量子化学作业 第四章 （2017-2018 学期）

1. Prove that, if a normalized function is expanded in terms of an orthonormal set of functions, the sum of the absolute squares of the expansion coefficients is unity.

2. Which of the following wave functions are normalized over the indicated two-dimensional intervals? Normalize those that aren't.

$$(a)\ e^{-(x^2+y^2)/2},\ 0 \le x < \infty, 0 \le y < \infty$$

$$(b)\ e^{-(x+y)/2},\ 0 \le x < \infty, 0 \le y < \infty$$

$$(c)\ (\frac{4}{ab})^{1/2} \sin(\frac{\pi x}{a}) \sin(\frac{\pi y}{b}),\ 0 \le x \le a, 0 \le y \le b$$

3. (a) Show that $\frac{d^2}{dx^2}$ and $\hat{T}_x$ are Hermitian.

(b) Show that $<T_x> = \frac{\hbar^2}{2m}\int\left|\frac{\partial\psi(x,y,z)}{\partial x}\right|^2 d\tau$, where $\psi(x,y,z)$ is the wave function of a 3-dimensional bounded system (which means the wave function vanishs at ∞).

4. Does the following operators meet the requirements for a quantum-mechanical operator that is to represent a physical quantity? (Consider that the wave function is well-behaved, which means that it vanishes at ∞)

$$(a)(\ \ )^{1/2} \qquad (b)\frac{d}{dx} \qquad (c)\frac{d^2}{dx^2} \qquad (d)i\frac{d}{dx}$$

5. Can the position and kinetic energy of an electron be measured simultaneously to arbitrary precision?

6. A theorem in quantum mechanics states that if two Hermitian operators $\hat{A}$ and $\hat{B}$ commute, they have a common complete set of eigenfunctions. We have proved it for nondegenerate cases in the textbook. Now prove it for degenerate cases.

7. For a 1-dimension particle-in-a-box system, where the length of the box is l, the state is represented by this function:

$$f(x) = \begin{cases} x, & 0 \le x \le \dfrac{l}{2} \\ l - x, & \dfrac{l}{2} < x \le l \end{cases}$$

Show the eigenfunction expansion of this function to the 4th degree, and calculate the probability that the particle is found in the ground state.

8. Generate an orthonormal set of polynomials $\{\phi_j(x), j = 1,2,3\}$ over the interval $-1 \le x \le 1$ starting with $f_0(x) = 1,\ f_1(x) = x,\ f_2(x) = x^2$.

9. What is the normalization constant for $\Psi(x,t) = \sum_{n=1}^{N} \psi_n(x) e^{-iE_n t/h}$ if the $\psi_n(x)$ are orthonormal?

10. We can define functions of operators through their Maclaurin series. For example, we define the operator $e^{\hat{S}}$ by

$$e^{\hat{S}} = \sum_{n=0}^{\infty} \frac{(\hat{S})^n}{n!}$$

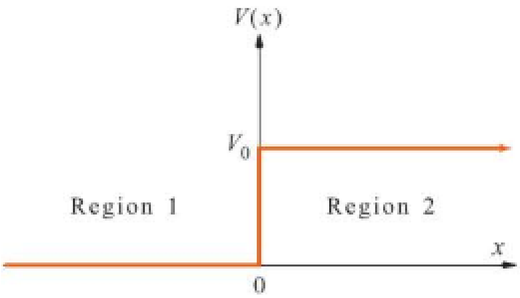
Under what conditions does the equality $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}}$ hold?

11. Give the quantum-mechanical operators for the following physical quantities

$$(a)\ p_y^3 \qquad (b)\ xp_y - yp_x \qquad (c)\ (xp_y)^2$$

12. Find the eigenfunctions and eigenvalues of $\int dx$

13. Consider a particle e moving in the potential energy:



whose mathematical form is

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

where V_0 is a constant. Show that if $E > V_0$, then the solutions to the Schrodinger equation in the two regions (1 and 2) are

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad x < 0 \quad (1)$$
$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad x > 0 \quad (2)$$

where

$$k_1 = (\frac{2mE}{\hbar^2})^{1/2} \quad \text{and} \quad k_2 = \left[\frac{2m(E - V_0)}{\hbar^2}\right]^{1/2} \qquad (3)$$

As we learned in Problem 3-35, e^{ikx} represents a particle traveling to the right and e^{-ikx} represents a particle traveling to the left. The physical problem we wish to set up is a particle of energy E traveling to the right and incident on a potential barrier of height V_0. If we wish to exclude the case of a particle traveling to the left in region 2, we set $D = 0$ in equation 2. The squares of the coefficients in equations 1 and 2 represent the probability that the particle is traveling in a certain direction in a given region. For example, $|A|^2$ is the probability that the particle is traveling with momentum $+\hbar k_1$ in the region $x < 0$. If we consider many particles, N_0, instead of just one, then we can interpret $|A|^2 N_0$ to be the number of particles with momentum $\hbar k_1$ in the region $x < 0$. The number of these particles that pass a given point per unit time is given by $v|A|^2 N_0$, where the velocity v is given by $\hbar k_1 / m$. Now apply the conditions that $\psi(x)$ and $d\psi / dx$ must be continuous at $x = 0$ to obtain

$$A + B = C$$

And

$$k_1(A - B) = k_2 C$$

Now define a quantity

$$r = \frac{\hbar k_1 |B|^2 N_0 / m}{\hbar k_1 |A|^2 N_0 / m} = \frac{|B|^2}{|A|^2}$$

And show that

$$r = (\frac{k_1 - k_2}{k_1 + k_2})^2$$

Similarly, define

$$t = \frac{\hbar k_2 |C|^2 N_0 / m}{\hbar k_1 |A|^2 N_0 / m} = \frac{k_2 |C|^2}{k_1 |A|^2}$$

$$t = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

and show that

The symbols r and t stand for reflection coefficient and transmission coefficient, respectively. Give a physical interpretation of these designations. Show that $r + t = 1$. Would you have expected the particle to have been reflected even though its energy, E, is greater than the barrier height, V_0? Show that $r \to 0$ and $t \to 1$ as $V_0 \to 0$.

14. Show that $r = 1$ for the system described in Problem 13 but with $E < V_0$. Discuss the physical interpretation of this result.

Mathematical Chapter:

1. Write out the expansion of $(1+x)^{1/2}$ through the quadratic term.

2. Numbers whose decimal formula are recurring decimals such as 0.272727... are rational numbers, meaning that they can be expressed as the ratio of two numbers (in other words, as a fraction). Show that 0.272727 ... = 27/99.

3. Series of the form

$$S(x) = \sum_{n=0}^{\infty} n x^n$$

occur frequently in physical problems. To find a closed expression for S(x), we start with

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n$$

Notice now that $S(x)$ can be expressed as

$$x\frac{d}{dx}\sum_{n=0}^{\infty}x^n = \sum_{n=0}^{\infty}nx^n$$

and show that $S(x) = x/(1-x)^2$

4. Using the method introduced in the previous problem, show that

$$\sum_{n=0}^{\infty}n^2x^n = \frac{x(1+x)}{(1-x)^3}$$

5. Evaluate the limit of

$$f(x) = \frac{e^{-x}\sin^2 x}{x^2}$$

as $x \to 0$