Quantum Mechanics 3 - Homework 1 Solution

Solution to question 1

The transition probability is presented in Fig. 1.

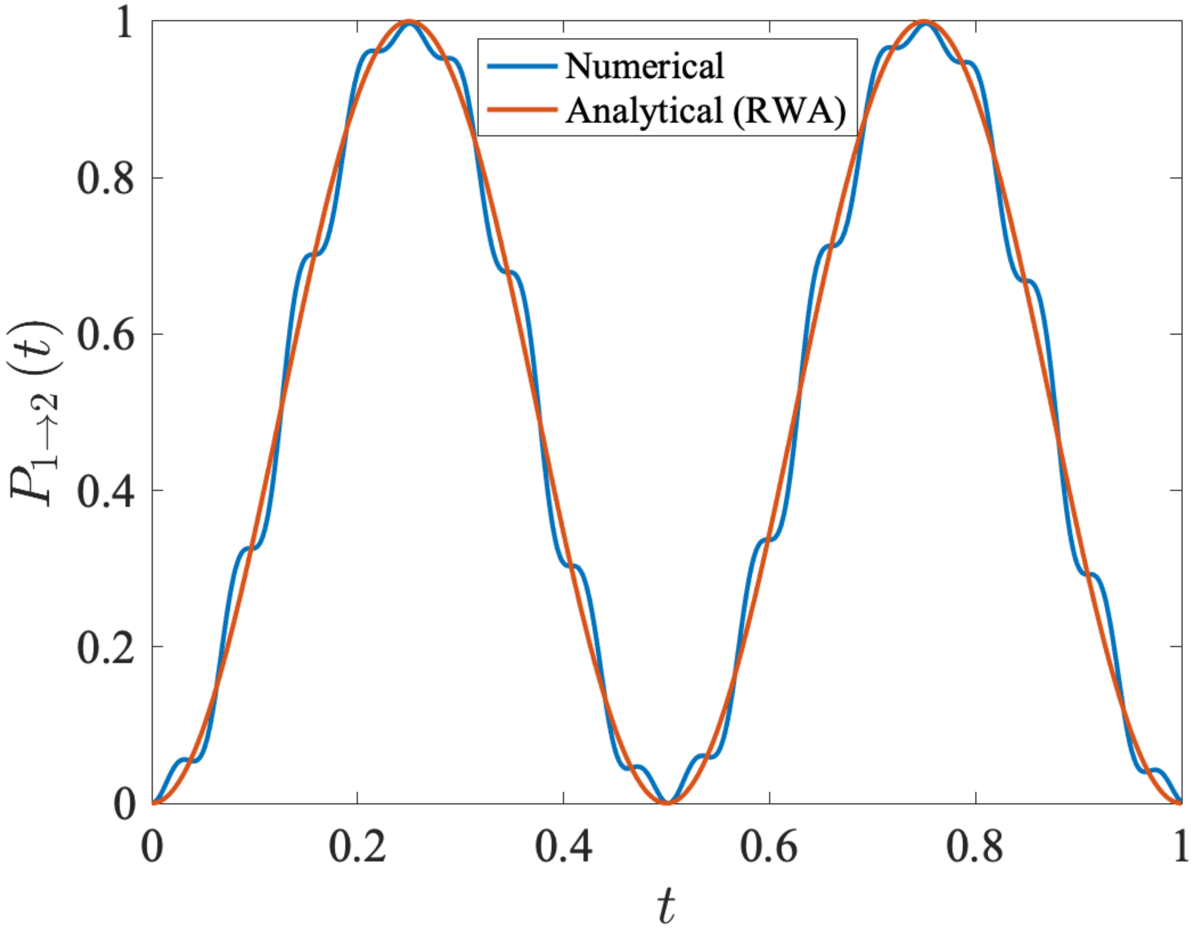


Figure 1: Transition probability as function of time.

We see that the numerical calculation agrees well with the analytical formula we derived in class. The small deviations between the results are due to the high frequency terms we neglected when we considered the rotating wave approximation.

Solution to question 2

The electric potential that is associated with an electric field $\vec{E}(t,\vec{r}) = A\delta(t)\hat{r}$ is

$$\vec{E} = -\vec{\nabla}\phi \implies \qquad \phi = -\int \vec{E}\cdot d\vec{r} = -Ar\delta(t), \tag{1}$$

where we chose to set $\phi = 0$ at the origin. The potential energy is

$$V(t,r) = e\phi(t,r) = -Aer\delta(t). \tag{2}$$

We now use Eq. (1.80) from the lecture notes,

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 \hat{V}_I(t_1)\hat{U}_I(t_1,t_0). \tag{3}$$

Since $\hat{U}_I(t,t_0) = \hat{U}_0^\dagger(t,t_0)\hat{U}(t,t_0)$, $\hat{V}_I(t) = \hat{U}_0^\dagger(t,t_0)\hat{V}(t)\hat{U}_0(t,t_0)$, we have

$$\begin{aligned}
\hat{U}(t,t_0) &= \hat{U}_0(t,t_0) - \frac{i}{\hbar}\hat{U}_0(t,t_0)\int_{t_0}^{t} dt_1 \hat{V}_I(t_1)\hat{U}_I(t_1,t_0) \\
&= \hat{U}_0(t,t_0) - \frac{i}{\hbar}\hat{U}_0(t,t_0)\int_{t_0}^{t} dt_1 \hat{U}_0^\dagger(t_1,t_0)\hat{V}(t_1)\hat{U}_0(t_1,t_0)\hat{U}_I(t_1,t_0) \\
&= \hat{U}_0(t,t_0) - \frac{i}{\hbar}\hat{U}_0(t,t_0)\int_{t_0}^{t} dt_1 \hat{U}_0^\dagger(t_1,t_0)\hat{V}(t_1)\hat{U}(t_1,t_0).
\end{aligned} \tag{4}$$

We now plug $V(t)$ from Eq. (2) to find[1]

$$\begin{aligned}
\hat{U}(t,t_0) &= \hat{U}_0(t,t_0) + \frac{i}{\hbar}\hat{U}_0(t,t_0)\int_{t_0}^{t} dt_1 \hat{U}_0^\dagger(t_1,t_0)Ae\hat{r}\delta(t_1)\hat{U}(t_1,t_0) \\
&= \hat{U}_0(t,t_0) + \frac{iAe}{\hbar}\hat{U}_0(t,t_0)\hat{U}_0^\dagger(0,t_0)\hat{r}\hat{U}(0,t_0)\Theta(t),
\end{aligned} \tag{5}$$

where $\Theta(t)$ is the Heaviside function. From here, we can isolate $\hat{U}(0,t_0)$ by plugging $t=0$ in the last equation,

$$\begin{aligned}
\hat{U}(0,t_0) &= \hat{U}_0(0,t_0) + \frac{iAe}{\hbar}\hat{U}_0(0,t_0)\hat{U}_0^\dagger(0,t_0)\hat{r}\hat{U}(0,t_0) \\
&= \hat{U}_0(0,t_0) + \frac{iAe\hat{r}}{\hbar}\hat{U}(0,t_0),
\end{aligned} \tag{6}$$

$$\implies \hat{U}(0,t_0) = \left(1 - \frac{iAe\hat{r}}{\hbar}\right)^{-1}\hat{U}_0(0,t_0). \tag{7}$$

With Eqs. (5) and (7) we can calculate the transition probability from the ground state to an excited state. Note that the potential of Eq. (2) only depends on r, thus angular momentum is conserved, and the only allowed value for ℓ and m is 0. Therefore, we calculate $P_{100\to200}$. In the limit $t_0 \to 0$ it is

$$\begin{aligned}
P_{100\to200} &= \left|\langle 200|\hat{U}(t,0)|100\rangle\right|^2 = \left|\langle 200|\hat{U}_0(t,0) + \frac{iAe}{\hbar}\hat{U}_0(t,0)\underbrace{\hat{U}_0^\dagger(0,0)}_{=1}\hat{r}\hat{U}(0,0)|100\rangle\right|^2 \\
&= \left|\langle 200|\hat{U}_0(t,0) + \frac{iAe}{\hbar}\hat{U}_0(t,0)\hat{r}\left(1 - \frac{iAe\hat{r}}{\hbar}\right)^{-1}|100\rangle\right|^2 \\
&= \left|\langle 200|\hat{U}_0(t,0)\left(1 + \frac{iAe\hat{r}}{\hbar}\left(1 - \frac{iAe\hat{r}}{\hbar}\right)^{-1}\right)|100\rangle\right|^2.
\end{aligned} \tag{8}$$

[1] Note that $\hat{U}^\dagger(0,t_0)\hat{r} \neq \hat{r}\hat{U}^\dagger(0,t_0)$. This is because $\hat{r}$ does not commute with the Hamiltonian.

Note that

$$\langle 200|\hat{U}_0(t,0) = \langle 200|\exp\left(-i\hat{H}_0 t/\hbar\right) = \langle 200|\exp\left(-iE_2 t/\hbar\right), \tag{9}$$

so

$$\begin{aligned} P_{100\to 200} &= \left|\langle 200|\exp\left(-iE_2 t/\hbar\right)\left(1+\frac{iAe\hat{r}}{\hbar}\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1}\right)|100\rangle\right|^2 \\ &= \left|\exp\left(-iE_2 t/\hbar\right)\right|^2\left|\langle 200|\left(1+\frac{iAe\hat{r}}{\hbar}\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1}\right)|100\rangle\right|^2 \\ &= \left|\langle 200|\frac{iAe\hat{r}}{\hbar}\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1}|100\rangle\right|^2. \end{aligned} \tag{10}$$

Note that we can simplify the operator inside the sandwich since

$$\frac{iAe\hat{r}}{\hbar}\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1} = \left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1} - \left(1-\frac{iAe\hat{r}}{\hbar}\right)\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1} = \left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1} - 1. \tag{11}$$

Thus

$$P_{100\to 200} = \left|\langle 200|\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1} - 1|100\rangle\right|^2 = \left|\langle 200|\left(1-\frac{iAe\hat{r}}{\hbar}\right)^{-1}|100\rangle\right|^2. \tag{12}$$

We can compute that sandwich in real space

$$P_{100\to 200} = \left|\int_0^\infty dr r^2 R_{20}(r)\left(1-\frac{iAer}{\hbar}\right)^{-1} R_{10}(r)\right|^2. \tag{13}$$

Recall that for the hydrogen atom, the radial part of the wavefunction (for $\ell = 0$) is given by

$$R_{n0}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-1)!}{2n\cdot n!}}\mathrm{e}^{-r/na_0}\;\frac{x^{-1}}{(n-1)!}\left(\frac{d}{dx}-1\right)^{n-1}x^n\Big|_{x=\frac{2r}{na_0}}, \tag{14}$$

where a_0 is the Bohr radius. So

$$R_{10}(r) = \frac{2}{a_0^{3/2}}\mathrm{e}^{-r/a_0}, \qquad R_{20}(r) = \frac{1}{2\sqrt{2}a_0^{3/2}}\mathrm{e}^{-r/2a_0}\left(2-\frac{r}{a_0}\right). \tag{15}$$

Therefore, we have

$$P_{100\to 200} = \frac{1}{2a_0^3}\left|\int_0^\infty dr r^2\mathrm{e}^{-3r/2a_0}\left(2-\frac{r}{a_0}\right)\left(1-\frac{iAer}{\hbar}\right)^{-1}\right|^2. \tag{16}$$

Let's define $x = 3r/2a_0$:

$$\boxed{P_{100\to 200} = \frac{2^7}{3^8}\left|\int_0^\infty dx x^2\mathrm{e}^{-x}(3-x)\left(1-\frac{2iAea_0}{3\hbar}x\right)^{-1}\right|^2 = \frac{2^7}{3^8}\left|\int_0^\infty dx x^2\mathrm{e}^{-x}\frac{3-x}{1-iyx}\right|^2}, \tag{17}$$

where we defined $y \equiv \frac{2Aea_0}{3\hbar}$.

For small enough A, i.e. $y \ll 1$, we can approximate the integral.

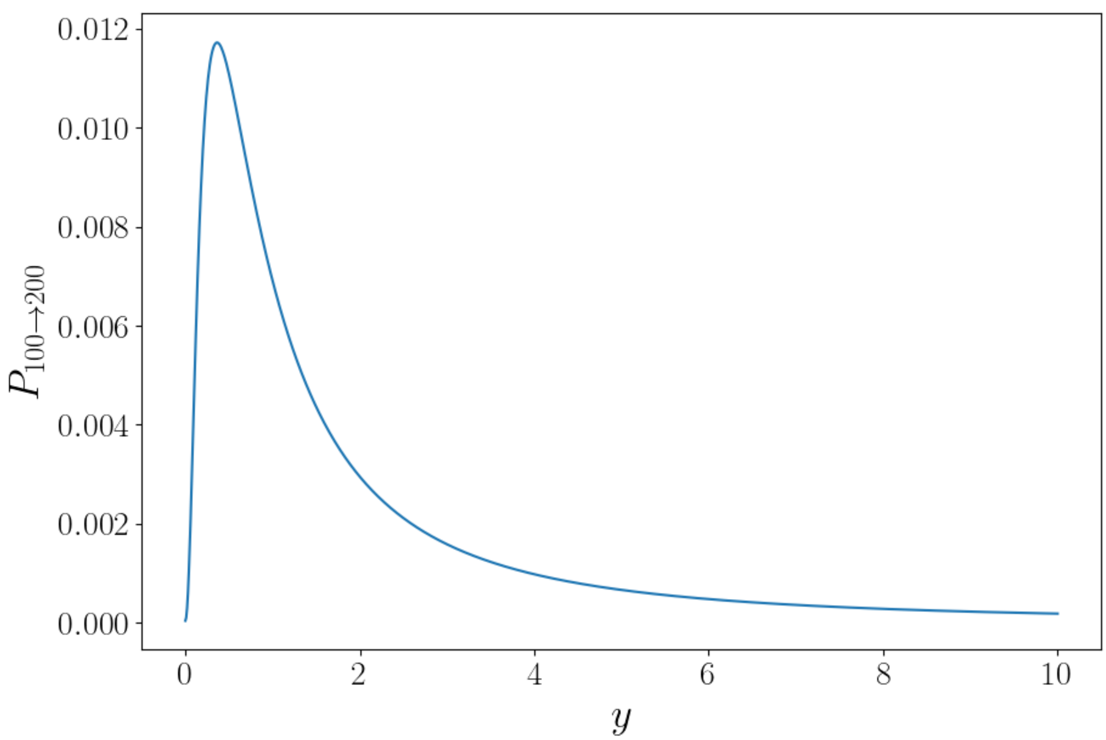
$$\begin{aligned} P_{100\to 200} &\approx \frac{2^7}{3^8}\left|\int_0^\infty dx x^2 \mathrm{e}^{-x}(3-x)(1+iyx)\right|^2 \\ &= \frac{2^7}{3^8}\left|\int_0^\infty dx \mathrm{e}^{-x}\left(3x^2-(1-3iy)x^3-iyx^4\right)\right|^2 \\ &= \frac{2^7}{3^8}\left|3\cdot 2!-(1-3iy)\,3!-iy\cdot 4!\right|^2 = \frac{2^7\cdot(4!-3\cdot 3!)^2}{3^8}y^2 \\ &= \frac{2^7\cdot 6^2}{3^8}\left(\frac{2Aea_0}{3\hbar}\right)^2 = \frac{2^{11}}{3^8}\left(\frac{Aea_0}{\hbar}\right)^2 \propto A^2. \end{aligned} \tag{18}$$

Indeed, the transition probability vanishes for $A=0$, as expected.

On the other hand, if $y \gg 1$,

$$\begin{aligned} P_{100\to 200} &= \frac{2^7}{3^8}\left|\int_0^\infty dx x^2 \mathrm{e}^{-x}\frac{3-x}{-iyx}\right|^2 \\ &\approx \frac{2^7}{3^8}\frac{1}{y^2}\left|\int_0^\infty dx \mathrm{e}^{-x}\left(3x-x^2\right)\right|^2 \\ &= \frac{2^7}{3^8}\frac{1}{y^2}\left|3-2!\right|^2 = \frac{2^7}{3^8}\frac{1}{y^2} = \frac{2^7}{3^8}\left(\frac{3\hbar}{2Aea_0}\right)^2 = \frac{2^5}{3^6}\left(\frac{\hbar}{Aea_0}\right)^2 \propto A^{-2}. \end{aligned} \tag{19}$$

Clearly, since the transition probability vanishes as $A \to 0$ and $A \to \infty$, it must reach a maximal value in between. To find the value of A for which the transition probability is maximal, we calculate it numerically.



The maximum of $P_{200\to 100}$ is at $y \approx 0.36$, which corresponds to $A = 0.36\frac{3\hbar}{2ea_0}$.

Solution to question 3

We can write the Hamiltonian (in Heisenberg picture) by using the ladder operators $a_{\rm H}$ and $a_{\rm H}^{\dagger}$,

$$\hat{H}=\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2-\hat{x}F\left(t\right)=\hbar\omega\left(\hat{a}_{\rm H}^{\dagger}\hat{a}_{\rm H}+\frac{1}{2}\right)-\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{\rm H}+\hat{a}_{\rm H}^{\dagger}\right)F\left(t\right). \tag{20}$$

The operator $\hat{a}_{\rm H}^{\dagger}$ evolves in time via the Heisenberg equation,

$$\begin{aligned}\frac{d\hat{a}_{\rm H}^{\dagger}}{dt} &= \frac{i}{\hbar}\left[\hat{H},\hat{a}_{\rm H}^{\dagger}\right]=\frac{i}{\hbar}\left[\hbar\omega\left(\hat{a}_{\rm H}^{\dagger}\hat{a}_{\rm H}+\frac{1}{2}\right)-\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{\rm H}+\hat{a}_{\rm H}^{\dagger}\right)F\left(t\right),\hat{a}_{\rm H}^{\dagger}\right]\\ &= i\omega\left[\hat{a}_{\rm H}^{\dagger}\hat{a}_{\rm H},\hat{a}_{\rm H}^{\dagger}\right]-\frac{i}{\sqrt{2m\hbar\omega}}F\left(t\right)\underbrace{\left[\hat{a}_{\rm H},\hat{a}_{\rm H}^{\dagger}\right]}_{=1}\\ &= i\omega\hat{a}_{\rm H}^{\dagger}\left[\hat{a}_{\rm H},\hat{a}_{\rm H}^{\dagger}\right]-\frac{i}{\sqrt{2m\hbar\omega}}F\left(t\right)=i\omega\hat{a}_{\rm H}^{\dagger}-\frac{i}{\sqrt{2m\hbar\omega}}F\left(t\right).\end{aligned} \tag{21}$$

This is the differential equation we need to solve. There are many methods for solving this equation, like adding the homogeneous and particular solutions. A neat trick we can do here is to multiply the equation by $\mathrm{e}^{-i\omega t}$. Then, we can write

$$\frac{d}{dt}\left(\hat{a}_{\rm H}^{\dagger}\mathrm{e}^{-i\omega t}\right)=-\frac{i}{\sqrt{2m\hbar\omega}}F\left(t\right)\mathrm{e}^{-i\omega t}. \tag{22}$$

Therefore,

$$\hat{a}_{\rm H}^{\dagger}\left(t\right)\mathrm{e}^{-i\omega t}-\hat{a}_{\rm H}^{\dagger}\left(t_0\right)\mathrm{e}^{-i\omega t_0}=-\frac{i}{\sqrt{2m\hbar\omega}}\int_{t_0}^{t}dt'F\left(t'\right)\mathrm{e}^{-i\omega t'}. \tag{23}$$

$$\hat{a}_{\rm H}^{\dagger}\left(t\right)=\hat{a}_{\rm H}^{\dagger}\left(t_0\right)\mathrm{e}^{i\omega(t-t_0)}-\frac{i}{\sqrt{2m\hbar\omega}}\mathrm{e}^{i\omega t}\int_{t_0}^{t}dt'F\left(t'\right)\mathrm{e}^{-i\omega t'}=\hat{a}_{\rm H}^{\dagger}\left(t_0\right)\mathrm{e}^{i\omega(t-t_0)}-B\left(t,t_0\right), \tag{24}$$

where we defined $B\left(t,t_0\right)$ (note that it is a number, not an operator!). What is the initial condition for this equation, i.e. $\hat{a}_{\rm H}^{\dagger}\left(t_0\right)$? By definition it is the ladder operator in Schrödinger picture, $\hat{a}^{\dagger}$. We now take $t_0\to-\infty$, where $\hat{a}^{\dagger}$ satisfies (since the force vanishes at $t\to-\infty$)

$$\frac{\left(\hat{a}^{\dagger}\right)^n}{\sqrt{n!}}|0\rangle=|n\rangle. \tag{25}$$

The transition probability to the n'th state is given by (we implicitly assume below that $t_0\to-\infty$)

$$\begin{aligned}P_n\left(t,t_0\right) &= \left|\langle n|\hat{U}\left(t,t_0\right)|0\rangle\right|^2=\left|\langle 0|\hat{U}^{\dagger}\left(t,t_0\right)|n\rangle\right|^2=\left|\langle 0|\hat{U}^{\dagger}\left(t,t_0\right)\frac{\left(\hat{a}^{\dagger}\right)^n}{\sqrt{n!}}|0\rangle\right|^2\\ &= \left|\langle 0|\hat{U}^{\dagger}\left(t,t_0\right)\frac{\left(\hat{U}\left(t,t_0\right)\hat{a}_{\rm H}^{\dagger}\left(t\right)\hat{U}^{\dagger}\left(t,t_0\right)\right)^n}{\sqrt{n!}}|0\rangle\right|^2\\ &= \frac{1}{n!}\left|\langle 0|\hat{U}^{\dagger}\left(t,t_0\right)\hat{U}\left(t,t_0\right)\left(\hat{a}_{\rm H}^{\dagger}\left(t\right)\right)^n\hat{U}^{\dagger}\left(t,t_0\right)|0\rangle\right|^2=\frac{1}{n!}\left|\langle 0|\left(\hat{a}_{\rm H}^{\dagger}\left(t\right)\right)^n\hat{U}^{\dagger}\left(t,t_0\right)|0\rangle\right|^2.\end{aligned} \tag{26}$$

We can use the binomial expansion to calculate $\left(\hat{a}_{\rm H}^{\dagger}\left(t\right)\right)^n$,

$$\left(\hat{a}_{\rm H}^{\dagger}\left(t\right)\right)^n=\left(\hat{a}^{\dagger}\mathrm{e}^{i\omega(t-t_0)}-B\left(t,t_0\right)\right)^n=\sum_{k=0}^{n}\binom{n}{k}\left(\hat{a}^{\dagger}\right)^k\mathrm{e}^{i\omega k(t-t_0)}B^{n-k}\left(t,t_0\right). \tag{27}$$

According to Eq. (26), we need to act on this operator with $\langle 0|$ from its left. Since $\langle 0|\hat{a}^\dagger = 0$, the only term that survives in Eq. (27) is the one that corresponds to $k = 0$. Thus

$$P_n(t, t_0) = \frac{|B(t, t_0)|^{2n}}{n!} \left|\langle 0|\hat{U}^\dagger(t, t_0)|0\rangle\right|^2 = \frac{|B(t, t_0)|^{2n}}{n!} \left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2. \tag{28}$$

We can try to calculate $\left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2$. This would be painful since the Hamiltonian does not commute with itself at different times! Instead, we claim the following argument: at $t \to +\infty$ the system must be found in one of its eigen-states, $|n\rangle$, thus

$$1 = \sum_{n=0}^{\infty} P_n = \sum_{n=0}^{\infty} \frac{B^{2n}}{n!} \left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2 = \left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2 \sum_{n=0}^{\infty} \frac{B^{2n}}{n!} = \left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2 \mathrm{e}^{B^2} \tag{29}$$

$$\Longrightarrow \left|\langle 0|\hat{U}(t, t_0)|0\rangle\right|^2 = \mathrm{e}^{-B^2}. \tag{30}$$

Therefore, we conclude

$$\boxed{P_n = \frac{B^{2n}}{n!} \mathrm{e}^{-B^2}}, \tag{31}$$

where

$$\boxed{B \equiv \frac{1}{\sqrt{2m\hbar\omega}} \left| \int_{-\infty}^{\infty} dt' F(t') \mathrm{e}^{-i\omega t'} \right| = \frac{1}{\sqrt{2m\hbar\omega}} \left| \tilde{F}(\omega) \right|}, \tag{32}$$

and we identified the Fourier transform of the force, $\tilde{F}(\omega)$.