Notes

Quantum Mechanics

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Contents

PART

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Caprice

1 Fall 2018

This section is based on my Quantum mechanics course in Fall 2018. The textbook we use is Sakurai's *Modern Quantum Mechanics*.

1.1 Derivation of (2.1.33)

Use iteration to prove it

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) &= H(t)\mathcal{U}(t,t_0)\\
\mathcal{U}(t,t_0) &= \mathbb{I} + \int_{t_0}^{t} dt_1 \frac{H(t_1)}{i\hbar}\mathcal{U}(t_1,t_0)\\
&= \mathbb{I} + \int_{t_0}^{t} dt_1 \frac{H(t_1)}{i\hbar}\left(\mathbb{I} + \int_{t_0}^{t_1} dt_2 \frac{H(t_2)}{i\hbar}\mathcal{U}(t_2,t_0)\right)\\
&\vdots\\
&= \mathbb{I} + \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1)H(t_2)\ldots H(t_n)
\end{aligned}$$

1.2 Postulate of quantum mechanics: inner product

The inner product postulate of quantum mechanics

$$\langle\alpha|\alpha\rangle \geq 0, \tag{1.1}$$

comes from the probability interpretation of quantum mechanics.

1.3 Probability postulate

The probability postulate can not be proved right nor wrong. So how can we use probability theory to study the world?

1.4 (1.4.46) and (1.4.47)

Which is larger? (1.4.47) should be larger, because there's more terms in the summation.

1.5 Translation Operator

Suppose a translation operator is given by

$$\hat{\mathscr{T}}(\mathrm{d}\mathbf{x}') = 1 - i\hat{\mathbf{K}}\cdot\mathrm{d}\mathbf{x}', \tag{1.2}$$

where $\hat{\mathbf{K}} = \hat{K}_j$, $j = 1,2,3$, is a vector with each component as Hermitian operator, $\mathrm{d}\mathbf{x}' = \mathrm{d}x_i'$, $i = 1,2,3$, is an infinitesimal displacement vector, which is just an array of numbers instead of operators.

$$\begin{aligned}
[\hat{\mathbf{x}}, \hat{\mathscr{T}}(d\mathbf{x}')]_i &= -i(\hat{\mathbf{x}}\mathbf{K}\cdot \mathrm{d}\mathbf{x}' - \mathbf{K}\cdot d\mathbf{x}'\hat{\mathbf{x}})_i \\
&= -i(\hat{x}_i\hat{K}_j\,\mathrm{d}x'_j - \hat{K}_j dx'_j\hat{x}_i) \\
&= -i([\hat{x}_i, \hat{K}_j])\,\mathrm{d}x'_j,
\end{aligned}$$

Also we know that

$$\begin{aligned}
[\hat{\mathbf{x}}, \hat{\mathscr{T}}(d\mathbf{x}')]_i &= \mathrm{d}x'_i \\
&= \mathrm{d}x'_j\delta_{ij},
\end{aligned}$$

Thus we have the commutation relation between $\hat{x}_i$ and $\hat{K}_j$

$$[\hat{x}_i, \hat{K}_j] = i\delta_{ij}. \tag{1.3}$$

1.6 Complete set of compatible operators

If we are given a CSCO, we can choose a basis for the space of states made of common eigenvectors of the corresponding operators. We can uniquely identify each eigenvector by the set of eigenvalues it corresponds to.

Why?

1.7 Typo a line above (1.4.57)

The value of λ is actually

$$\lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}. \tag{1.4}$$

1.8 Galilean Invariance in Schrodinger equation

Consider a Galileo transformation:

$$\begin{aligned}
x &= x' + vt', \\
t &= t',
\end{aligned}$$

then

$$f(x', t') \to f(x - vt, t), \tag{1.5}$$

If we do the partial derivatives, then we will find

$$\frac{\partial f}{\partial x'} = \frac{\partial f}{\partial x}, \tag{1.6}$$

$$\frac{\partial f}{\partial t'} = \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial t}, \tag{1.7}$$

The reason that (1.7) has a plus $v\partial_x f$ term is that when we do partial derivative $\partial_{t'}$, what we really want to do is to do time derivative only on the second argument in $f(x - vt, t)$, without touching the t in the first argument. However, if we simply do $\partial_t f$ what we will get is actually $\partial_{t'} f - v\partial_x f$

$$\partial_t f(x - vt, t) = \partial_{t'} f(x - vt, t') - v\partial_x f(x - vt, t),$$

or

$$\partial_{t'} f(x', t') = \partial_t f(x - vt, t) + v\partial_x f(x - vt, t). \tag{1.8}$$

Thus we have

$$\partial_{x'} = \partial_x, \tag{1.9}$$
$$\partial_{t'} = \partial_t + v\partial_x. \tag{1.10}$$

1.9 Residue Theorem and A Line Integral

We want to evaluate this integral

$$\int_0^\infty \frac{\ln x}{x^2+a^2}dx, \tag{1.11}$$

where $a > 0$. To do it, we loop around the entire complex plane in the following way:

see the picture.

Therefore the contour integral can be written as

$$\begin{aligned}
\int_0^\infty \frac{\ln x}{x^2+a^2}dx &= \int_\delta^R \frac{\ln x}{x^2+a^2}dx + \int_{C_R} \frac{\ln z}{z^2+a^2}dz + \int_R^\delta \frac{\ln x + 2\pi i}{x^2+a^2}dx + \int_{C_\delta} \frac{\ln z}{z^2+a^2}dz \\
&= 2\pi i \sum_{\mathbb{C}} \operatorname{Res}\left(\frac{\ln z}{z^2+a^2}\right) \\
&= 2\pi i \left(\frac{\ln a + i\pi/2}{2ia} + \frac{\ln a + i3\pi/2}{-2ia}\right) \\
&= -i\frac{\pi^2}{a}.
\end{aligned}$$

Since $\lim_{z\to 0} z\ln z = 0$ and $\lim_{z\to\infty} \ln z/z = 0$, we eliminate two circle integrals

$$\int_{C_\delta} \frac{\ln z}{z^2+a^2}dz = 0,$$
$$\int_{C_R} \frac{\ln z}{z^2+a^2}dz = 0,$$

Therefore, after taking limit $R\to\infty$ and $\delta\to 0$, we obtain

$$\int_0^\infty \frac{\ln x}{x^2+a^2}dx - \int_0^\infty \frac{\ln x + 2\pi i}{x^2+a^2}dx = -i\frac{\pi^2}{a}. \tag{1.12}$$

Although the integrals along both the banks of the branch cut are related to the integral we want to compute, but they cancel out each other and leave an integral which is not the one we want

$$\int_0^\infty \frac{1}{x^2+a^2} = \frac{\pi}{2a}. \tag{1.13}$$

On the other hand, this indicates us that if we want to compute $\int_0^\infty f(x)\ln x dx$, we should consider the complex integral $\oint_C f(z)\ln^2 z dz$, because in this case function $\ln^2 z$ on the two banks of branch cut partially cancel out, and leave the $\ln x$ term which is what we want.

$$\begin{aligned}
\int_0^\infty \frac{\ln^2 x}{x^2+a^2}dx - \int_0^\infty \frac{(\ln x + 2\pi i)^2}{x^2+a^2}dx &= 2\pi i \sum_{\mathbb{C}} \operatorname{Res}\left(\frac{(\ln z)^2}{z^2+a^2}\right) \\
&= 2\pi i \left(\frac{(\ln a + i\pi/2)^2}{2ia} + \frac{(\ln a + i3\pi/2)^2}{-2ia}\right) \\
&= -i\frac{2\pi^2 \ln a}{a} + \frac{2\pi^3}{a}.
\end{aligned}$$

Thus

$$-4\pi i\int_0^\infty \frac{\ln x}{x^2+a^2}dx + 4\pi^2\int_0^\infty \frac{1}{x^2+a^2}dx = -i\frac{2\pi^2\ln a}{a} + \frac{2\pi^3}{a}. \tag{1.14}$$

Therefore, we compute the integral

$$\int_0^\infty \frac{\ln x}{x^2+a^2}dx = \frac{\pi}{2a}\ln a. \tag{1.15}$$

1.10 Order $\ln x$ and $-1/x$ at $x=0$

Consider the domain $x \in (0,1)$, then we want to compare $\ln x$ and $-1/x$

$$r(x) = \frac{\ln x}{-1/x} = \frac{|\ln x|}{|1/x|} = -x\ln x, \tag{1.16}$$

First we notice that $r(x) = -x\ln x > 0$ if $x \in (0,1)$. Second, we do the derivative of this ratio and get

$$\frac{dr(x)}{dx} = -(\ln x + 1), \tag{1.17}$$

where $r'(x) > 0$ if $x < 1/e$, $r'(x) < 0$ if $x > 1/e$, $r'(x) = 0$ if $x = 1/e$, so $r(x)$ takes maximum at $x = 1/e$, and $r(1/e) = 1/e$,

$$0 < r(x) < 1/e < 1. \tag{1.18}$$

Therefore

$$|\ln x| < |-1/x|, \quad x \in (0,1), \tag{1.19}$$

or equivalently

$$\ln x > -1/x, \quad x \in (0,1). \tag{1.20}$$

1.11 Saddle point approximation

Suppose we want to evaluate the following integral

$$I = \int_{-\infty}^{\infty} dx \mathrm{e}^{-f(x)} \tag{1.21}$$

where

$$\lim_{x\to\pm\infty} f(x) = \infty \tag{1.22}$$

Since the negative exponential function vanished very quickly when $f(x)$ becomes large, we only need to look at the contribution when $f(x)$ is at its minima. We can expand $f(x)$ around its minima x_0

$$f(x) = f(x_0) + \frac{1}{2}f''(x_0)(x-x_0)^2 + \dots \tag{1.23}$$

Then the integral can be written as

$$\begin{aligned} I &\approx \int_{-\infty}^{\infty} dx \exp\left[-f(x_0) - \frac{1}{2}f''(x_0)(x-x_0)^2)\right] \\ &= \mathrm{e}^{-f(x_0)}\int_{-\infty}^{\infty} dx \exp\left[-\frac{1}{2}f''(x_0)(x-x_0)^2)\right] \\ &= \mathrm{e}^{-f(x_0)}\sqrt{\frac{2\pi}{f''(x_0)}} \end{aligned}$$

If $f(x)$ has several local minima $\{x_i\}$, we should sum over all the contribution from the minima

$$I \approx \sum_i \mathrm{e}^{-f(x_i)} \sqrt{\frac{2\pi}{f''(x_i)}} \tag{1.24}$$

1.12 Qubit

All qubit states ω may be represented as 2×2 matrices

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & 1 - x_3 \end{pmatrix}, \quad \underline{x} \in \mathbb{R}^3 \tag{1.25}$$

$$\rho \geq 0, \quad \mathrm{tr}(\rho) = 1 \tag{1.26}$$

Example. Show $\rho \geq 0 \Leftrightarrow |\underline{x}| \leq 1$. Thus $\underline{x} = (x_1, x_2, x_3)$ is in ball of radius 1.

$$\rho = \frac{1}{2}(\mathbb{I} + x_1\sigma_x + x_2\sigma_y + x_3\sigma_z) \tag{1.27}$$

Proof. the eigenvalues of ρ is $\frac{1}{2}(1 \pm |\underline{x}|)$. For $\rho \geq 0$, $\exists X \in \mathbb{C}^{2\times 2}$, such that $\rho = X^H X$. Equivalently speaking, the eigenvalues of ρ are all greater than or equal to 0. Therefore $|\underline{x}| \leq 1$. □

For pure states of a qubit, the possible vector $\underline{x}$ is in a sphere of radius 1, which is called the Bloch sphere. But unfortunately the idea of Bloch sphere in 2D quantum system cannot be generalized to higher dimension.

1.13 The improved Bohr-Sommerfeld quantization formula

Theorem 1.1. From the boundary condition (or connection condition) of WKB approximation at the classical turning points, we are able to write down the semiclassical quantization formula as follows

$$\oint p(x)\,\mathrm{d}x = 2\pi\hbar(n + \mu/4) \quad \text{with} \quad \mu = N_{\text{soft}} + 2N_{\text{hard}} \tag{1.28}$$

where $n = 0, 1, 2, \ldots$, and μ is called *Maslov index* and counts the number of classical turning points with smooth potential (soft wall) plus twice the number of classical turning points with Dirichlet boundary conditions (hard wall).

1.14 Landau level for a electron in unifrom magnetic field

A electron is moving in the presence of a uniform magnetic field in the z-direction ($\mathbf{B} = B\hat{z}$). Define the kinematical (or mechanical) momentum

$$\mathbf{\Pi} = m\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{p} - \frac{e\mathbf{A}}{c} \tag{1.29}$$

We can compute the commutator between componets of kinematical momentum

$$\begin{aligned}
[\Pi_i, \Pi_j] &= [p_i - eA_i(x)/c, p_j - eA_j(x)/c] \\
&= [p_i, p_j] - \frac{e}{c}\{[A_i(x), p_j] + [p_i, A_j(x)]\} + \frac{e^2}{c^2}[A_i(x), A_j(x)] \\
&= \frac{i\hbar e}{c}\left[\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_i}\right] \\
&= \frac{i\hbar e}{c}\epsilon_{ijk}B_k
\end{aligned}$$

1.15 Order of even permutation group (alternating groyp)

The subset of the permutation group S_n formed by even permutations is a group, called the alternating group A_n. We can check that it satisfies the definition of a group

- The identity is the do-nothing permutation $\sigma = ()$, and its determinant is 1 and $\mathrm{sign}(()) = 1$, that is $()$ is even.

- The composition of two even permutations is even, thus closure is satisfied.

- The inverse of an even permutation must be even. To show this, we know

$$P_\sigma^\top P_\sigma = I, \tag{1.30}$$

so $\det\left(P_\sigma^\top\right) = \det(P_\sigma)$ implies $\det\left(P_\sigma^\top\right) = 1$ if $\det(P_\sigma) = 1$.

The size of A_n is $\frac{1}{2}n!$, since for every even permutation, one can uniquely associate an odd one by exchanging the first two elements.

Proof. Say $A_n = a_i$, and a_i is the element of alternating group. E is the transposition that exchanges the first two elements, which means Ea_i is odd. Next we want to show that $Ea_i \neq Ea_j$ if $a_i \neq a_j$. Well, one can immediately prove this by saying that permutations are bijective, thus injective. Or we can do the following: Suppose $Ea_i = Ea_j$ for some $a_i \neq a_j$, then $EEa_i = EEa_j$, which implies $a_i = a_j$, because $E^2 = I$. Contradiction. □

1.16 Cross product

Actually, there does not exist a cross product vector in space with more than 3 dimensions. The fact that the cross product of 3 dimensions vector gives an object which also has 3 dimensions is just pure coincidence. However, we can always define the cross product tensor in any dimension n, such that the cross product of $\mathbf{a}$ and $\mathbf{b}$ is defined as

$$c_{ij} = a_i b_j - a_j b_i. \tag{1.31}$$

Therefore the cross product tensor is of rank 2 and it is antisymmetric. So the cross product tensor has $n(n-1)/2$ independent elements.

The cross product in 3 dimensions is actually a tensor of rank 2 with 3 independent coordinates. We can create a 3-vector in 3 dimensions to represent these 3 independent elements.

$$c_{ij} = \begin{pmatrix} 0 & c_3 & -c_2 \\ -c_3 & 0 & c_1 \\ c_2 & -c_1 & 0 \end{pmatrix} = \epsilon_{ijk} c_k, \tag{1.32}$$

where $\mathbf{c}$ is the cross product vector of $\mathbf{a}$ and $\mathbf{b}$ in 3 dimensions and defined as

$$c_i = (\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk} a_j b_k. \tag{1.33}$$

In addition to (1.32), we can also express the cross product vector $\mathbf{c}$ interms of the cross product tensor c_{ij}

$$c_i = \tfrac{1}{2}\epsilon_{ijk} c_{jk} \tag{1.34}$$

Using the definition (1.31) and (1.33), we can immediately show this.

$$
\begin{aligned}
\tfrac{1}{2}\epsilon_{ijk}c_{jk} &= \tfrac{1}{2}\epsilon_{ijk}(a_j b_k - a_k b_j) \\
&= \tfrac{1}{2}\epsilon_{ijk}a_j b_k - \tfrac{1}{2}\epsilon_{ijk}a_k b_j \\
&= \epsilon_{ijk}a_j b_k = c_i.
\end{aligned}
$$