i|j\rangle = 0$)

The result is important enough to carry the name Fermi’s golden rule. You should find

$$P_{i \rightarrow j}(t) = \frac{\sin(\omega t/2)^2}{(\omega/2)^2} |\langle i|H_I|j\rangle|^2$$

(54)

with the frequency of oscillation given by $\omega = E_j - E_i$. As example, consider the Hamiltonian

$$H = H_0 + H_I = \begin{pmatrix} E & 0 & \delta \\ 0 & -E & \delta \\ \delta & \delta & 0 \end{pmatrix}$$

(55)

where $|\delta| \ll E$.

Q 3.3 Find the energies and eigenstates for $\delta = 0$. Then use the result of Q 3.2 to find the transition amplitude between the two energy levels to leading order in $\delta$.

Q 3.4 Calculate to leading order the transition probability between different levels of the harmonic oscillator, $H_0 = \frac{1}{2} \{a, a^\dagger\}$, under the anharmonic perturbation $H_I = \epsilon x^3$. (Tip: Express $x^3$ in terms of $a, a^\dagger$.)

Q* 3.5 Calculate the correction to next-to-leading order.

You will have noticed that the computation is tremendously simplified when computing transitions between eigenstates of the unperturbed system. Recall that the Schrödinger and Heisenberg picture are different, yet equivalent, assignments of time evolution between the state and the operators. We can now make use of the above observation by introducing a half-way picture: since we know the evolution of the state $\psi$ by the unperturbed, exactly solvable Hamiltonian $H_0$, we absorb this into the definition of the state, i.e.

$$|\psi\rangle_I = \exp(itH_0)|\psi\rangle_S ,$$

(56)

where $|\psi\rangle_I$ and $|\psi\rangle_S$ are the state in interaction and Schrödinger picture respectively, which the perturbation as its only explicit time dependence. Comparison with the Schrödinger equation yields that in this picture the state and the operators have to satisfy the equations

$$i\partial_t|\psi\rangle = \hat{H}_I|\psi\rangle \quad \text{and} \quad \frac{d}{dt}\hat{O} = i[\hat{H}_0, \hat{O}] .$$

(57)

Q 3.6 Verify this.

For the next two terms you will be working mainly in this picture.