Summary of SI2380 Advanced Quantum Mechanics

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Abstract

This is a summary of SI2380 Advanced Quantum Mechanics.

Contents

1 Basic Concepts

Observables An observable is a Hermitian operator whose orthonormal eigenvectors form a basis.

The Postulates of Quantum Mechanics The postulates of quantum mechanics are:

- At any fixed time the state of a physical system is specified by a ket in Hilbert space.
- Every measurable physical quantity corresponds to an operator on Hilbert space. This is a Hermitian observable. The possible outcomes of a measurement are the eigenvalues of A.
- The probability of measuring the value a of operator A in a normalized state $|\Psi\rangle$ is $P(a) = \langle\Psi|P_a|\Psi\rangle$, where P_a is the projector onto the subspace corresponding to the eigenvalue a given by $P_a = |a\rangle\langle a|$.
- If a measurement of an observable A gives an outcome a, the state of the system immediately after the measurement is the projection of the state onto the subspace with eigenvalue a.
- The time evolution of a state is governed by the Schrödinger equation.

Consequences of the Probability Picture The form of writing the projection operator implies $P(a) = |\langle a|\Psi\rangle|^2$, or $P(a)\,\mathrm{d}a = |\langle a|\Psi\rangle|^2\,\mathrm{d}a$ in the continuous case. In order for the probability interpretation to be consistent, i.e. for the sum of all probabilities to amount to 1, it must hold that $\langle\Psi|\Psi\rangle = 1$.

Expectation Values Expectation values are given by

$$\langle A\rangle = \sum aP(a) = \sum a\,\langle\Psi|P_a|\Psi\rangle = \langle\Psi|\sum a\,|a\rangle\,\langle a|\Psi\rangle = \langle\Psi|A|\Psi\rangle\,.$$

Physical States Modifying a state by a phase factor $e^{i\alpha}$ does not change any expectation values.

Pure and Mixed States Pure states are states with a well-defined state vector. Mixed states are states wherein the state vector is not well-defined.

Density Matrix The density matrix is defined as

$$\rho = |\Psi\rangle\langle\Psi|\,.$$

It has some cool properties. For instance:

$$\begin{aligned}
&\mathrm{tr}\{\rho\} = \sum_n \langle n|\rho|n\rangle = \left\langle \psi\middle|\sum_n |n\rangle\langle n|\middle|\psi\right\rangle = \langle\Psi|\Psi\rangle = 1,\\
&\rho^\dagger = \rho,\\
&\langle A\rangle = \sum_{n,m}\langle\Psi|n\rangle\,\langle n|A|m\rangle\,\langle m|\Psi\rangle = \sum_{n,m}\langle m|\Psi\rangle\,\langle\Psi|n\rangle\,\langle n|A|m\rangle = \sum_{n,m}\langle m|\rho|n\rangle\,\langle n|A|m\rangle = \mathrm{tr}(\rho A),\\
&\rho^2 = \rho.
\end{aligned}$$

Note that the latter is only true for pure states. Mixed states have a density matrix of the form

$$\rho = \sum_j P_j\,|\Psi_j\rangle\langle\Psi_j|\,,$$

where the P_j are the probability that the state of the system is $|\Psi_j\rangle$.

The Time Evolution Operator Suppose that there exists an operator $u_{t'}(t)$ which evolves $|\Psi(t')\rangle$ to $|\Psi(t)\rangle$. Such an operator should satisfy

- $u_{t'}(t) = u_{t''}(t)u_{t'}(t'')$ for consistency.
- $u_{t'}(t)$ is unitary to preserve the normalization.
- $u_t(t) = 1$.

Inserting this into the Schrödinger equation yields

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}u_{t'}(t)\left|\Psi(t')\right\rangle = Hu_{t'}(t)\left|\Psi(t')\right\rangle,$$
$$i\hbar\partial_t t' = Hu_{t'}(t).$$

In the case of a time-independent Hamiltonian, the solution must be of the form $u_{t'}(t) = u(t-t')$, and the equation above can be integrated to yield

$$u_{t'}(t) = e^{-i\frac{t-t'}{\hbar}H}.$$

Symmetries in Quantum Mechanics A symmetry in a quantum mechanics context is any transformation acting on Hilbert space that leaves all probabilities invariant.

Wigner's Theorem Wigner's theorem states that any operator that is a symmetry is either unitary or anti-unitary ($\langle\Phi|U^\dagger U|\Psi\rangle = \langle\Psi|\Phi\rangle$).

Transformation of Operators Consider a symmetry operator u. In order for this to be a symmetry, it must also act on all operators according to $A \to uAu^\dagger$.

Time Evolution From Symmetry Consider some system with time translation symmetry - that is, any system for which time translations do not change the theory. Introduce the transformation operator

$$u_\tau\left|\Psi(t)\right\rangle = \left|\Psi(t+\tau)\right\rangle.$$

This transformation is a smooth map acting on a manifold - namely, Hilbert space. Hence we can use the language of Lie algebra to treat this (if you know nothing about Lie algebra, pretend that I didn't write this and carry on. If you want some reference material, please look at my summary of SI2360). We expand the transformation operator around the identity as

$$u_\tau = 1 - i\frac{\tau}{\hbar}H$$

for some operator H. The requirement that this be unitary yields $H^\dagger - H = 0$, and hence the generator H is self-adjoint. By continuous application of this we obtain

$$u_\tau = e^{-i\frac{\tau}{\hbar}H}.$$

This reproduces the Schrödinger equation, tying it all together neatly. It also demonstrates that the Hamiltonian generates time translation in a mathematical sense.

Space Translation Consider the space operator x^i. A space translation u transforms x^i to $x^i + a^i$, meaning $ux^iu^\dagger = x^i + a^i$. Expanding the translation around the identity yields

$$u = 1 + i\frac{a^i}{\hbar}p_i$$

for some operator p_i. The requirement that u be unitary implies that p is self-adjoint. The transformation rule yields

$$(1 + i\frac{a^i}{\hbar}p_i)x^i(1 - i\frac{a^i}{\hbar}p_i) = x^i + i\frac{a^i}{\hbar}\left\{p_i, x^i\right\}$$

and the requirement

$$\left[p_i, x^i\right] = -i\hbar.$$

Time Evolution of the Density Matrix The time evolution of the density matrix is given by

$$\rho(t) = \sum P_i u_{t_0}(t) |\Psi_i\rangle \langle\Psi_i| u_{t_0}(t)^\dagger = u_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger.$$

This implies

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho = Hu_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger - u_{t_0}(t)\rho(t_0)u_{t_0}(t)^\dagger H = H\rho(t) - \rho(t)H = [H, \rho].$$

The Heisenberg Equation Heisenberg's outlook starts from preserving expectation values under time translations in such a way that all (total) time evolution is contained in the operators, arriving at the transformation rule

$$A_\mathrm{H} = u_{t_0}^\dagger(t)A_\mathrm{S}u_{t_0}(t).$$

A_H is the operator according to Heisenberg and A_S is the operator according to Schrödinger. We now have

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A_\mathrm{H}\rangle &= -u_{t_0}^\dagger(t)HA_\mathrm{S}u_{t_0}(t) + u_{t_0}^\dagger(t)(i\hbar\partial_t A_\mathrm{S})u_{t_0}(t) + u_{t_0}^\dagger(t)A_\mathrm{S}Hu_{t_0}(t) \\
&= -u_{t_0}^\dagger(t)Hu_{t_0}(t)u_{t_0}^\dagger(t)A_\mathrm{S}u_{t_0}(t) + u_{t_0}^\dagger(t)(i\hbar\partial_t A_\mathrm{S})u_{t_0}(t) + u_{t_0}^\dagger(t)A_\mathrm{S}u_{t_0}(t)u_{t_0}^\dagger(t)Hu_{t_0}(t) \\
&= -H_\mathrm{H}A_\mathrm{H} + u_{t_0}^\dagger(t)(i\hbar\partial_t A_\mathrm{S})u_{t_0}(t) + A_\mathrm{H}H_\mathrm{H} \\
&= -H_\mathrm{H}[A_\mathrm{H}, +](i\hbar\partial_t A_\mathrm{S})_\mathrm{H}.
\end{aligned}$$

Propagators The probability amplitude at some point x at time t is given by

$$\Psi(x,t) = \langle x|\Psi(t)\rangle = \langle x|u_0(t)|\Psi(0)\rangle = \int \mathrm{d}x' \left\langle x\middle|u_0(t)\middle|x'\right\rangle \left\langle x'\middle|\Psi(0)\right\rangle.$$

Defining the propagator $G_{x',t'}(x,t) = \langle x|u_{t'}(t)|x'\rangle$, we arrive at

$$\Psi(x,t) = \int \mathrm{d}x'\, G_{x',0}(x,t)\left\langle x'\middle|\Psi(0)\right\rangle = \int \mathrm{d}x'\, G_{x',0}(x,t)\Psi(x',0).$$

Hence the propagator acts as a Green's function with respect to time, in some sense.

Arriving at Path Integrals The general propagator of some state is given by

$$G_{x',t'}(x,t) = \sum_\gamma G_{\gamma;x',t'}(x,t),$$

where the summation is performed over all possible paths γ between the two points.

Suppose now that the time evolution is divided into steps such that

$$u_{t'}(t) = \prod_{k=1}^n u_{t_{k-1}}(t_k),\ t_0 = t',\ t_n = t,\ t_k - t_{k-1} = \delta t.$$

Then

$$G_{x',t'}(x,t) = \left\langle x\middle|\prod_{k=1}^n u_{t_{k-1}}(t_k)\middle|x'\right\rangle.$$

For every k we now introduce an identity according to

$$\begin{aligned}
G_{x',t'}(x,t) &= \left\langle x\middle|\prod_{k=1}^n u_{t_{k-1}}(t_k)\int \mathrm{d}x_k\, |x_{k-1}\rangle\langle x_{k-1}|\middle|x'\right\rangle \\
&= \left\langle x\middle|\prod_{k=1}^n \int \mathrm{d}x_k\, u_{t_{k-1}}(t_k)\, |x_{k-1}\rangle\langle x_{k-1}|\middle|x'\right\rangle \\
&= \int\prod_{k=1}^n \mathrm{d}x_k\, \langle x_k|u_{t_{k-1}}(t_k)|x_{k-1}\rangle.
\end{aligned}$$

The time translation operator has the form $u_{t_{k-1}}(t_k) = e^{-i\frac{\Delta t}{\hbar}H}$. For a Hamiltonian of the form $H = \frac{p^2}{2m} + V(\mathbf{x})$, the terms do not necessarily commute. However, to second order we have

$$\begin{aligned}
e^{\alpha A}e^{\alpha B} &= \left(1 + \alpha A + \frac{1}{2}\alpha^2 A^2 + \dots\right)\left(1 + \alpha B + \frac{1}{2}\alpha^2 B^2 + \dots\right), \\
e^{\alpha(A+B)} &= 1 + \alpha A + \alpha B + \frac{1}{2}\alpha^2(A^2 + B^2 + AB + BA) + \dots, \\
&= e^A e^B \left(1 - \frac{1}{2}\alpha^2 AB + \frac{1}{2}\alpha^2 BA + \dots\right) \\
&= e^{\alpha A}e^{\alpha B}e^{\frac{1}{2}\alpha^2[A,B]}.
\end{aligned}$$

Ignoring the second-order term yields

$$\begin{aligned}
G_{x',t'}(x,t) &= \int \prod_{k=1}^{n} \mathrm{d}x_k \, \langle x_k | e^{-i\frac{\Delta t}{\hbar}(T+V)} | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \, \langle x_k | e^{-i\frac{\Delta t}{\hbar}T} | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \left\langle x_k \middle| e^{-i\frac{\Delta t}{\hbar}T} \int \mathrm{d}p_k \, |p_k\rangle\langle p_k| \middle| x_{k-1} \right\rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \left\langle x_k \middle| \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{\hbar}T} \, |p_k\rangle\langle p_k| \middle| x_{k-1} \right\rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}p_k^2} \, \langle x_k | p_k \rangle \, \langle p_k | x_{k-1} \rangle \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}p_k^2} \frac{1}{2\pi\hbar} e^{i\frac{p_k(x_k - x_{k-1})}{\hbar}} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \frac{1}{2\pi\hbar} \int \mathrm{d}p_k \, e^{-i\frac{\Delta t}{2m\hbar}\left(p_k - \frac{m}{\Delta t}(x_k - x_{k-1})\right)^2} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \sqrt{\frac{m}{2\pi^2\hbar\Delta t i}} \int \mathrm{d}v_k \, e^{-v_k^2} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \, e^{-i\frac{\Delta t}{\hbar}V(x_{k-1})} e^{i\frac{m}{2\hbar\Delta t}(x_k - x_{k-1})^2} \sqrt{\frac{m}{2\pi\hbar\Delta t i}} \\
&= \int \prod_{k=1}^{n} \mathrm{d}x_k \sqrt{\frac{m}{2\pi\hbar\Delta t i}} e^{i\frac{1}{\hbar}\sum_{k=1}^{n}\left(\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\Delta t}\right)^2 - V(x_{k-1})\right)\Delta t}.
\end{aligned}$$

In the continuous limit the exponent becomes

$$i\frac{1}{\hbar}\int \mathrm{d}t \, \frac{1}{2}m\dot{x}^2 - V(x) = i\frac{S}{\hbar}$$

where S is the action. The remaining factor, termed the measure, is

$$D(x(t)) = \lim_{\Delta t \to 0} \prod_{k=1}^{n} \mathrm{d}x_k \sqrt{\frac{m}{2\pi\hbar\Delta t i}}.$$

Finally the propagator is given by

$$G_{x',t'}(x,t) = \int D(x(t)) e^{-i\frac{S}{\hbar}}.$$

This is termed the path integral.

As a side note, if the action is large compared to $\hbar$, the action varies strongly, causing destructive interference from all paths except for the one such that

$$\frac{\delta S}{\delta x} = 0.$$

This is Hamilton's principle, the fundamental postulate of classical mechanics.

The Harmonic Oscillator The Hamiltonian of the harmonic oscillator is

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2.$$

To diagonalize it we introduce the lowering operator

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right)$$

and its adjoint, the raising operator. Their commutator is

$$\begin{aligned}
\left[a, a^\dagger\right] &= \left[\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right), \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \frac{i}{\sqrt{m\omega\hbar}}p\right)\right] \\
&= \left[\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x, -\frac{1}{\sqrt{2}}\frac{i}{\sqrt{m\omega\hbar}}p\right] + \left[\frac{1}{\sqrt{2}}\frac{i}{\sqrt{m\omega\hbar}}p, \frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x\right] \\
&= \frac{1}{2}\frac{i}{\hbar}\left([x, -p] + [p, x]\right) \\
&= 1.
\end{aligned}$$

The definition of the raising and lowering operators may be inverted to obtain

$$x = \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}(a^\dagger + a),\ p = \frac{i}{\sqrt{2}}\sqrt{m\omega\hbar}(a^\dagger - a).$$

The Hamiltonian may now be written in terms of these operators as

$$\begin{aligned}
H &= \frac{1}{2m}\cdot -\frac{1}{2}m\omega\hbar(a^\dagger - a)^2 + \frac{1}{2}m\omega^2\frac{1}{2}\frac{\hbar}{m\omega}(a^\dagger + a)^2 \\
&= -\frac{1}{4}\hbar\omega(a^\dagger - a)^2 + \frac{1}{4}\hbar\omega(a^\dagger + a)^2 \\
&= \frac{1}{4}\hbar\omega\left((a^\dagger)^2 + a^\dagger a + aa^\dagger + a^2 - \left((a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2\right)\right) \\
&= \frac{1}{2}\hbar\omega\left(a^\dagger a + aa^\dagger\right) \\
&= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).
\end{aligned}$$

We now define the operator $n = a^\dagger a$. It is Hermitian, meaning that an orthonormal basis of its eigenvectors exists (fortunately, as it constitutes the Hamiltonian). These eigenvectors must be studied next. To do this, we use the commutation relations[1]

$$[n, a] = a^\dagger[a, a] + \left[a^\dagger, a\right]a = -a,\ \left[n, a^\dagger\right] = a^\dagger\left[a, a^\dagger\right] + \left[a^\dagger, a^\dagger\right]a = a^\dagger$$

applied to some eigenvector $|\nu\rangle$ with eigenvalue ν to obtain

$$na\left|\nu\right\rangle = (an - a)\left|\nu\right\rangle = (\nu - 1)a\left|\nu\right\rangle.$$

Hence, if some eigenvalue ν exists, we can repeat this argument to show that $\nu - 1,\ \nu - 2, \dots$ are also eigenvalues, assuming no value in this sequence is zero. The length of these eigenvectors is given by

$$\langle\nu|a^\dagger a|\nu\rangle = \nu\left\langle\nu|\nu\right\rangle \geq 0,$$

[1] What might inspire this? A suggestion might be the fact that if n and the raising and lowering operators commuted, we would find that they share eigenvectors.

where the latter is due to the positivity of the inner product. In order for this to work, no negative eigenvalues may exist. This only fits with the previous sequence of eigenvalues if $\nu = 0$ is an eigenvalue.

Having established that, we rename the eigenvalues to n. Next, we have

$$n a^\dagger |n\rangle = (a^\dagger n + a^\dagger) |n\rangle = (n+1) a^\dagger |n\rangle .$$

Hence the sequence $n+1, n+2, \dots$ also consists of eigenvalues of n. The length of such vectors is

$$\langle n | a a^\dagger | n \rangle = \langle n | a^\dagger a + 1 | n \rangle = (n+1) \langle n | n \rangle > 0.$$

Now the eigenvalues of the Hamiltonian are found to be

$$H_n = \hbar\omega \left(n + \frac{1}{2} \right), \; H |n\rangle = H_n |n\rangle .$$

With respect to degeneracy, suppose there is a set of eigenvectors denoted by the index k such that $a |0, k\rangle = 0$. In the coordinate basis we obtain

$$\left\langle x \middle| \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} x + \frac{i}{\sqrt{m\omega\hbar}} p \right) \middle| 0, k \right\rangle = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} x + \sqrt{\frac{\hbar}{m\omega}} \frac{\mathrm{d}}{\mathrm{d}x} \right) \Psi_{0,k} = 0.$$

The solution to this differential equation is unique, hence the ground state is non-degenerate. The linearity of the raising operator therefore implies that the other eigenvalues are non-degenerate as well.

With respect to normalization, we may require all states to be normalized. Then

$$\begin{aligned} a^\dagger |n\rangle &= c_{n+1} |n+1\rangle , \\ |c_{n+1}|^2 &= \langle n | a a^\dagger | n \rangle = \langle n | n+1 | n \rangle = n+1, \\ c_n &= \sqrt{n}. \end{aligned}$$

Next we have

$$\begin{aligned} a a^\dagger |n-1\rangle &= \sqrt{n} a |n\rangle \\ n |n-1\rangle &= \sqrt{n} a |n\rangle , \\ a |n\rangle &= \sqrt{n} |n-1\rangle . \end{aligned}$$

Finally, the excited states may be found according to

$$|n\rangle = \frac{1}{\sqrt{n}} a^\dagger |n-1\rangle = \cdots = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle ,$$

which when applied to the ground state will reproduce some special function.