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.

Mixed States

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

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

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

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

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

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

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

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

Defining the propagator $G_{x',t'}(x,t) = \left\langle x \middle| u_{t'}(t) \middle| x'\right\rangle$, 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

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

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.