Problem 1. The Time Energy Uncertainty Principal

It is well known that the uncertainty principal in he form of $\Delta E \Delta t \sim h$ has a very different meaning compared to $\Delta p \Delta x \sim h$ since time is not an operator in quantum mechanics. Previously we have introduced one possible interpretation by referring to Δt to the "*amount of time it takes for the expectation value of an observable Q to change by one standard deviation*". Here we would like to explore another interpretation of the principle by referring to the first order time-dependent perturbation results. This approach was first proposed by Landau. We shall see that the Δt according to this will be interpreted as "*the time it takes to measure a transition energy involving an energy uncertainty of* ΔE".

Part (a)

Let is refer to the case of harmonic time perturbation (similar arguments can be applied to the case of constant perturbation). For the case of stimulated emission, one can show from Eq. 25.2, Lecture notes, that the first order transition probability can be expressed as:

$$\left| c_f^{(1)}(t) \right|^2 = 4 \left| H_{fi}^{r_0} \right|^2 \left(\frac{t}{2\hbar} \right)^2 \frac{\sin^2 x}{x^2} \tag{1}$$

where

$$x = \left(\frac{E_f - E_i + \hbar\omega}{2\hbar} \right) t \tag{2}$$

Give a sketch of $\left| c_f^{(1)}(t) \right|^2$ as a function of x.

Solution

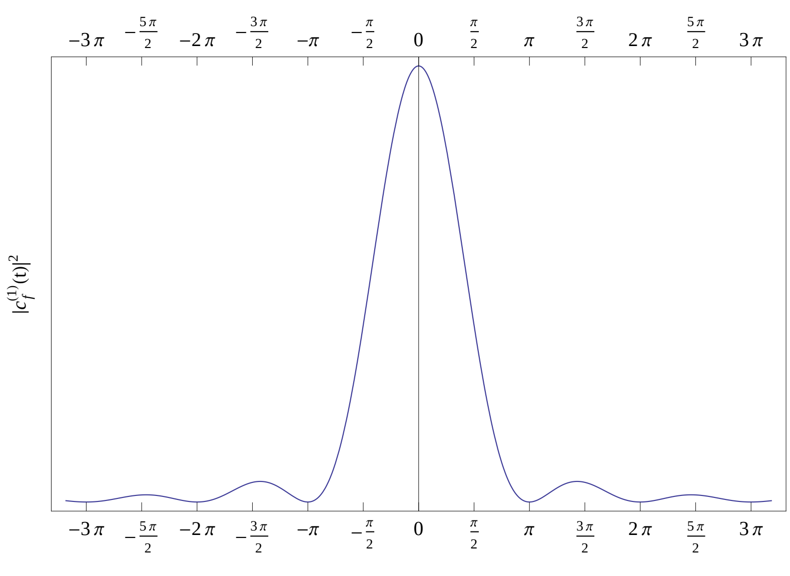

Figure 1: Sketch of $\left| c_f^{(1)}(t) \right|^2$ as a function of x

Part (b)

Let us consider a system (e.g. an atom) and we are measuring the energy states E_m and $E_n (< E_m)$. We do this by by using a macroscopic apparatus to induce the atom to make a transition from E_m to E_n and measure the emitted photon energy ($\hbar\omega$) by means of the same apparatus. The value of the measured photon energy can in principle be assumed knowable exactly. Try to use the result in a. to introduce a relevant time duration Δt and hence formulate the time-energy uncertainty principal in this context.

Solution

We see from the plot in part (a) that there is a central peak around $x = 0$ and it rapidly drops off when $x < \pi$ indicating that there is a negligible transition probability beyond that point. Introducing Δt, the time it takes for the transition form energy state E_m to E_n to occur, to Equation (2) we arrive at the condition for stimulated emission.

$$x = \left(\frac{E_f - E_i + \hbar\omega}{2\hbar}\right)\Delta t < \pi \tag{3}$$

Remembering that $\Delta E = E_f - E_i$ is the energy difference between the two energy levels, and that $\Delta E = \hbar\omega$ is the energy emitted by the photon during stimulation, we can simplify this further:

$$\left(\frac{2\Delta E}{2\hbar}\right)\Delta t < \pi \tag{4}$$

$$\Delta t\Delta E < \hbar\pi \tag{5}$$

$$\Delta t\Delta E \approx h \tag{6}$$

Part (c)

Can you generalize the above to introduce the concepts of "line width" and "lifetime" for an excited state of an atomic system and establish a relationship between them?

Solution

We can define a transition probability per unit time, W by summing the individual transmission probabilities (1) and dividing it by time.

$$W = \frac{1}{t}\sum_f \left|c_f^{(1)}(t)\right|^2 \tag{7}$$

From here, we can define a "lifetime" as

$$\tau = \frac{1}{W} \tag{8}$$

which is referred to as the "Golden Rule".

From the time uncertainty principal (6), we can define a “line width” of the excited state m as

$$\Gamma_m \equiv \Delta E_m = \frac{h}{\tau} \tag{9}$$

by substituting $\Delta E \to \Delta E_m$ and $t \to \tau$.

Problem 2. The Thomas-Reiche-Kuhn (TRK) sum rule

A. Approach 1: The dipole oscillator strength f_{mn} is a very useful quantity in calculating intensities of spectral lines in atomic physics. In terms of the dipole transition matrix elements, the oscillator strength is defined as:

$$f_{mn} = f^x_{mn} + f^y_{mn} + f^z_{mn} = \frac{2m\omega_{mn}}{\hbar}\left[|x_{mn}|^2 + |y_{mn}|^2 + |z_{mn}|^2\right] \tag{10}$$

where

$$\hbar\omega_{mn} = E_m - E_n \tag{11}$$

$$x_{mn} = \int u^*_m x u_n d\tau \text{...etc.} \tag{12}$$

Part (a)

Show that f^*_{mn} can be written in a slightly different form as:

$$f^*_{mn} = \frac{m}{\hbar}(\omega_{mn}x_{mn}x_{nm} - \omega_{nm}x_{nm}x_{mn}) \tag{13}$$

Solution

Lets first by establishing some useful relationships. Looking at x_{mn} and x_{nm}:

$$x^*_{mn} = \int u^*_n x u_m d\tau \tag{14}$$

$$x_{nm} = \int u^*_n x u_m d\tau \tag{15}$$

$$x_{nm} = x^*_{mn} \tag{16}$$

we also see the relationship between ω_{mn} and ω_{nm}:

$$\hbar\omega_{mn} = E_m - E_n \tag{17}$$

$$\hbar\omega_{nm} = E_n - E_m \tag{18}$$

$$-\hbar\omega_{mn} = E_n - E_m \tag{19}$$

$$-\hbar\omega_{mn} = \hbar\omega_{nm} \tag{20}$$

$$-\omega_{mn} = \omega_{nm} \tag{21}$$

such that

$$2\hbar\omega_{mn} = 2(E_m - E_n) \tag{22}$$

$$= E_m - E_n - E_n + E_m \tag{23}$$

$$= \hbar\omega_{mn} - \hbar\omega_{nm} \tag{24}$$

$$2\omega_{mn} = \omega_{mn} - \omega_{nm} \tag{25}$$

Now we can start plugging in Equation (21) and Equation (25) to f^x_{mn}.

$$f^x_{mn} = \frac{2m\omega_{mn}}{\hbar} |x_{mn}|^2 \tag{26}$$

$$= \frac{m}{\hbar}(\omega_{mn} - \omega_{nm}) |x_{mn}|^2 \tag{27}$$

$$= \frac{m}{\hbar}(\omega_{mn} - \omega_{nm}) x^*_{mn} x_{mn} \tag{28}$$

$$= \frac{m}{\hbar}(\omega_{mn} - \omega_{nm}) x_{mn} x_{nm} \tag{29}$$

$$\boxed{f^x_{mn} = \frac{m}{\hbar}(\omega_{mn} x_{mn} x_{nm} - \omega_{nm} x_{mn} x_{nm})} \tag{30}$$

Part (b)

From the procedures shown in the Lecture Notes [Eq. (25.16)-(25.18)], show that

$$(p_x)_{mn} = im\omega_{mn}x_{mn} \tag{31}$$

where $(p_x)_{mn}$ is the transition matrix element for the x-component of the momentum and m is the mass of the electron.

Solution

From the notes (25.17), we know that

$$[x_i, H_0] = \frac{1}{2m}[x_i, p_i^2] = \frac{1}{2m}[x_i, p_i]p_i + \frac{1}{2m}p_i[x_i, p_i] = \frac{i\hbar}{m}p_i \tag{32}$$

where

$$[x_i, p_i] = i\hbar \tag{33}$$

from the quantum condition. In order to find $(p_x)_{mn}$ we need to operate on $\langle m|n\rangle$ with $[x, H_0]$ and solve for p_x to find the mn'th element of p_x.

$$\langle m| [x, H_0] |n\rangle = \frac{i\hbar}{m}(p_x)_{mn} \tag{34}$$

$$\langle m| xH_0 - H_0x |n\rangle = \tag{35}$$

$$(E_n - E_m) \langle m| x |n\rangle = \qquad \text{where } (E_n - E_m) = -\hbar\omega_{mn} \tag{36}$$

$$-\hbar\omega_{mn}x_{mn} = \qquad \text{and } \langle m| x |n\rangle = x_{mn} \tag{37}$$

$$-\frac{m}{i\hbar}\hbar\omega_{mn}x_{mn} = (p_x)_{mn} \tag{38}$$

$$\boxed{(p_x)_{mn} = im\omega_{mn}x_{mn}} \tag{39}$$

Part (c)

Hence, using (a) and (b), show that f^*_{mn} can be written as:

$$f^x_{mn} = \frac{i}{\hbar}\left(p_{nm}x_{mn} - x_{nm}p_{mn}\right) \tag{40}$$

Solution

Comparing Equation (30) and Equation (31), we see that it will be useful to write

$$\frac{(p_x)_{mn}}{im} = \omega_{mn}x_{nm} \qquad \frac{(p_x)_{nm}}{im} = \omega_{nm}x_{mn} \tag{41}$$

which can be substituted into Equation (30) directly.

$$f^x_{mn} = \frac{m}{\hbar}\left(\frac{(p_x)_{mn}}{im}x_{nm} - \frac{(p_x)_{nm}}{im}x_{mn}\right) \tag{42}$$

$$= \frac{1}{i\hbar}\left((p_x)_{mn}x_{nm} - (p_x)_{nm}x_{mn}\right) \tag{43}$$

$$\boxed{f^x_{mn} = \frac{i}{\hbar}((p_x)_{nm}x_{mn} - (p_x)_{mn}x_{nm})} \tag{44}$$

$$\tag{45}$$

Part (d)

Using the closure property of the wave functions in the following form:

$$\sum_m u_m^*(\vec{r})u_m(\vec{r'}) = \partial(\vec{r} - \vec{r'}) \tag{46}$$

(can you prove this?), derive the following TRK sum rule:

$$\sum_m f_{mn}^x = 1 \tag{47}$$

$$\sum_m f_{mn} = 3 \tag{48}$$

Solution

No Dirac notation allowed! Or at least any of the fancy shortcuts it prohibits. This is a messy operation so hang on tight. Since $\sum_m f_{mn}$ is simply the sum of $\sum_m f_{mn}^x$, $\sum_m f_{mn}^y$ and $\sum_m f_{mn}^z$ [1], all we need to do is find one and we have the others. Lets find $\sum_m f_{mn}^x$.

$$\sum_m f_{mn}^x = \sum_m \frac{i}{\hbar}((p_x)_{nm}x_{mn} - (p_x)_{mn}x_{nm}) \tag{49}$$

$$= \frac{i}{\hbar}(\sum_m (p_x)_{nm}x_{mn} - \sum_m (p_x)_{mn}x_{nm}) \tag{50}$$

We know from Equation (12) that

$$x_{mn} = \int u_m^* x u_n d\tau \qquad (p_x)_{mn} = \int u_m^* p_x u_n d\tau \tag{51}$$

$$x_{nm} = \int u_n^* x u_m d\tau \qquad (p_x)_{nm} = \int u_n^* p_x u_m d\tau \tag{52}$$

so that at this point Equation (50) is a matter of tedious algebra, notation and calculus trickery. It is at this point that I begin clamoring for Dirac notation, but its not allowed.

$$\sum_m f_{mn}^x = \frac{i}{\hbar}(\sum_m (p_x)_{nm}x_{mn} - \sum_m (p_x)_{mn}x_{nm}) \tag{53}$$

$$= \frac{i}{\hbar}\left(\sum_m \int u_n^*(\vec{r'})p_x u_m(\vec{r'})d\tau' \int u_m^*(\vec{r})x u_n(\vec{r})d\tau - \sum_m \int u_m^*(\vec{r'})p_x u_n(\vec{r'})d\tau' \int u_n^*(\vec{r})x u_m(\vec{r})d\tau\right) \tag{54}$$

$$= \frac{i}{\hbar}\left(\int\int \sum_m u_n^*(\vec{r'})p_x u_m(\vec{r'})u_m^*(\vec{r})x u_n(\vec{r})d\tau' d\tau - \int\int \sum_m u_m^*(\vec{r'})p_x u_n(\vec{r'})u_n^*(\vec{r})x u_m(\vec{r})d\tau' d\tau\right) \tag{55}$$

[1] See Equation (10)

Using the closure property see in Equation (46) and the fact $\delta x = \delta{-x}$ we see that our discrete summation reduced to Dirac delta functions.

$$\sum_m f^x_{mn} = \frac{i}{\hbar}\left(\int\int u^*_n(\vec{r'})p_x\delta(\vec{r}-\vec{r'})xu_n(\vec{r})d\tau' d\tau - \int\int u^*_n(\vec{r})x\delta(\vec{r}-\vec{r'})p_x u_n(\vec{r'})d\tau' d\tau\right) \tag{56}$$

Performing one of the integrals we see that $\vec{r'} = \vec{r}$ due to the delta functions, otherwise the matrix elements are of 0 value.

$$\sum_m f^x_{mn} = \frac{i}{\hbar}\left(\int u^*_n(\vec{r})p_x x u_n(\vec{r})d\tau - \int u^*_n(\vec{r})x p_x u_n(\vec{r})d\tau\right) \tag{57}$$

At this point the math is just screaming commutator rules, but we mush push on. Remembering that $p_x = (-i\hbar)\frac{d}{dx}$

$$\sum_m f^x_{mn} = \frac{i}{\hbar}\left(\int u^*_n(\vec{r})(-i\hbar)\frac{d}{dx}x u_n(\vec{r})d\tau - \int u^*_n(\vec{r})x(-i\hbar)\frac{d}{dx}u_n(\vec{r})d\tau\right) \tag{58}$$

$$= \left(\int u^*_n(\vec{r})\frac{d}{dx}x u_n(\vec{r})d\tau - \int u^*_n(\vec{r})x\frac{d}{dx}u_n(\vec{r})d\tau\right) \tag{59}$$

$$= \left(\int u^*_n(\vec{r})\frac{dx}{dx}u_n(\vec{r})d\tau + \int u^*_n(\vec{r})x\frac{du_n(\vec{r})}{dx}d\tau - \int u^*_n(\vec{r})x\frac{du_n(\vec{r})}{dx}d\tau\right) \tag{60}$$

$$= \left(\int u^*_n(\vec{r})\frac{dx}{dx}u_n(\vec{r})d\tau\right) \tag{61}$$

$$\boxed{\sum_m f^x_{mn} = 1} \tag{62}$$

using the closure property. Finally,

$$\sum_m f_{mn} = \sum_m f^x_{mn} + \sum_m f^y_{mn} + \sum_m f^z_{mn} \tag{63}$$

$$\boxed{\sum_m f_{mn} = 1+1+1 = 3} \tag{64}$$

I get it. Dirac notation is really nice sometimes, as a simple $\langle u_m|\,[x,p_x]\,|u_n\rangle = -i\hbar$ would really be nice about now.

B. Approach 2: Let us re-derive the above sum rule using Dirac notation. We shall see the beautiful result for closure obtained in this notation, i.e.: $\sum_k |k\rangle \langle k| = 1$ will lead to a much simpler proof of the above result. It is sufficient for us to just derive the result of the x-dipole transition matrix element here. Consider a non-relativistic atom with Hamiltonian:

$$H = \frac{\vec{p}^2}{2m} + V(r) \qquad \vec{r} = (x, y, z) \tag{65}$$

Part (e)

Use the quantum condition to derive the following result for the "double commutator":

$$[x, [x, H]] = -\frac{\hbar^2}{m} \tag{66}$$

Solution

Looking back to the notes (25.17) or Equation (32) we know

$$[x_i, H_0] = \frac{i\hbar}{m} p_i \tag{67}$$

Simply plugging this into Equation (66) and using the quantum condition we arrive at our goal:

$$\left[x, \frac{i\hbar}{m} p_i\right] = \frac{i\hbar}{m}[x, p_i] = \frac{i\hbar}{m} i\hbar \tag{68}$$

$$\boxed{[x, [x, H]] = -\frac{\hbar^2}{m}} \tag{69}$$

Part (f)

Hence derive the TRK sum rule in the form:

$$\sum_k (E_k - E_n) |x_{kn}|^2 = \frac{\hbar^2}{2m}, \text{ where } x_{kn} = \langle k| x |n\rangle \text{ and } H|n\rangle = E_n |n\rangle \tag{70}$$

Solution

Following the hint's give in Gasiorowicz we can write the quantum condition as:

$$\langle n| [p, x] |n\rangle = -i\hbar \tag{71}$$

$$\langle n| px - xp |n\rangle = -i\hbar \tag{72}$$

$$\langle n| px |n\rangle - \langle n| xp |n\rangle = -i\hbar \tag{73}$$

using closure

$$\sum_k \langle n| p |k\rangle \langle k| x |n\rangle - \sum_k \langle n| x |k\rangle \langle k| p |n\rangle = -i\hbar \tag{74}$$

Solving (67) for p, we can sub into (74)

$$[x_i, H_0] = \frac{i\hbar}{m} p_i \tag{75}$$

$$\frac{m}{i\hbar}[x_i, H_0] = p_i \tag{76}$$

so that

$$\frac{m}{i\hbar}\left(\sum_k \langle n| [x_i, H_0] |k\rangle \langle k| x |n\rangle - \sum_k \langle n| x |k\rangle \langle k| [x_i, H_0] |n\rangle\right) = -i\hbar \tag{77}$$

$$\frac{m}{i\hbar}\left(\sum_k (E_k - E_n) \langle n| x |k\rangle \langle k| x |n\rangle + \sum_k (E_k - E_n) \langle n| x |k\rangle \langle k| x |n\rangle\right) = -i\hbar \tag{78}$$

$$\frac{m}{i\hbar}\left(\sum_k (E_k - E_n) \langle k| x |n\rangle^* \langle k| x |n\rangle + \sum_k (E_k - E_n) \langle k| x |n\rangle^* \langle k| x |n\rangle\right) = -i\hbar \tag{79}$$

$$\frac{m}{i\hbar}\left(\sum_k (E_- E_n) \left|\langle k| x |n\rangle\right|^2 + \sum_k (E_k - E_n) \left|\langle k| x |n\rangle\right|^2\right) = -i\hbar \tag{80}$$

$$\frac{2m}{i\hbar}\sum_k (E_k - E_n) \left|\langle k| x |n\rangle\right|^2 = -i\hbar \tag{81}$$

$$\sum_k (E_k - E_n) \left|\langle k| x |n\rangle\right|^2 = \frac{\hbar^2}{2m} \tag{82}$$

$$\boxed{\sum_k (E_k - E_n) \left|x_{kn}\right|^2 = \frac{\hbar^2}{2m}} \tag{83}$$

Problem 3. The adiabatic Theorem

This theorem states that if the Hamiltonian of a system is changed very slowly from H_0 to H, then the system in a given eigenstate of H_0 will simply go over the corresponding eigenstate of H, without making any transitions. To illustrate this, let us a system being in the ground state u_0 of H_0 defined by : $H_0 u_0 = E_0^0 u_0$. Now let H_0 go over very slowly to $H = H_0 + V$, V being small, the theorem requires that the state of the system must go over from u_0 to the ground state w_0 of H, defined by $Hw_0 = E_0 w_0$. Let is prove this as follows:

Part (a)

Consider a time-dependent perturbation to $H_0 : H'(t) = f(t)V$ where $f(t)$ is a slowly varying function from 0 to 1 as shown. Using integration by parts, establish the following results for the integral:

$$\int_0^t f(t') e^{i\omega_{mn}t'} dt' = \int_0^t f(t') \frac{1}{i\omega_{mn}} \frac{d}{dt'} e^{i\omega_{mn}t'} dt' \approx \frac{1}{i\omega_{mn}} f(t) e^{i\omega_{mn}t} \tag{84}$$

Solution

We will use simple integration by parts:

$$\int f(x)g'(x)dx = f(x)g(x) - \int g(x)f'(x)dx \tag{85}$$

Selecting f and g to be:

$$f = f(t') \qquad g' = \frac{1}{i\omega_{mn}} \frac{d}{dt} e^{i\omega_{mn}t'} = e^{i\omega_{mn}t'} \tag{86}$$

$$f' = \frac{df(t')}{dt'} \qquad g = \frac{1}{i\omega_{mn}} e^{i\omega_{mn}t'} \tag{87}$$

we can perform the integral now

$$\int_0^t f(t') \frac{1}{i\omega_{mn}} \frac{d}{dt'} e^{i\omega_{mn}t'} dt' = f(t') \frac{1}{i\omega_{mn}} e^{i\omega_{mn}t'} \bigg|_0^t - \int_0^t \frac{1}{i\omega_{mn}} e^{i\omega_{mn}t'} \frac{df(t')}{dt'} dt' \tag{88}$$

We can drop the second term because our system is going through an adiabatic transition, meaning that that the time derivative of f is going to be nearly 0, so we are left with:

$$\boxed{\int_0^t f(t') \frac{1}{i\omega_{mn}} \frac{d}{dt'} e^{i\omega_{mn}t'} dt' \approx \frac{1}{i\omega_{mn}} f(t) e^{i\omega_{mn}t}} \tag{89}$$

Part (b)

Using first order time-dependent perturbation theory, show that the time-dependent wave function $\Psi(t)$ can be expressed as :

$$\Psi(t) = \sum_n c_n(t) e^{-i\omega_m t} u_n \tag{90}$$

$$\text{where } \omega_n = E_n^0/\hbar \tag{91}$$

and the coefficients $c_n(t)$ are given by

$$c_0 = 1 + \frac{1}{i\hbar} V_{00} \int_0^t f(t')dt' \tag{92}$$

and for $n \neq 0$,

$$c_n = \frac{1}{i\hbar} V_{n0} \int_0^t f(t') e^{i\omega_{n0}t'} dt' \tag{93}$$

$$\text{with } V_{n0} = \int u_n^* V u_0 d\tau \tag{94}$$

$$\text{and } \omega_{n0} = \frac{E_n^0 - E_0^0}{\hbar} \tag{95}$$

Solution

Lets find $\Psi(x)$ for a system made up of a single eigenfunction then generalize to the full set of eigenfunctions, following Griffiths 2nd edition page 371. If the system is in the n'th eigenstate we have

$$H\psi_n = E_n \psi_n \qquad\qquad \langle \psi_n | \psi_m \rangle = \delta_{nm} \tag{96}$$

At time $t = 0$ we perturb the system so that the total Hamiltonian is

$$H = H_0 + H'(t) \tag{97}$$

which when we generalize our perturbed two state system

$$\Psi(t) = c_a(t)\psi_a e^{-iE_a t/\hbar} + c_b(t)\psi_b e^{-iE_b t\hbar} \tag{98}$$

reads

$$\boxed{\Psi(t) = \sum c_n(t)\psi_n e^{-iE_n t\ \hbar}} \tag{99}$$

where

$$\boxed{c_n(t) \approx 1 - \frac{i}{\hbar} \int_0^t H'_{nn}(t')dt'} \tag{100}$$

$$\boxed{c_{m\neq n}(t) \approx \frac{-i}{\hbar} \int_0^t H'_{mn}(t') e^{i(E_m - E_n)t'/\hbar} dt'} \tag{101}$$

$$\Psi_n = \psi_n e^{-iE_n t/\hbar} \tag{102}$$

Part (c)

Using the results in a, show that for large t:

$$\Psi(t) \approx \left[\left(1 - i\frac{V_{00}A}{\hbar}\right)u_0 - \sum_{n\neq 0}\frac{V_{n0}}{E_n^0 - E_0^0}u_n\right]e^{-i\omega_0 t} \tag{103}$$

where

$$A = \int_0^t f(t')dt' \tag{104}$$

Solution

Using the results from (A) Equation (90)

$$\Psi(t) = \sum_n c_n(t)e^{-i\omega_n t}u_n \tag{105}$$

At this point we just start filling this out, separating out $n = 0$ and $n \neq 0$. Using Equations (92) - (95)

$$\Psi(t) \approx \left(1 - \frac{iV_{00}}{\hbar}\int_0^t f(t')dt'\right)e^{-i\omega_0 t}u_0 + \sum_{n\neq o}c_n(t)e^{-i\omega_n t}u_n \qquad \text{Using Eq. (104)} \tag{106}$$

$$\Psi(t) \approx \left(1 - \frac{iV_{00}}{\hbar}A\right)e^{-i\omega_0 t}u_0 + \sum_{n\neq o}c_n(t)e^{-i\omega_n t}u_n \tag{107}$$

$$\Psi(t) \approx \left(1 - \frac{iV_{00}}{\hbar}A\right)e^{-i\omega_0 t}u_0 + \sum_{n\neq o}\left(\frac{-V_{n0}}{\hbar\omega_{n0}}f(t)e^{i\omega_{n0}t}e^{-i\omega_n t}u_n\right) \qquad \text{using Eq.(89)} \tag{108}$$

$$\Psi(t) \approx \left[\left(1 - \frac{iV_{00}}{\hbar}Au_0\right) + \sum_{n\neq o}\left(\frac{-V_{n0}}{\hbar\omega_{n0}}f(t)u_n\right)\right]e^{-i\omega_0 t}u_0 \qquad e^{it(\omega_{n0}-\omega_n)} = e^{-i\omega_0 t} \tag{109}$$

$$\Psi(t) \approx \left[\left(1 - \frac{iV_{00}}{\hbar}Au_0\right) + \sum_{n\neq o}\left(\frac{-V_{n0}}{E_n^0 - E_0^0}f(t)u_n\right)\right]e^{-i\omega_0 t}u_0 \qquad \text{using Eq. (95)} \tag{110}$$

$$\boxed{\Psi(t) \approx \left[\left(1 - \frac{iV_{00}}{\hbar}Au_0\right) + \sum_{n\neq o}\left(\frac{-V_{n0}}{E_n^0 - E_0^0}u_n\right)\right]e^{-i\omega_0 t}u_0} \qquad f(t\to\infty) = 1 \tag{111}$$

Part (d)

From the time-independent perturbation theory we have:

$$w_0 = u_0 + \sum_{k \neq 0} \frac{V_{k0}}{E_0^0 - E_k^0} u_k \tag{112}$$

Use the results in c. to show that:

$$|\langle \Psi(t)|w_0\rangle|^2 \equiv \left| \int \Psi^*(t) w_0 d\tau \right|^2 \rightarrow 1 \text{ to the first order in } V \tag{113}$$

Solution

We have to just calculate this out but I am totally confused and tired at this point.

Problem 4. Energy Time Commutator

In the Hilbert space formalism of quantum mechanics, the equation of motion of a system given by the quantum condition expressed in terms of the commutators of paris of conjugate variable. When one projects these back to a certain specific representation, one obtains back the corresponding familiar "wave equations" in conventional wave mechanics. For example, $[\hat{x}, \hat{p}] = i\hbar$ leads back to the "momentum wave equation" in the coordinate representation:

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - p\right)\Psi_p(x) = 0 \tag{114}$$

Hence, *if one can also have an "energy-time commutator":* $[\hat{H}, \hat{t} = i\hbar]$, with the energy and time both represented by self-adjoint operators, then one would expect the TDSE:

$$\left(\hbar i\frac{\partial}{\partial t} - H\right)\Psi_E(x) = 0 \tag{115}$$

should also be obtained in the x–representation. However, one can show (Pauli, 1933) that such a self-adjoint operator for $\hat{t}$ can never exist (see below). Hence one should regard the operator representation of $\hat{H} : \hat{H} = i\hbar\frac{\partial}{\partial t}$ as a separate postulate in the formulation of Q.M.[2] and is valid in any representation. To demonstrate Pauli's proof:

Part (a)

Let E_a and Ψ_a be certain eigenvalue and eigenfunction of $\hat{H} : \hat{H}\Psi_a = E_a\Psi_a$. Show that if such a $\hat{t}$ operator exists such that $[\hat{H}, \hat{t}] = i\hbar$, then the following eigenvalue equation will be valid:

$$\hat{H}\left(e^{i\varepsilon\hat{t}/\hbar}\Psi_a\right) = (E_a - \varepsilon)\left(e^{i\varepsilon\hat{t}/\hbar}\Psi_a\right) \tag{116}$$

where ε is an arbitrary real constant.[3]

[2] In classical mechanincs, it is known that H is the generator of time evolution (Goldstein, 2nd ed., p.407-408). Therefore, if one *postulates* that it *plays the same role in Q.M., then one can also establish TDSE in this way (Ref.: excerpt from "Quantum Mechanics by Peebles.")*

[3] **Hint**: Try to establish the result for the following commutator:

$$\left[\hat{H}, e^{i\varepsilon\hat{t}/\hbar}\right] = -\left(\frac{i\varepsilon}{\hbar}\right)(-i\hbar)e^{i\varepsilon\hat{t}/\hbar} = -\varepsilon e^{i\varepsilon\hat{t}/\hbar} \tag{117}$$

Solution

Following the advice of the hint, the first thing we do is to establish the commutator from Equation (117).

$$\left[\hat{H}, e^{i\varepsilon\hat{t}/\hbar}\right]\psi = \hat{H}e^{i\varepsilon\hat{t}/\hbar}\psi - e^{i\varepsilon\hat{t}/\hbar}\hat{H}\psi \tag{118}$$

$$= i\hbar\frac{\partial}{\partial t}e^{i\varepsilon\hat{t}/\hbar}\psi - e^{i\varepsilon\hat{t}/\hbar}i\hbar\frac{\partial}{\partial t}\psi \qquad \text{remembering that } \hat{H} = i\hbar\frac{\partial}{\partial t} \tag{119}$$

$$= i\hbar\frac{i\varepsilon}{\hbar}e^{i\varepsilon\hat{t}/\hbar} + i\hbar e^{i\varepsilon\hat{t}/\hbar}\frac{\partial\psi}{\partial t} - i\hbar e^{i\varepsilon\hat{t}/\hbar}\frac{\partial\psi}{\partial t} \tag{120}$$

$$\left[\hat{H}, e^{i\varepsilon\hat{t}/\hbar}\right]\psi = -\varepsilon e^{i\varepsilon\hat{t}/\hbar}\psi \tag{121}$$

$$\boxed{\left[\hat{H}, e^{i\varepsilon\hat{t}/\hbar}\right] = -\varepsilon e^{i\varepsilon\hat{t}/\hbar}} \tag{122}$$

thus the eigenvalue Equation (116) would be valid by treating $\hat{t}$ as an operator rather than a parameter.

Part (b)

Hence provide an argument from the result in (a) that such and operator $\hat{t}$ cannot exist.

Solution

Because $\hat{H}$ and $\hat{t}$ no longer commute by treating $\hat{t}$ as an operator, and we are able to arrive at Equation (116), we find some wacky results. We see that a ground state energy no longer exists, because you can always lower it more by some arbitrary ε amount. This either means that we are apart of the Matrix and someone introduced a software bug, or physical reality as we know it would not exist.

Problem 5. Probability Distributions Revisited

Consider the eigenkets of the position and momentum of a 1-D free particle as follows:

$$\hat{x}\,|x\rangle = x\,|x\rangle \qquad \hat{p}\,|p\rangle = p\,|p\rangle \tag{123}$$

$$\langle x|x'\rangle = \delta(x-x') \qquad \langle p|p'\rangle = \delta(p-p') \tag{124}$$

$$\int dx\,|x\rangle\langle x| = 1 \qquad \int dp\,|p\rangle\langle p| = 1 \tag{125}$$

Part (a)

By considering $\langle x|\,\hat{p}\,|p\rangle$, and using the results derived in the notes: $\langle x|\,\hat{p}\,|\psi\rangle = \frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$, find the differential equation satisfied by the function $\langle x|p\rangle$ and show that the solution is

$$\langle x|p\rangle \propto e^{ipx/\hbar} \tag{126}$$

Use the normalization condition to determine the constant of proportionality.

Solution

To find the differential equation, we have to expand out our momentum operator using its position representation and momentum representation. In it's position representation, it is a differential operator. It's momentum representation is simply an eigenvalue p.

Remembering Equation (123) we see that using the momentum representation we get

$$\langle x|\,\hat{p}\,|p\rangle = p\,\langle x|p\rangle \tag{127}$$

and using the position representation of $\hat{p}$ we get

$$\langle x|\,\hat{p}\,|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle \tag{128}$$

which allows us to find our differential equation satisfied by $\langle x|p\rangle$:

$$p\,\langle x|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle \tag{129}$$

Using separation of variables

$$p\,\langle x|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle \tag{130}$$

$$pdx = -i\hbar\frac{d\,\langle x|p\rangle}{\langle x|p\rangle} \tag{131}$$

$$\int pdx = -i\hbar\int\frac{d\,\langle x|p\rangle}{\langle x|p\rangle} \tag{132}$$

$$px + C = -i\hbar\ln\langle x|p\rangle \tag{133}$$

$$\frac{ipx}{\hbar} + C = \ln\langle x|p\rangle \tag{134}$$

$$e^{\frac{ipx}{\hbar}+C} = \langle x|p\rangle \tag{135}$$

$$\boxed{Ae^{\frac{ipx}{\hbar}} = \langle x|p\rangle} \tag{136}$$

we arrive at a solution.

Now we must find our constant of proportionality, A. Combining Equation (124) of orthonormality, as well as Equation (125) of closure in order to perform a change of basis, as well as the Fourier expansion of $\delta(x)$, we can solve for A.

$$\langle x|x'\rangle = \delta(x-x') \tag{137}$$

$$\int \langle x|p\rangle \langle p|x'\rangle \, dp = \delta(x-x') \qquad \langle p|x'\rangle = \langle x'|p\rangle^* \text{ from (136)} \tag{138}$$

$$\int \langle x|p\rangle \langle x'|p\rangle^* \, dp = \delta(x-x') \qquad \& \ \langle x'|p\rangle^* = A^* e^{\frac{-ipx'}{\hbar}} \tag{139}$$

$$\int A e^{\frac{ipx}{\hbar}} A^* e^{\frac{-ipx'}{\hbar}} dp = \delta(x-x') \tag{140}$$

$$\int |A|^2 e^{\frac{ip}{\hbar}(x-x')} dp = \delta(x-x') \tag{141}$$

Remembering that the Fourier expansion of $\delta(x-x')$:

$$\delta(x-x') = \frac{1}{2\pi}\int e^{ik(x-x')} dk \tag{142}$$

with a simple substitution of

$$k = \frac{p}{\hbar} \tag{143}$$

$$dk = \frac{dp}{\hbar} \tag{144}$$

such that

$$\delta(x-x') = \frac{1}{2\pi\hbar}\int e^{\frac{ip}{\hbar}(x-x')} dp \tag{145}$$

it becomes trivial to see (145) going into (141) resulting in our proportionality constant A.

$$\int |A|^2 e^{\frac{ip}{\hbar}(x-x')} dp = \delta(x-x') \tag{146}$$

$$|A|^2 \int e^{\frac{ip}{\hbar}(x-x')} dp = \frac{1}{2\pi\hbar}\int e^{\frac{ip}{\hbar}(x-x')} dp \tag{147}$$

$$|A|^2 = \frac{1}{2\pi\hbar} \tag{148}$$

$$\boxed{A = \frac{1}{\sqrt{2\pi\hbar}}} \tag{149}$$

Part (b)

Consider a state vector $|\psi\rangle$, with $\langle\psi|\psi\rangle = 1$. The position representation of this state vector is the wave function $\psi(x) = \langle x|\psi\rangle$, and the momentum representation : $\phi(p) = \langle p|\phi\rangle$. The probability distribution in the result of the measurement of the momentum in the state $|\psi\rangle$ is

$$d\wp = |\langle p|\psi\rangle|^2 \, dp \tag{150}$$

Use the result in (a) to express this probability distribution in terms of the position wave function $\psi(x) = \langle x|\psi\rangle$.

Solution

With what we know now, this is a simple change of bases. Starting with Equation (150), we use the closure property, Equation (125), to represent this probability distribution in terms of the position wave function $\psi(x)$.

$$d\wp = \left| \int \langle p|x\rangle \langle x|\psi\rangle \, dx \right|^2 dp \tag{151}$$

$$d\wp = \left| \int \langle p|x\rangle \, \psi(x) dx \right|^2 dp \tag{152}$$

$$d\wp = \left| \int \langle x|p\rangle^* \, \psi(x) dx \right|^2 dp \tag{153}$$

$$\boxed{d\wp = \left| \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{-ipx}{\hbar}} \psi(x) dx \right|^2 dp} \tag{154}$$