TFY4205 Quantum Mechanics II
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SUGGESTED SOLUTION

Problem 1
Let us start by defining the quantity $\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[V(x)-E]}$. To describe an incident particle from the left region $x<0$, as well as the possibility that it may be reflected, we write for the wavefunction:

$$\psi = \mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx},\ x<0. \tag{1}$$

In the right region, $x>a$, we write down a plane-wave moving toward positive x. This represents the possibility that the incident particle has been transmitted through the potential region, and thus

$$\psi = F\mathrm{e}^{\mathrm{i}kx},\ x>0. \tag{2}$$

In the central region, $0<x<a$, the WKB approximation gives the following solution according to our treatment in the lectures:

$$\psi \simeq \frac{C}{\sqrt{\kappa(x)}}\mathrm{e}^{\int_0^x \kappa(t)dt} + \frac{D}{\sqrt{\kappa(x)}}\mathrm{e}^{-\int_0^x \kappa(t)dt},\ 0<x<a. \tag{3}$$

We have here absorbed some numerical prefactors into the unknown coefficients C and D, which can be done without loss of generality. We have four unknown coefficients $\{B,C,D,F\}$ and four boundary conditions (continuity of the wavefunction and its derivative at $x=0$ and $x=a$), so all coefficients may be determined. In turn, this allows us to compute the transmission probability $T=|F|^2$. Note that since we expect the wavefunction to decrease exponentially with respect to x between $[0,a]$, the higher the potential, the smaller the coefficient C should be.

Problem 2
The solution to the paradox is as follows. We see that the first order term in the expansion of $a_b = a_{b\to b}$ contributes to $|a_b|^2$. However, the second order term of in the expansion of a_b, which is not included, will also contribute to $|a_b|^2$. These two contributions will partly cancel each other forcing $P_{b\to b}\leq 1$.

A toy example: for a real c_1, the equation $a = 1+\mathrm{i}\lambda c_1$ gives $|a|^2 = 1+\lambda^2 c_1^2 > 1$. However, the equation $a = 1+\mathrm{i}\lambda c_1 + \lambda^2 c_2$ gives $|a|^2 = 1+\lambda^2(c_1^2+c_2+c_2^*)+O(\lambda^3)$, which is not necessary larger than 1 since $(c_1^2+c_2+c_2^*)$ may be a negative number.

The order of the perturbation is given as powers of λ in the toy example and also in the real problem if we write the perturbing potential as λV instead of V. Now, you are encouraged to compute the transition probability to second order instead of first. Start with the exact equation

$$da_n/dt = \frac{1}{\mathrm{i}\hbar}\sum_k \lambda V_{nk}(t)\mathrm{e}^{\mathrm{i}\omega_{nk}t}a_k(t). \tag{4}$$

We now expand the coefficients in λ according to:

$$a_n = a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)} + \dots \tag{5}$$

Inserted into the exact equation, we then get the following equations order for order:

$$\begin{aligned}
\lambda^0 &: da_n^{(0)}/dt = 0, \\
\lambda^1 &: da_n^{(1)}/dt = \frac{1}{\mathrm{i}\hbar}\sum_k V_{nk}(t)\mathrm{e}^{\mathrm{i}\omega_{nk}t}a_k^{(0)}(t), \\
\lambda^2 &: da_n^{(2)}/dt = \frac{1}{\mathrm{i}\hbar}\sum_k V_{nk}(t)\mathrm{e}^{\mathrm{i}\omega_{nk}t}a_k^{(1)}(t).
\end{aligned} \tag{6}$$

Assuming the system is initially in state b, the solution to the zeroth order equation is $a_n^{(0)}(t) = \delta_{nb}$. Inserting this value into the first order equation, only one term survives: $k = b$. Time integration gives

$$a_n^{(1)}(t) = \frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t} V_{nb}(\tau)\mathrm{e}^{\mathrm{i}\omega_{nb}\tau}d\tau. \tag{7}$$

Inserting this into the second order equation, we obtain for $a_b^{(2)}$:

$$\frac{da_b^{(2)}(t)}{dt} = \frac{1}{\mathrm{i}\hbar}\sum_k V_{bk}(t)\mathrm{e}^{\mathrm{i}\omega_{bk}t}a_k^{(1)}(t) = \frac{1}{(\mathrm{i}\hbar)^2}\sum_k V_{bk}(t)\mathrm{e}^{\mathrm{i}\omega_{bk}t}\int_{t_0}^{t} V_{kb}(\tau)\mathrm{e}^{\mathrm{i}\omega_{kb}\tau}d\tau. \tag{8}$$

We can thus find $a_b^{(2)}$ by integrating the above equation. In total, to second order in λ the probability amplitude for the system to remain in state b at time t becomes a sum of three terms:

$$a_b(t) = 1 + \frac{\lambda}{\mathrm{i}\hbar}\int_{t_0}^{t} V_{bb}(\tau)d\tau - \frac{\lambda^2}{\hbar^2}\sum_k \int_{t_0}^{t} V_{bk}(\tau_1)\mathrm{e}^{\mathrm{i}\omega_{bk}\tau_1}\int_{t_0}^{\tau_1} V_{kb}(\tau)\mathrm{e}^{\mathrm{i}\omega_{kb}\tau}d\tau d\tau_1 + O(\lambda^3). \tag{9}$$

Using that $V_{kb}^* = V_{bk}$ and $\omega_{bk} = -\omega_{kb}$, we get that

$$\begin{aligned}
|a_b(t)|^2 = 1 + \frac{\lambda^2}{\hbar^2}\Bigg[&\Big(\int_{t_0}^{t} V_{bb}(\tau)d\tau\Big)^2 - \int_{t_0}^{t}\int_{t_0}^{\tau_1}\sum_k V_{bk}(\tau_1)V_{kb}(\tau)\mathrm{e}^{\mathrm{i}\omega_{bk}\tau_1 + \mathrm{i}\omega_{kb}\tau}d\tau d\tau_1 \\
&- \int_{t_0}^{t}\int_{t_0}^{\tau_1}\sum_k V_{bk}^*(\tau_1)V_{kb}^*(\tau)\mathrm{e}^{-\mathrm{i}\omega_{bk}\tau_1 - \mathrm{i}\omega_{kb}\tau}d\tau d\tau_1\Bigg].
\end{aligned} \tag{10}$$

Using the above relations for V and ω and interchanging the variables in the last double integral, we see that the integrands are identical. The limits in the first double integral are such that we integrate over $t_0 \le \tau < \tau_1 \le t$. Afer the variable change in the second double integral we integrate over $t_0 \le \tau_1 < \tau \le t$. Together, this means that we integrate over $t_0 \le \tau \le t$ and $t_0 \le \tau_1 \le t$. Therefore, we end up with

$$|a_b(t)|^2 = 1 + \frac{\lambda^2}{\hbar^2}\Bigg[\Big(\int_{t_0}^{t} V_{bb}(\tau)d\tau\Big)^2 - \sum_k \Big|\int_{t_0}^{t} V_{bk}(\tau)\mathrm{e}^{\mathrm{i}\omega_{bk}\tau}d\tau\Big|^2\Bigg]. \tag{11}$$

The term $k = b$ in the sum exactly cancels the first term inside the brackets, and so

$$P_{b\to b} = |a_b(t)|^2 = 1 - \sum_{k\neq b}\frac{\lambda^2}{\hbar^2}\Big|\int_{t_0}^{t} V_{bk}(\tau)\mathrm{e}^{\mathrm{i}\omega_{bk}}\tau d\tau\Big|^2. \tag{12}$$

The paradox is then resolved since $P_{b\to b} < 1$. More precisely, we see that the final result is nothing but a statement of probability conservation:

$$\sum_k |a_k|^2 = 1. \tag{13}$$

A moral which can be taken away is then that it is easier to calculate 1 minus the probability for the system to leave state b than to directly calculate the probability for the system to remain in state b.

Problem 3

1. We write the state at time t in terms of stationary states of the oscillator:

$$\Psi(q,t) = \sum_{n=0}^{\infty} a_n(t)\psi_n(q)\mathrm{e}^{-\mathrm{i}E_n t/\hbar}. \tag{14}$$

To first order in time-dependent perturbation theory, we find for $n \neq 1$ that:

$$a_n(t) = \frac{1}{\mathrm{i}\hbar}\int_0^t \langle n|(a+a^\dagger)|1\rangle V_0 \mathrm{e}^{-t'/\tau}\mathrm{e}^{\mathrm{i}(E_n-E_1)t'/\hbar}dt'. \tag{15}$$

For the oscillator, we have that $E_n - E_1 = (n-1)\hbar\omega$ and

$$\langle n|(a+a^\dagger)|1\rangle = \begin{cases} 1 \text{ for } n=0 \\ \sqrt{2} \text{ for } n=2 \\ 0 \text{ otherwise} \end{cases} \tag{16}$$

Therefore, evaluation of the integral gives

$$\begin{aligned} \mathrm{i}\hbar a_0(t) &= V_0 \frac{1-\mathrm{e}^{-[\tau^{-1}+\mathrm{i}\omega]t}}{\tau^{-1}+\mathrm{i}\omega} \\ \mathrm{i}\hbar a_2(t) &= \sqrt{2}V_0 \frac{1-\mathrm{e}^{-[\tau^{-1}-\mathrm{i}\omega]t}}{\tau^{-1}-\mathrm{i}\omega} \\ \mathrm{i}\hbar a_n(t) &= 0 \text{ for } n>2. \end{aligned} \tag{17}$$

From the relation $\sum_n |a_n(t)|^2 = 1$, we see that $a_1(t) = 1 - O(V_0^2)$. Let us show this in more detail. Since $|a_1(t)|^2 = 1 - |a_0(t)|^2 - |a_2(t)|^2 = 1 - KV_0^2 + O(V_0^3)$ where $K > 0$ is a real positive constant, we can write in general that

$$a_1 = 1 + c_1V_0 + c_2V_0^2 + O(V_0^3). \tag{18}$$

Here, c_1 and c_2 are complex coefficients. It follows that

$$|a_1|^2 = 1 + (c_1 + c_1^*)V_0 + (c_2 + c_2^* + |c_1|^2)V_0^2 + O(V_0^3). \tag{19}$$

Since we know that $|a_1|^2 = 1 - KV_0^2$, the first-order term in V_0 has to be zero. This is accomplished in one of two ways. The first way is if we set $c_1 = 0$, and then we have proven that

$a_1(t) = 1 - O(V_0^2)$. The second way is if $c_1 = -c_1^*$, meaning that c_1 is a purely imaginary number. In that case, we may write $c_1 = \mathrm{i}C$ where C is a real constant. It then follows that

$$a_1 = 1 + \mathrm{i}CV_0 \tag{20}$$

to first order in V_0 (same order as the coefficients in Eq. (17)). But if that is the case, then $|a_1|^2 > 1$ which is not reasonable for a probability amplitude. Therefore, setting $c_1 = 0$ ensures that the probability does not exceed 1. Thus, we have proven that the lowest order acceptable correction to a_1 is of order $O(V_0^2)$.

Hence, the wavefunction is

$$\Psi(q,t) = a_0(t)\psi_0 + \psi_1 + a_2(t)\psi_2 + O(V_0^2) \tag{21}$$

to first order in V_0.

2. When $t \to \infty$, the wavefunction above becomes

$$\Psi(q,t) = \frac{V_0}{\tau^{-1} + \mathrm{i}\omega}\psi_0 \mathrm{e}^{-\mathrm{i}\omega t/2} + \psi_1 \mathrm{e}^{-3\mathrm{i}\omega t/2} + \frac{\sqrt{2}V_0}{\tau^{-1} - \mathrm{i}\omega}\psi_2 \mathrm{e}^{-5\mathrm{i}\omega t/2} + O(V_0^2). \tag{22}$$

Hence, the three energy eigenvalues $\hbar\omega/2, 3\hbar\omega/2, 5\hbar\omega/2$ are the most probable results of such a measurement. The respective probabilities $P(E)$ are given by the absolute square of the coefficients in front of ψ_0, ψ_1, ψ_2.

If the absolute square of the coefficients are used uncritically, one obtains $P(3\hbar\omega/2) = 1$, correct only to first order of V_0. The value of $P(3\hbar\omega/2)$ can be determined to second order in V_0 by using that the sum of the probabilities is 1.