

(Non-relativistic) Quantum Mechanics

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Here is a collected notes on physics readings.

Contents

1	Kinematics	2
2	Dynamics	3
2.1	Notes	3
2.2	QA and comments	5

§1 Kinematics

§2 Dynamics

§2.1 Notes

- Conservation of probability implies time evolution is **unitary**. Unitary operators are just operators that preserve the norm of the wavefunction (which must be 1 because probabilities add to 1). They are generalizations of rotations for vectors in hilbert space. ¹

$$\underbrace{\mathcal{U}(t, t_0)}_{\text{time evolution}} |\psi(t_0)\rangle \equiv |\psi(t)\rangle$$

$$\mathcal{U}^\dagger \mathcal{U} = \mathbb{I} \rightarrow \langle \psi | \psi \rangle(t) = 1 \forall t$$

- In general, unitary operators can be written as exponentiated hermitian operators. This can be seen with a short taylor expansion.

$$\mathcal{U} = \exp\left(-\frac{i}{\hbar} \hat{H} t\right) \approx \mathbb{I} - \frac{i}{\hbar} \hat{H} t + \mathcal{O}(t^2)$$

The hermitian operator \hat{H} that **generates** ² time evolution is defined/called the **Hamiltonian** of a system. It has units of energy and corresponds to the energy operator (eigenvalues are the energy levels).

- This directly implies **Schrodinger's equation**:

$$i\hbar \frac{\partial}{\partial t} \mathcal{U}(t) = \hat{H} \mathcal{U}$$

or equivalently

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

Time evolution in quantum mechanics is *linear* ³.

- The **Dyson Series** solution to the schrodinger equation is ⁴:

$$\begin{aligned} \mathcal{U}(t, t_0) &= \underbrace{\mathcal{T}}_{\equiv \text{time ordered}} \exp\left(-\frac{i}{\hbar} \int_0^t dt' \hat{H}(t')\right) \\ &\equiv \mathbb{I} - \frac{i}{\hbar} \int_0^t \hat{H}(t') dt' - \left(\frac{i}{\hbar}\right)^2 \int_{t_1}^t dt' \int_0^{t_1} dt'' \hat{H}(t') \hat{H}(t'') + \dots \end{aligned}$$

- An equivalent solution to schrodinger time evolution is via the so called **path integral** ⁵

$$\langle x_1(t_1) | \mathcal{U}(t, 0) | x_0(t_0) \rangle = \underbrace{\int \mathcal{D}x}_{\sum \text{ over paths with boundary conditions on } x}^{x(t_2)=x_2, x(t_1)=x_1} \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t_1} dt \mathcal{L}(x, \dot{x}, t)\right)$$

- If the hamiltonian is time independent, the solution is easier, by working in the eigenbasis of the hamiltonian:

$$\begin{aligned} \hat{H} |n\rangle &\equiv E_n |n\rangle \\ \mathcal{U}(t) &= \sum_n e^{-i \frac{E_n t}{\hbar}} |n\rangle \langle n| \\ |\psi(t)\rangle &= \sum_n e^{-i \frac{E_n t}{\hbar}} |n\rangle \langle n | \psi(0) \rangle \end{aligned}$$

This is the motivation behind finding the energy eigenvalues E_n and eigenvectors $|n\rangle$ of the hamiltonian. The states $|n\rangle$ are called **stationary** because it remains in that subspace modulo a complex phase factor over time.

¹Unitary time evolution means you cannot "destroy" parts of the wavefunction. This trivial statement underlies many statements like "quantum mechanics requires information to be conserved" and debates regarding the black hole information paradox

²An operator A that "generates" a continuous change parametrized by $\alpha \in \mathbb{R}$ transforms the state as $|\psi\rangle \rightarrow \exp(i\alpha A) |\psi\rangle$

³The **linearity** of time evolution underlies "no-cloning" theorems for example

⁴This series solution is mostly useful for formal manipulations, but most of the time it is not practical to compute

⁵Many partial differential equations beside the schrodinger equation also admit path integral solutions. Examples are the black-scholes equation in finance (why wall street hires physicists?), the diffusion equation etc...

- An alternate way to compute time evolution is to time evolve the operators while keeping the state vector fixed. This is called the **Heisenberg Picture**:

$$\frac{d}{dt}\hat{O}(t) = \frac{1}{i\hbar}[\hat{H}, \hat{O}(t)]$$

- A useful trick called the **Baker-Campbell-Hausdorff (BCH)** lemma can be used to transform operators⁶:

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \dots$$

$$e^{\frac{i\hat{p}a}{\hbar}} \hat{x} e^{-\frac{i\hat{p}a}{\hbar}} = \hat{x} + a$$

$$e^{i\sigma_x} \sigma_y e^{-i\sigma_x} =$$

- The harmonic oscillator is arguably the most important classical and quantum system that has an analytical solution. This is because around any minimum, the potential energy looks quadratic.
- The stationary states of the harmonic oscillator can be "solved" by factoring the hamiltonian in terms of **creation and annihilation** operators:

$$\hat{H} = \hbar\omega (a^\dagger a + 1)$$

$$[a, a^\dagger] = 1$$

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

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

The ground state is a gaussian in the position representation, and the excited states are hermite polynomials times gaussians.

- Eigenvectors of a are called **coherent states**⁷. They are called so because they look like localized wavepackets that under time evolution oscillate back and forth like a classical mass-spring system:

$$\frac{d}{dt}a = ae^{-i\omega t} \text{ use heisenberg equation}$$

- The **WKB** approximation is a way to solve a PDE when the wavelength is small relative to the change in the potential $V(x)$ ⁸.

$$\psi(x) \propto \exp\left(\frac{i}{\hbar} \int dx \sqrt{2m(E - V(x))}\right)$$

This formula is handy to calculate tunneling amplitudes when $E < V(x)$ (classically disallowed!).

- In general, one can use the saddle-point approximation to evaluate the path integral in the limit $\hbar \rightarrow 0$. This is called the **semi-classical** expansion which connects quantum mechanics to the hamilton-jacobi equation which is classical mechanics.
- Linear PDE's can be solved for arbitrary conditions via superposition. This implies that if you know the solution to schrodinger's equation for a dirac delta at a given time, you know the solution for any initial condition by superposing them. The **propagator**⁹ is the solution to schrodinger's equation for a dirac delta function:

$$K(x'', t''; x', t') \equiv \underbrace{\langle x'', t'' | x', t' \rangle}_{\text{amplitude to start at } x', t' \text{ and end at } x'', t''}$$

⁶A common notation is to write $e^A B e^{-A} \equiv \exp_{\text{Ad}A} B$. The fancy mathspeak is A is a "generator" of [blahblah] transformation and it lives in the **adjoint** representation of that [blahblah] group of transformations.

⁷ a and a^\dagger are **not** hermitian operators. Their eigenstates actually do not form an orthogonal basis. In fact coherent states form an overcomplete basis

⁸In optics, one talks about the **eikonal** approximation which is the first order WKB approximation.

⁹Electrical engineers call it the **impulse response function** It is also called the **kernel** or **green function**

Superpose solutions: ¹⁰

$$\underbrace{\psi(x'', t'')}_{\text{evolved wavefunction}} = \int dx' K(x'', t''; x', t') \underbrace{\psi(x', t')}_{\text{initial condition}}$$

For example the propagator for the free schrodinger equation is:

$$K(x'', t''; x', t') = \sqrt{\frac{m}{2\pi\hbar i(t'' - t')}} \exp\left(\frac{im(x'' - x')^2}{2\hbar(t'' - t')}\right)$$

As you see the wavepacket of a free particle just spreads into a gaussian with variance $\propto t$. The propagator for the simple harmonic oscillator is:

$$K(x'', t''; x', t') = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega(t'' - t'))}} \exp\left(\frac{im\omega}{2\hbar i \sin(t'' - t')} \times [2(x'' + x')^2 \cos(\omega t) - 2x'x'']\right)$$

One can solve these propagators by evolving a dirac delta function *or* by evaluating the transition amplitude using the path integral. The path integral for these simples systems is just a (*very big*) gaussian integral.

- Classical electromagnetism is an example of a **gauge theory**: it exhibits **gauge invariance**, which is that the physics is unchanged by a gauge transformation ¹¹:

$$H = \frac{1}{2m}\left(p - \frac{qA}{c}\right)^2 + q\phi$$

$$A \rightarrow A + \nabla\lambda, \phi \rightarrow \phi - \frac{1}{c}\partial_t\lambda, H \rightarrow H$$

- Quantum mechanically, the wavefunction picks up a phase factor under gauge transformation. $\psi \rightarrow e^{\frac{i\lambda}{\hbar c}}\psi$. For a pure spacial gauge transformation, $\lambda(x) \propto \int \mathbf{A} \cdot d\mathbf{x}$
- When there is a magnetic field, $\nabla \times \mathbf{A}$ is not 0. This implies that the phase factor acquired by the wavefunction depends on the path taken by the particle, *even when the particle does not cross through a region with the magnetic field*. This is the **Aharonov Bohm** (AB) effect ¹²
- The existence of a single magnetic monopole of charge value e_M and the requirement the wavefunction be single valued implies the quantization of charge:

$$\frac{2ee_M}{\hbar c} \in \mathbb{Z}$$

This was realized by Paul Dirac.

§2.2 QA and comments

Question 2.1: What is the intuition behind the propagator for the free schrodinger equation?

The schrodinger equation is the same as the equation for diffusion in imaginary time.

$$i\hbar \frac{\partial}{\partial t} \psi = - \underbrace{\#}_{\text{some constant}} \nabla^2 \psi$$

$$t \rightarrow it : \quad \underbrace{-\hbar \frac{\partial}{\partial t} \psi = -(\#) \nabla^2 \psi}_{\text{diffusion eqn with diffusion rate } \propto \hbar}$$

¹⁰This is also known as a convolution

¹¹One perspective on gauge invariance is that it is a constrained system (since not all dynamical variable is physical). Note that gauge invariance is not a symmetry like rotation in the sense a gauge transformation does not map physical states to each other. It is a "do-nothing" operation.

¹²The AB effect variants appears in many other areas of physics. Some examples include quantum-hall systems (Berry phase and curvature), spin 1/2 particle Berry phase, Wilson lines in QCD etc...

The diffusion kernel is a gaussian due to the central limit theorem ¹³. Note that $\int dx |K(x, t)|^2 = 1$ so the crazy normalization constant in from of the propagator is just to normalize the wavefunction. The interesting physics is all contained in the exponential:

$$K(x, t, x' = 0, t' = 0) = \underbrace{\sqrt{\frac{m}{2\pi\hbar it}}}_{\text{normalization}} \underbrace{\exp\left[\frac{imx^2}{2\hbar t}\right]}_{\text{gaussian}}$$

What is the rate of diffusion? Note that as you take the limit of $\hbar \rightarrow 0$, the variance $\frac{\hbar t}{im}$ goes to 0. This implies there is no spreading of the wavepacket when quantum mechanics is "turned off". The spreading is a fundamental quantum mechanical effect due to uncertainty: since you localized the wavefunction by imposing a $\delta(x, t = 0)$ initial condition, the particle's momentum is completely uncertain and causes the spreading.

Question 2.2: *What is the intuition behind the path integral?*

The path integral solution fundamentally comes from the property that quantum evolution is **markovian** in nature. This means that the evolution has a composition rule that "don't care" about anything else other than the current state of affairs:

$$\mathcal{U}(t, 0) = \mathcal{U}(t, t_1)\mathcal{U}(t_1, 0)$$

You can repeat this ad infinitum and add complete set of states:

$$\begin{aligned} \mathcal{U}(t, 0) &= \mathcal{U}(t, t_n)\mathcal{U}(t_n, t_{n-1})\dots\mathcal{U}(t_1, 0) \\ &= \int dx_1 \int dx_2 \dots \int dx_{n-1} \mathcal{U}(t, t_n) |x_{n-1}\rangle \langle x_{n-1}| \mathcal{U}(t_n, t_{n-1}) |x_{n-2}\rangle \langle x_{n-2}| \dots |x_1\rangle \langle x_1| \mathcal{U}(t_1, 0) \end{aligned}$$

What you have integrated over is over all possible set of interpolating points between $x(t = 0) \rightarrow x(t)$ which which means you have summed over all "paths":

$$\int dx_1 \int dx_2 \dots \int dx_{n-1} = \sum_{\text{paths}} \equiv \int \mathcal{D}x$$

For more discussion of this topic, Zinn Justin's book "Path Integrals and Quantum Mechanics" is a good read.

Question 2.3: *What is the link between classical and quantum mechanics?*

I think there are 2 ways to see it. One direct way is through heisenberg's equations of motions:

$$\frac{d}{dt}\mathcal{O} = \frac{1}{i\hbar}[H, \mathcal{O}]$$

For example for the momentum and position operator, we have:

$$\begin{aligned} \frac{d}{dt}\hat{x} &= \frac{\hat{p}}{m} \\ \frac{d}{dt}\hat{p} &= \frac{1}{i\hbar}[H, \hat{p}] = -V'(\hat{x}) \end{aligned}$$

Note the similarity to the classical equation $F = ma = \frac{dp}{dt} = -V'(x)$ and $\frac{p}{m} = \dot{x}$.

If you sandwich any operator with a state you have:

$$\frac{d}{dt}\langle \hat{x} \rangle = \langle \frac{\hat{p}}{m} \rangle$$

What this means is that *on average*, the quantum values will match the classical values. This is just a restatement of **Ehrenfest's theorem** (see Griffiths).

¹³Diffusion processes for example brownian motion can be seen as a random walk with roughly IID steps. In the limit of large number of steps, the central limit theorem states the limiting distribution is gaussian

The other way to see it is by evaluating the semiclassical expansion of the path integral. This is a very useful trick in more advanced applications since very often that's the only thing we can do! This approximation is called **saddle-point integration**¹⁴. Suppose we have a function $f(x)$ which has a minimum at $x = x_0$. The saddle point approximation says in the limit $\hbar \rightarrow 0$:

$$\int dx e^{-\frac{1}{\hbar} f(x)} \approx \int dx e^{-\frac{1}{\hbar} f(x_0) + \frac{1}{2} \frac{1}{\hbar} f''(x_0)(x-x_0)^2 + \dots} \approx_{\hbar \rightarrow 0} e^{-\frac{1}{\hbar} f(x_0)} \sqrt{\frac{2\pi}{f''}}$$

Similarly, the path integral admits a saddle point approximation, except now expanded around the solution $x(t)$ which minimizes the **action** S .

$$S \equiv \int dt \mathcal{L}$$

$$\int \mathcal{D}x e^{-\frac{i}{\hbar} S} \approx_{\hbar \rightarrow 0} e^{-\frac{i}{\hbar} S_{cl}} \sqrt{\frac{2\pi}{\det(H)}} = \exp \left(-\frac{i}{\hbar} \left[\underbrace{S_{cl}}_{\text{classical action}} - \underbrace{\frac{\hbar}{2} \text{Tr} \ln(H)}_{\text{quantum correction} \propto \hbar} + \text{stuff that matters less} \right] \right)$$

$$H_{x(t_i), x(t_j)} \equiv \frac{\delta^2}{\delta x(t_i) \delta x(t_j)} S[x(t)]$$

Here is the **Hessian** of the action functional, and is the analog of f'' above. Solving $F = ma$ involves minimizing the action and therefore the dominant contribution to the path integral is the classical solution.

Path integrals are pretty well discussed in Feynman's book (pretty cheap on Dover) or Zinn Justin's book.

¹⁴The reason behind the name complex analysis. One deforms the integration contour in the complex plane around a "saddle" of an analytical function