PHY 304, II-Semester 2023/24, Tutorial 7 solution

Stage 1 Time dependent perturbation theory

(i) Discuss what is the mission objective of time-dependent perturbation theory. When do we need it? What are alternatives to it?
Solution: It typically seeks to find a simple (approximate) answer to the question "what is the probability make a transition into some final state $|\,f\,\rangle$, starting from some initial state $|\,i\,\rangle$?". We need it when the complete Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{H}'(t)$ is too complex to solve the TDSE. Whenever we can solve the TDSE on a computer we do not need perturbation theory, but it might still be nice to gain some analytical insights.

(ii) Revise the general formula for the transition from state $|\,i\,\rangle$ to state $|\,f\,\rangle$ in first order time-dependent perturbation theory, and describe the key terms in it and their interpretation.
Solution: See Eq. (9.10) in the lecture:

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_0^t dt' \;\underbrace{e^{i(E_f^{(0)}-E_i^{(0)})t'/\hbar}}_{=A}\underbrace{\langle\,\phi_f^{(0)}\,|\hat{H}'(t')|\,\phi_i^{(0)}\,\rangle}_{=B} \tag{1}$$

The key-pieces are marked with $\underbrace{\cdots}_{A/B}$. A depends only on energy differences between the two states and will thus have to contain information an how energetically accessible the transition is. The matrix element B will also contain some time dependence from $\hat{H}'$ (which helps decide if the perturbation can "supply/substract the missing/excess energy", but it also encodes the operator structure of $\hat{H}'$. This often encodes whether the perturbation has the right symmetry/shape to cause the transition in question. We had seen examples of how this works in Assignment 5.

(iii) Discuss the special case for a periodic perturbation and what physical requirements on the quantum state transition the different mathematical terms encode.
Solution: For a periodic perturbation $\hat{H}'(t) = \hat{V}\cos(\omega t)$ with frequency ω we had further boiled down Eq. (1) into Eq. (9.24) of the lecture:

$$P_f(t) = \frac{|V_{fi}|^2}{\hbar^2|\omega_{fi}-\omega|^2}\sin^2\left[(\omega_{fi}-\omega)\frac{t}{2}\right]]. \tag{2}$$

Here we see all the statement from (ii) even more clearly: $V_{fi} = \langle\,f\,|\hat{V}|\,i\,\rangle$ decides if the perturbation contains "the right operator" to cause this transition. For example for the particle in the box we had seen that a spatially constant oscillating force can not cause direct transitions from even symmetry states to even symmetry states. The term $|\omega_{fi}-\omega|^2$

directly tells us that transitions where there is a large mismatch between the energy associated with the perturbation ($\hbar\omega$), and the transition energy $\hbar\omega_{fi}$ will be less likely.

Stage 2 Rabi oscillations: Discuss Rabi oscillations in section 9.3.5 on your table for the resonant case ($\Delta = 0$).

(i) Then run the app http://www.falstad.com/qmatomrad/ , which handles transitions between electronic states of a Hydrogen atom coupled with a periodically oscillating electric field in various choosable directions. The Hamiltonian thus is:

$$\hat{H} = \hat{H}_{hyd} + e\mathbf{E}_0 \cdot \hat{\mathbf{r}} \cos(\omega t) \tag{3}$$

with $\mathbf{E}_0 = E_0 \mathbf{e}_{x,y,z}$ with the direction of $\mathbf{E}_0$ indicated in the app. The app only considers resonant perturbations, such that $\hbar\omega = E_n - E_m$ for two Hydrogen states n and m. Discuss how features you see in the animation relate to what you learnt about Rabi-oscillations, what information decides which two Hydrogen states are involved, and why only two become relevant in this app.
Solution: We can see how the electronic state changes completely from the initial state to the final state. In between, we have a quantum superposition of both, which causes the electron density to oscillate in time, with a frequency equal to the transition frequency. We see that the initial state, electric field direction and excitation frequency together decide which two states are showing Rabi oscillations. The field direction enters $\langle f|\hat{V}|i\rangle$, see equation (9.43), (9.44), and in the perturbative regime the frequency "selects" one of the states with non-vanishing $\langle f|\hat{V}|i\rangle$ since all other-states will be "off-resonant" and thus not participate due to Eq. (2).

(ii) **Bonus:** Also discuss what behavior of the electron dipole $\langle e\hat{\mathbf{r}}\rangle$ corresponds to the electron wavefunctions shown, and how this relates to the emission of absorption of radiation (thinking about the latter in terms of classical electromagnetism for now).
Solution: The oscillating charge density of the electron represents an oscillating dipole, the frequency of which matches that of the radiation field. We can think of this as either the dipole emitting radiation or absorbing radiation, which it is depends on the relative phase between dipole oscillation and field.

(iii) **Bonus:** You can also check out http://www.falstad.com/qm1drad/ , which handles dynamics of the particle in the box subject to a periodically oscillating force along the x-direction, just as we had seen in QM-1 assignment5Q2 and are presently seeing in assignment 6 Q4 (see those for the Hamiltonian). In contrast to the first app, it allows you to chose an

arbitrary frequency ω and strength F_0 for the perturbation. Play with those and discuss what happens and understand why.
Solution: We can choose a very strong field such that we can see its effect in the potential itself. In that case the particle wavefunction will get strongly excited in many excited states and complicated dynamics ensues. Here we are outside of the range of applicability of perturbation theory [see stage 3(i)(c)]. For weaker perturbations, we generally see that just a few of the excited state amplitudes (little rotating arrows at the bottom) become relevant. Overall, this app would be nicer if one could control the frequency in a way that one can hit a resonance on purpose.

Stage 3 Interaction of electro-magnetic waves with matter: Consider an arbitrary quantum system for which we assume we know the unperturbed spectrum

$$\hat{H}^{(0)}|\,\phi_n\,\rangle = E_n|\,\phi_n\,\rangle. \tag{4}$$

The system contains particles that are affected by electro-magnetic fields, such that the system is subject to a perturbing Hamiltonian

$$\hat{H}'(t) = \hat{V}\cos(\omega t) \tag{5}$$

if a monochromatic electro-magnetic wave of frequency ω hits it. Consider $\hbar\omega$ to be of the order of the $E_n - E_m$. Note that this a very general setting throughout physics, the states could describe eigen-energies of (nuclei/atoms/molecules) or quasi-particle energies in materials (excitons/phonons/polarons etc.) and waves can span the entire spectrum from gamma rays to radio. We assume the system is in the ground-state $|\,\phi_0\,\rangle$ initially.

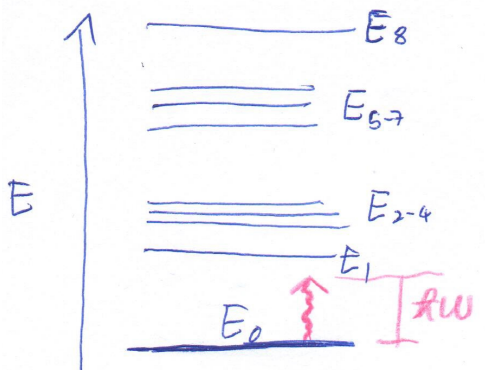

Figure 1: (**stage 3**) Cartoon of a quantum system with discrete energies, interrogated by monochromatic radiation.

(i) Initially assume all $\langle\,\phi_m\,|\hat{V}|\,\phi_n\,\rangle = V_0 \neq 0$. Consider the cases where (a) ω is closer to $E_k - E_0$ than to any other energy differences but $|\hbar\omega - (E_k - E_0)| \gg V_0$, (b) $\hbar\omega = E_k - E_0$ for some k, and

$|\hbar\omega - (E_n - E_0)| \gg V_0$ for all other $n \neq k$ and (c) $V_0 \gg |\hbar\omega - (E_n - E_0)|$ for a large number of n. In each case discuss qualitatively (or quantitatively if possible) what you expect to happen once the elm. wave hits the system and how you can know this.
Solution: (a) $[\hbar\omega - (E_k - E_0)] = \hbar\Delta$ *is called the detuning. Thanks to* $[\hbar\omega - (E_k - E_0)] \ll V_0$ *we can hope to apply perturbation theory. Then based on (2) we see that in this case we get the picture from page 222 or bottom page 232 (red line): This is called detuned Rabi-oscillations, only a small probability of maximum* $p_k = |V_0/\hbar\Delta|^2$ *is reached in state* $|\,k\,\rangle$*, which oscillates as* $\sim \sin^2(\Delta t/2)$*. For all other states* $|\,m\,\rangle$ $|\hbar\omega - (E_m - E_0)| = \hbar|\Delta_m|$ *will be way larger, so these can be neglected. (b) In this case the perturbation is fully resonant with the* $|\,0\,\rangle \to |\,k\,\rangle$ *transition. We had seen in section 9.3.5 that in this case the population in* $|\,k\,\rangle$ *will at some point reach* 1 *which necessarily invalidates perturbation theory (since the time evolving perturbation of the state cannot be considered small compared to the initial state). We instead see coherent Rabi oscillations as discussed in section 9.3.5 with Rabi frequency* $\hbar\Omega = V_0$*. Even in this case we can use perturbative arguments to justify why we only needed to consider two states: For all other ones again* $\hbar\Delta_m$ *will be very large, so we can neglect them. (c) If* $V_0 \gg |\hbar\omega - (E_n - E_0)|$ *for a large number of n neither perturbation theory nor a two-level picture will do us much good. With similar arguments as above, we would have to consider many levels and dynamics can be quite complicated. See app in Stage 2 (ii).*

(ii) Typically the $\langle\,\phi_m\,|\hat{V}|\,\phi_n\,\rangle$ will not be all equal. Discuss what information they contain and through which principles you can often infer which ones are non-zero.
Solution: Content see Stage 1. Principles: Symmetry and conservation laws.

(iii) **Bonus:** While the discussion above forms the basis of interactions of electro-magnetic waves with matter, there is lots and lots of complications, details and effects that are not yet considered and you will learn later. Brainstorm some.
Solution: Polarisation, inhomogeneous fields, non-monochromatic fields, incoherent fields, backaction between quantum system and field (i.e. absorption or amplification), QED. See PHY402 for some of those.

(iv) What changes in the picture if we do not start in the ground-state, but an excited state $|\,\phi_e\,\rangle$?
Solution: All the above also applies to downwards transitions in energy. The classical electromagnetic field assumed here makes no distinction between up and down in energy. See discussion of absorption versus stimu-

lated emission in the lecture, and more in PHY402.