PHY 304, II-Semester 2023/24, Assignment 6 solution

(1) Kicked quantum dot [12 pts] Consider the particle in an infinite square well potential, as discussed in QM-I, section 2.2.1, which is initially in the ground-state $n = 1$ and then subject to a briefly pulsed perturbation

$$\hat{H}'(t) = \kappa\left(\hat{x} - \frac{a}{2}\right)^3 \sin^2(\pi t/T) \text{ for } 0 < t < T, \tag{1}$$

and again $\hat{H}'(t) = 0$ afterwards.

(a) To first order in κ, find the transition probabilities from the ground state $n = 1$ initially, to any other state n'. [6 pts]
Solution: This is a pulsed perturbation (not periodic since we are just looking at a single half cycle of the sine), hence referring to section 9.1.1 from the lecture, Eq. (9.10) gives us the transition amplitude between the two states as:

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_0^T e^{i(E_f^0 - E_i^0)t'/\hbar}\langle\, \phi_f^0\, |H'(t')|\, \phi_i^0\, \rangle dt' \tag{2}$$

in the given state, the particle performs the transition from the ground state n=1 to any final state n'. Thus, the above equation (2) is modified as:

$$d_{n'}(t) = \delta_{n'1} - \frac{i}{\hbar}\int_0^T e^{i(E_{n'}^0 - E_1^0)t'/\hbar}\langle\, \phi_{n'}^0\, |H'(t')|\, \phi_1^0\, \rangle dt' \tag{3}$$

We already know that $\phi_{n'}^0 = \sqrt{\frac{2}{a}}\sin(\frac{n'\pi x}{a})$ and $E_{n'}^0 = \frac{n'^2\pi^2\hbar^2}{2ma^2}$, so that Eq. (3) reads:

$$d_{n'}(t) = \delta_{n'1} - \frac{2}{a}\frac{i}{\hbar}\int_0^T e^{i(n'^2-1)\frac{\pi^2\hbar^2}{2ma^2}t'/\hbar}\langle\, sin\left(\frac{n'\pi x}{a}\right)|\kappa\left(\hat{x} - \frac{a}{2}\right)^3 sin^2\left(\frac{\pi t}{T}\right)|\, sin\left(\frac{\pi x}{a}\right)\rangle dt \tag{4}$$

We see that this decomposes into two pieces, the spatial matrix element M_{fi} and the integration over the time-dependence of the pulse and the oscillatory factors from initial and final state energies, I_t. We evaluate both of them separately.
The spatial matrix element

$$\begin{aligned} M_{n'i} &= \frac{2}{a}\int_0^a dx \sin\left(\frac{n'\pi x}{a}\right)\left(x - \frac{a}{2}\right)^3 \sin\left(\frac{\pi x}{a}\right) \\ &= -\frac{6a^3 n'(1 + (-1)^{n'})(-16(1 + n'^2) + (-1 + n'^2)^2\pi^2)}{2(-1 + n'^2)^4\pi^4} \end{aligned} \tag{5}$$

and the time integral

$$\begin{aligned} I_t &= -\frac{i}{\hbar}\int_0^T e^{i(1-n'^2)\frac{E_1 t'}{\hbar}}\; k_0 \sin^2\left(\frac{\pi t}{T}\right) \\ &= -\frac{2}{\hbar}\,\frac{\left(e^{iE_1(n'^2-1)T/\hbar} - 1\right)e^{-iE_1(n^2-1)T/\hbar}\pi^2 k_0}{\frac{4E_1}{\hbar}(n^2-1)\pi^2 - (E_1/\hbar)^3(n^2-1)^3T^2} \end{aligned} \tag{6}$$

We then combine all this into the transition probability

$$P_{n'} = |d_{n'}(t)|^2 = |M_{n'i} I_t|^2. \tag{7}$$

The matrix elements in Eq. (5) provide "selection rules". We see that they are non-zero only if n' is even. Even quantum numbers correspond to anti-symmetric (odd symmetry) wave functions. We see that since we have an odd perturbation $\sim x^3$, we can only make a transition from the initially even state to an odd state. These considerations are similar to those providing us the dipole selections rules for atomic transition (see e.g. example 50 and section 9.3.4.)

(b) Checkout these probabilities in the limits $T \to 0$ and $T \to \infty$ and justify those based on physical arguments. [2pts]
Solution: From Eq. (6), it is seen that in the limits $T \to 0$ and $T \to \infty$

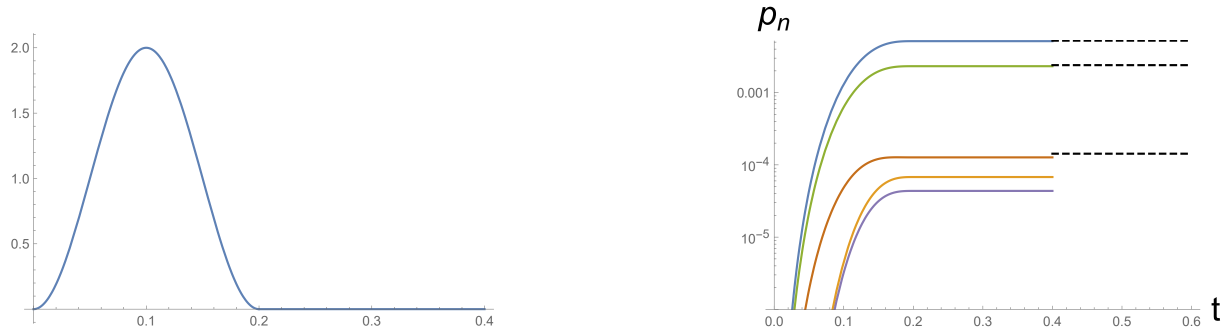
$$\lim_{T\to 0} P_{n'} = 0 \quad \textit{and} \quad \lim_{T\to\infty} P_{n'} = 0$$

We expect $P_f \to 0$ in both limits. In the first case because the pulse is sudden and can make no change in the state (see section 9.1.2.). For $T \to \infty$, it is because the quantum state will adiabatically follow the initial state, and thus return to the ground-state after the pulse with unit probability so that there is no transition(see section 9.2.2).

(c) Use `assignment6_question1_draft.nb`, which solves the above scenario numerically, to verify your calculation from part (a) by implementing your solution in the indicated spot. Discuss where you see agreement, what differs, and why that might be. [2 pts]
Solution: See Fig. 1. The PT for all even numbered states are very good. For odd numbered states there is a qualitative difference: The full solution populates these while PT does not. The reason is that the full solution contained higher order PT contributions where the system can reach e.g. state 3 via going through state 2 (both transitions $1 \to 2$, $2 \to 3$ are allowed by the selection rules we found in part (a).
Discuss results: I expect that the probabilities from initial state (Even) to all the odd symmetry states are OK. The other ones are analytically zero but numerically not. The reason for that is that the numerics contains sequential transitions ($1 \to 2 \to 3$), which would only appear in <u>second order perturbation theory</u> (see week10).

(2) Shift of a harmonic oscillator: [5 pts] Assume a particle of mass m is initially for $t < 0$ in the ground-state of a harmonic oscillator potential with frequency ω:

$$V(x) = \frac{1}{2} m\omega x^2. \tag{8}$$



(a) Pulse. (b) Probability.

Figure 1: (left) Perturbation pulse shape in time ($\sin(\pi t/T)$ for $0 < t < T$). (right) Populations of states other than groundstate from full TDSE: blue p_2, yellow p_3, green p_4, violet p_5, red p_6. Black dashed lines are p_2, p_4, p_6 from perturbation theory, while $p_k = 0$ for all odd k in PT.

Now at $t = 0$, we suddenly shift the potential by a displacement x_0:

$$V(x, t > 0) = \frac{1}{2} m\omega \left(x - x_0\right)^2. \tag{9}$$

What is the state of the oscillator immediately after this shift and why? Also find the probability distribution of the particle position at all $t > 0$. What is the fastest velocity with which we could shift the potential slowly from being centered at 0 to being centered at x_0, without causing significant excitations of the oscillator?

Solution: Immediately after the shift, the oscillator remains in the earlier ground-state $\phi(x) \sim e^{-x^2/(2\sigma^2)}$ since it did not have any time to evolve and thus respond to the perturbation (see section 9.2.1.). Onwards from immediately after the change the potential remains as Eq. (12) and we can thus consider the evolution according to a constant Hamiltonian with initial-state $\phi(x, t \approx 0) = \mathcal{N} e^{-x^2/(2\sigma^2)}$. It is now easiest to shift the origin of our x-axis to x_0, such that the potential Eq. (12) becomes the usual harmonic oscillator potential but the initial state is now:

$$\phi(x, t \approx 0) = \mathcal{N} e^{-\frac{(x-x_0)^2}{2\sigma^2}}. \tag{10}$$

We can now solve the TDSE as usual to find the time evolution of the initial state in Eq. (10) which is the ground state of the harmonic oscillator displaced from the equilibrium. This gives us a coherent state in which the probability density

$$\left|\psi^{(\alpha)}(x, t)\right|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{m\omega}{\hbar}\left(x - \langle\hat{x}(t)\rangle\right)^2\right). \tag{11}$$

oscillates as a Gaussian wavepacket about the minimum of the harmonic potential.

From the discussion of the quantum adiabatic theorem in section 9.2.2 (Eq 9.36 in particular), it is clear that the fastest time scale allowed from the adiabatic theorem will be set by $\sim \frac{\hbar}{(E_1 - E_0)}$.

To be more specific, let us parametrise the centre of the trap by $x_c(t) = 0 + \frac{x_0}{T}t$, such that it takes a time T to reach from $x_c(t) = 0$ to $x_c(t) = x_0$. The potential energy is then is then

$$V(x, 0 < t < T) = \frac{1}{2}m\omega\left(x - x_c(t)\right)^2. \tag{12}$$

such that

$$\frac{\partial \hat{H}}{\partial t} = m\omega\left(x - x_c(t)\right)\frac{x_0}{T}. \tag{13}$$

By Eq. (9.36) the key quantity controlling non-adiabatic transitions from the ground to the first excited state is

$$\begin{aligned}
&\frac{\langle\, \phi_1(t)\,|\frac{\partial}{\partial t}\hat{H}(t)|\,\phi_0(t)\,\rangle}{E_1(t) - E_0(t)} \\
&= \frac{m\omega\frac{x_0}{T}\int dx\; \varphi_1^*(x - x_c(t))\,(x - x_c(t))\,\varphi_0(x - x_c(t))}{\hbar\omega} \\
&\overset{e.g.\ mathematica}{=} \frac{m\omega x_0}{\hbar\omega T}\underbrace{\frac{\sigma}{\sqrt{2}}}_{=\sqrt{\hbar/(2m\omega)}} = \frac{x_0}{T\omega\sigma} \ll 1
\end{aligned} \tag{14}$$

We can interpret this as follows: Consider the time τ it takes to shift the oscillator potential by one unit of the ground-state position uncertainty σ: This time is σ/v for shift-velocity v, which is here x_0/T. Hence this time is $\tau = \frac{x_0}{T\sigma}$. To avoid non-adiabatic excitations, it must be much longer than one oscillation period $2\pi/\omega$.

If you wrote a much more qualitative discussion, stating that $\sim 1\omega$ is the key time-scale, that was fine too.

(3) Charged particle in 3D within quantum dot [5 pts] A particle of mass m with electric charge q is confined to a three-dimensional cubical box of side length L and in the ground-state until $t = 0$. It now feels an electric field $\mathbf{E} = E_0 e^{-\alpha t}\mathbf{e}_x$ for $t > 0$ only, where α is a constant, and $\mathbf{e}_x$ is the unit vector in the x-direction. Calculate the probability that the charged particle is excited to the first excited state by the time $t = \infty$. Discuss the dependence of your result on α, how can you separately understand the limits $\alpha = 0, \infty$?

Solution. The energy eigenfunctions and eigenvalues of a particle in a cubical box of side L are given by

$$E_{jkl} = \frac{\pi^2\hbar^2}{2mL^2}(j^2 + k^2 + l^2), \quad j, k, l = 1, 2, 3, \ldots \tag{15}$$

and

$$\Psi_{jkl} = \frac{\sqrt{8}}{\sqrt{L^3}}\sin\left(\frac{j\pi x}{L}\right)\sin\left(\frac{k\pi y}{L}\right)\sin\left(\frac{l\pi z}{L}\right) = |\, jkl\,\rangle \tag{16}$$

respectively.
The ground state is $|\,111\,\rangle$ *and the first excited states are* $|\,211\,\rangle, |\,121\,\rangle, |\,112\,\rangle$. *As the electric field is along the x-axis, then the perturbation due to the dipole moment* $\boldsymbol{\mu} = qx\mathbf{e}_x$ *is*

$$\hat{H}' = -\boldsymbol{\mu}\cdot\mathbf{E} = -qE_0 x e^{-\alpha t} \tag{17}$$

The transition probability for a transition from state n *to state* m *is*

$$P = \left| \frac{1}{\hbar^2}\int_0^\infty \hat{H}'_{mn}\exp(i\omega_{mn}t')dt' \right|^2 \tag{18}$$

where $\omega_{mn} = (E_m - E_n)/\hbar$, *and* H'_{mn} *is the transition matrix element between states* m *and* n. *For our case*

$$\begin{aligned} H'_{mn} = \langle\,111\,|\,\hat{H}'|211\,\rangle &= \langle\,111\,|-qE_0 x e^{-\alpha t}|211\,\rangle \\ &= -eE_0 e^{-\alpha t}\langle\,111\,|\,x\,\,|211\,\rangle \\ &= -\frac{8qE_0 e^{-\alpha t}}{L^3}\int_0^L x\sin\frac{\pi x}{L}\sin\frac{2\pi x}{L}dx\int_0^L \sin^2\frac{\pi y}{L}dy\int_0^L\sin^2\frac{\pi z}{L}dz \\ &= \frac{8qE_0 e^{-\alpha t}}{L^3}\left(-\frac{8L^2}{9\pi^2}\right)\times\frac{L}{2}\times\frac{L}{2} = \frac{16qE_0 L e^{-\alpha t}}{9\pi^2} \end{aligned} \tag{19}$$

The terms

$$\langle\,111\,|\,x\,\,|121\,\rangle = \int_0^L x\sin^2\frac{\pi x}{L}dx\underbrace{\int_0^L \sin\frac{\pi y}{L}\sin\frac{2\pi y}{L}dy}_{=0}\int_0^L\sin^2\frac{\pi z}{L}dz \tag{20}$$

and

$$\langle\,111\,|\,x\,\,|112\,\rangle = \int_0^L x\sin^2\frac{\pi x}{L}dx\underbrace{\int_0^L \sin\frac{\pi y}{L}\sin\frac{2\pi y}{L}dy}_{=0}\int_0^L\sin^2\frac{\pi z}{L}dz \tag{21}$$

go to zero because of the orthogonality of sine functions. Therefore, Eq. (18) reduces to

$$P = \left(\frac{16qE_0}{9\pi^2\hbar}\right)^2\left|\int_0^\infty \exp(-\alpha t + i\omega_{21}t)dt\right|^2 = \left|\frac{16qE_0}{9\pi^2\hbar}\right|^2\frac{1}{\alpha^2+\omega_{21}^2} \tag{22}$$

where $w_{21} = \frac{E_2-E_1}{\hbar} = \frac{3\pi^2\hbar}{2mL^2}$.

From Eq. (22) it is evident that as α *tends to* ∞, *the probability tends to zero. This is intuitive because for* $\alpha = 0$ *the electric field is zero and there is no perturbation that can cause transitions. At* $\alpha = 0$, *one has just a constant electric field* E_0 *such that the probability of transition is*

$$P = \left(\frac{16q}{27\pi^2}\right)^2. \tag{23}$$

(4) Driven quantum dot [10 pts] Let us change the perturbation of the (otherwise unchanged) quantum dot in Q1 to

$$\hat{H}'(t) = F_0 \left(\hat{x} - \frac{a}{2}\right)^3 \sin(\omega t) \tag{24}$$

at all t. We are showing numerical solution of the TDSE similar to example 46 page 144 in Fig. 2, from the initial state $|\Psi(0)\rangle = |\phi_1\rangle$ [See online code, we used a Hamiltonian in matrix form as in QM1, assn5 Q2(c), but that is not important for this question].

(a) See the attached Mathematica notebook `assignment6_question4_code_v1(a).nb`.

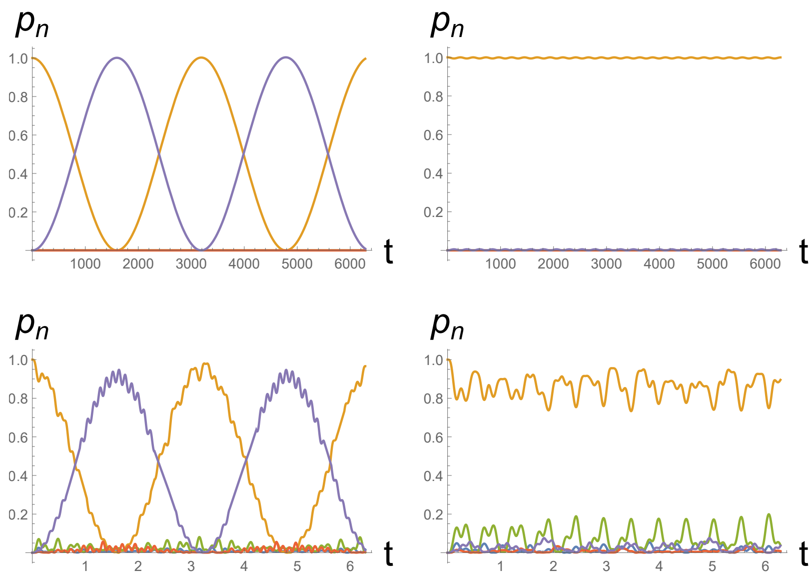


Figure 2: (**Q4**) Probability $p_k = |\langle \phi_k | \Psi(t) \rangle|^2$ for the PIB to be in eigenstate k while subject to (24) from $t = 0$ for $k = 1$ (blue), $k = 2$ (orange). Parameters are (top left) $a = 2$, $F_0 = 0.02$, $\omega = (E_5 - E_2)/\hbar$, (top right) same but $\omega = 0.999(E_5 - E_2)/\hbar$, (bottom left) Same as top left but $F_0 = 20$, (bottom right) same as bottom left but $\omega = 0.7(E_5 - E_2)/\hbar$.

(b) Using the parameters provided in the caption, *quantitatively explain* all features of the dynamics (amplitude and period of main oscillation, choice of states, why is there which oscillation). We are using dimensionless units with $\hbar = m = 1$. [4pts] *Solution:(a) In this case we have resonant Rabi oscillations, with Rabi frequency* $\Omega = 0.0019705$. *Hence the period of population oscillations is* $T = \frac{2\pi\hbar}{\Omega} = 3188.62$ *as seen in the figure. (b) Here we are looking at detuned Rabi oscillations, which no longer allow* 100 % *population transfer, but only to a maximum of* $p_2 = (\Omega/\Delta)^2 = 0.0025$. *The period of these fast oscillations is given approximately by* $T = 400$ *[set by* Δ *in this case]. (c) In cases (a,b) due to the small* F_0 *the Rabi frequency was small compared to the frequency* ω *of the perturbation. Thus transitions between states* $|2\rangle$ *and* $|1\rangle$ *happen on time-scales that are a lot slower than the period of the perturbation, which means the rotating wave approximation (RWA) (see section 9.3.5) is fulfilled* *very well. For (c,d) the new $\Omega = 1.9705$ actually becomes much close to ω, so that the RWA fails to be fully valid. We still see a qualitatively similar picture, but now there are some superimposed faster oscillations, caused by the terms we had neglected under the RWA.*

(c) Using `assignment6_question4_code_v1.nb`: Moderately vary the perturbation amplitude F_0 (but keep it $F_0 < 0.05$ here) and discuss what happens. Change the frequency to $\omega = (E_3 - E_2)/\hbar$ and $\omega = (E_2 - E_1)/\hbar$ instead of the default ($\omega = (E_5 - E_2)/\hbar$). Discuss what happens and why. [4pts]
Solution:
In plotting following functions, the parameter $F_0 = 0.04$ and the time period of the oscillation decreases as $T \propto \frac{1}{F_0}$.

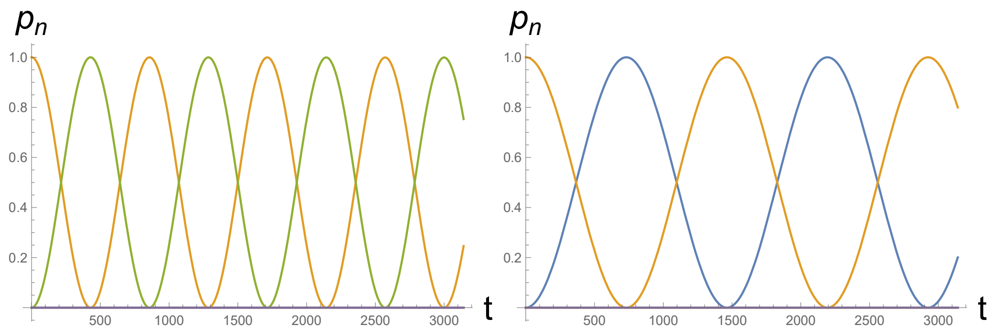


Figure 3: The above plots show transition between E3 and E2 levels (Left) and E2 and E1 levels (right) with $F_0 = 0.04$. The periodic modulation of the external field 'F' has a frequency matching the transition frequency $\omega_{mn} = (Em - En)/\hbar$ between two levels, probability portrays the periodic oscillations. This condition corresponds to resonant driving.

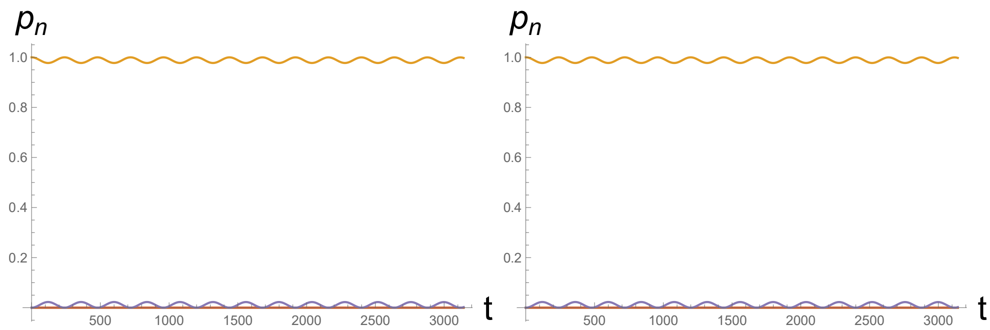


Figure 4: Shows that irrespective of the strength of external force '$F_0 = 0.04$' (less than 0.05), the transition between the states with energy (left) E3 and E2 and with energy (right) E2 and E1 shows like behaviour. The condition is similar to off-resonant driving.

(d) Now go to large $1 < F_0 < 10$. Discuss what you see and why? [2pts] *Solution:*

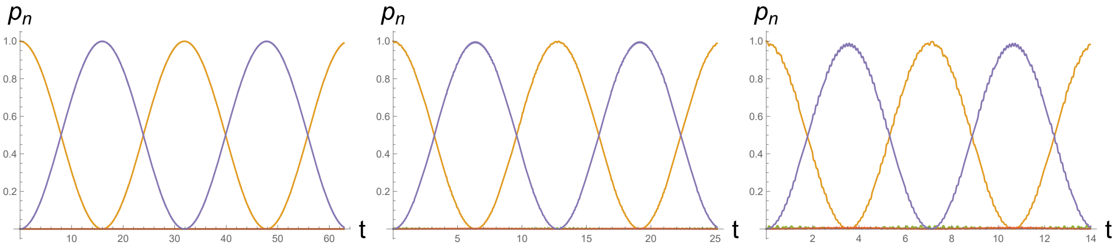


Figure 5: The transition between the level E5 and E2 with parameter F_0 value as (left) F_0=2, (center) F_0=5, (right) F_0=9..With increasing F_0, we can see that the probability curves are not varying smoothly anymore as RWA fails to be fully valid. (Detailed discussion in (b))

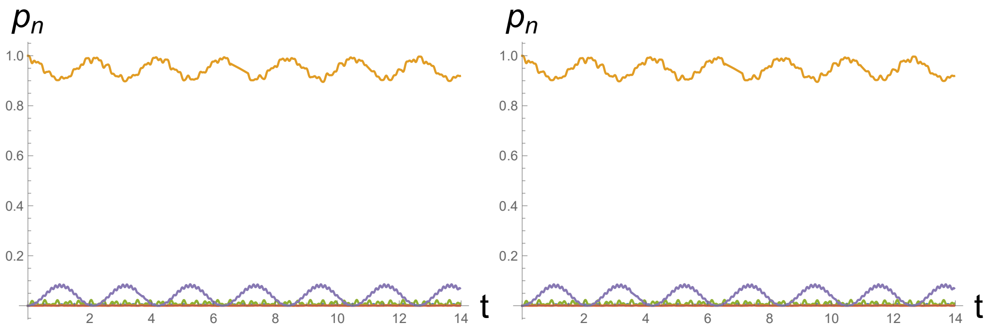


Figure 6: The strength of external force is 'F_0=9' and the transition between the states with energy (left) E3 and E2 and with energy (right) E2 and E1 shows similar off-resonance behaviour as in Fig. 4.