(Non-relativistic) Quantum Mechanics

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Nov 2021

Here is a collected notes on physics readings.

Contents

1 Kinematics 2

2 Dynamics 3

§1 Kinematics

§2 Dynamics

- 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]

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

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

- 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 *linear* [3].

- The solution to the schrodinger equation is [4]:

$$\mathcal{U}(t,t_0) = \underbrace{\mathrm{T}}_{\equiv\text{time ordered}} \quad \exp\left(-\frac{i}{\hbar}\int_0^t dt'\hat{H}(t')\right)$$

$$\equiv \mathbb{I} - \frac{i}{\hbar}\int_0^t \hat{H}(t')dt' - \left(\frac{i}{\hbar}\right)^2\int_{t_1}^t dt'\int_0^{t_1} dt''\hat{H}(t')\hat{H}(t'') + \ldots$$

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

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

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

$$\hat{H}|n\rangle \equiv E_n|n\rangle$$

$$\mathcal{U}(t) = \sum_n e^{-i\frac{E_n t}{\hbar}}|n\rangle\langle n|$$

$$|\psi(t)\rangle = \sum_n e^{-i\frac{E_n t}{\hbar}}|n\rangle\langle n|\psi(0)\rangle$$

  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.

[1] Unitary 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

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

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

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

[5] Many 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-Haussdorf (BCH)** lemma can be used to transform operators[6]:

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

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

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

- 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 annahilation** operators:

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

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

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

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

  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 localled 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 evalute the path integral. 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:

$$K(x'', x', t'', t') \equiv \langle x'', t''|x', t'\rangle$$

[6] A common notation is to write $e^A B e^{-A} \equiv \exp_{\mathrm{Ad}A} B$. 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 a orthogonal basis. In fact coherent states form an overcomplete basis

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

[9] Electrical engineers call it the **impulse response function**. The superposition integral is call **convolution**

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

For example the propagator for the free schrodinger equation is:

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

The propagator for the simple harmonic oscillator is:

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

- Classical electromagnetism is an example of a **gauge theory**: it exhibits **gauge invariance**, which is that the physics is unchanged by a gauge transformation [10]:

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

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

- Quantum mechanically, the wavefunction picks up a phase factor under gauge transformation. $\psi \to e^{\frac{i\lambda}{\hbar c}}\psi$. For a pure spacial gauge transformation, $\lambda(x) \propto \int \mathbf{A} \cdot \mathbf{dx}$

- 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 [11]

- 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.

[10] One 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.

[11] The 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...