Approximation Scheme for Time Dependent Problems
24.3 Resonance transitions*

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§1 Probability for Resonance Transitions

The case of periodic perturbation with a single frequency is an important one for many physical situations including the interaction of radiation with matter Assuming that H' varies periodically with time with a single frequency ω we write

$$H' = Fe^{i\omega t} + F^* e^{-i\omega t} \tag{1}$$

where F is an operator which does not depend on t explicitly. Let us substitute Eq.(1) in Eq.(**??**) and integrate to get

$$C_f^{(1)}(t) = \langle f|F|i\rangle \left[\frac{e^{i(\omega_{fi}-\omega)t} - 1}{-\hbar(\omega_{fi} - \omega)}\right] + \langle f|F^\dagger|i\rangle \left[\frac{e^{-i(\omega_{fi}+\omega)t} - 1}{-\hbar(\omega_{fi} + \omega)}\right] \tag{2}$$

Further analysis of the above relations depends on whether the final state f corresponds to some discrete energy level or to a state in continuum.

In this section we consider the case of resonance transition from an initial discrete level i to a final discrete level f when the applied perturbation varies harmonically in time. Here the term level refers to an energy level of H_0. The first order perturbation result for a transitions between two discrete levels is

$$C_f^{(1)}(t) = \langle f|F|i\rangle \left[\frac{e^{i(\omega_{fi}-\omega)t} - 1}{-\hbar(\omega_{fi} - \omega)}\right] + \langle f|F^\dagger|i\rangle \left[\frac{e^{-i(\omega_{fi}+\omega)t} - 1}{-\hbar(\omega_{fi} + \omega)}\right] \tag{3}$$

When the frequency $\hbar\omega$ is close to one of the two differences $E_i - E_f$, or $E_f - E_i$, the above result blows up and the perturbation theory breaks down. In this case we must get back to the exact equations and analyze them again making a different kind of approximation. We will do so and *solve the resulting approximate equations exactly.*

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We start with Eq.(**??**) after substituting

$$H' = Fe^{i\omega t} + F_1 e^{-i\omega t}. \tag{4}$$

we get

$$\begin{aligned} i\hbar\frac{dC_m(t)}{dt} &= \sum_n \exp\big(i(\omega_{mn}+\omega)t\big)\langle m|F|n\rangle C_n(t) \\ &\quad + \sum_n \exp\big(i(\omega_{mn}-\omega)t\big)\langle m|F^\dagger|n\rangle C_n(t). \end{aligned} \tag{5}$$

In the perturbation approximation after integration, the large coefficients came from those terms which were multiplied with an exponential with a small argument. For a given ω when there are two energy levels i and f such that $|E_f - E_i|$ matches with ω, we need to retain *all* the terms involving the two coefficients C_i and C_f in the summation in the right hand side of Eq.(5). Thus the resulting approximate equations to be solved assume the form

$$i\hbar\frac{dC_f(t)}{dt} = e^{i(\omega_{fi}+\omega)t}\langle f|F|i\rangle C_i(t) \quad + \quad e^{i(\omega_{fi}-\omega)t}\langle f|F^\dagger|i\rangle C_i(t), \tag{6}$$

and

$$i\hbar\frac{dC_i(t)}{dt} = e^{i(\omega_{if}+\omega)t}\langle i|F|f\rangle C_f(t) \quad + \quad e^{i(\omega_{if}-\omega)t}\langle i|F^\dagger|f\rangle C_f(t). \tag{7}$$

In these equations we retain only those exponentials which have small arguments. Taking $\hbar\omega \approx (E_f - E_i)$, using the notation $\nu \equiv \omega_{fi} - \omega$, and therefore writing $\omega_{if} + \omega = -\nu$, we get

$$i\hbar\frac{dC_f(t)}{dt} = \langle f|F^\dagger|i\rangle e^{i\nu t} C_i(t) \tag{8}$$

$$i\hbar\frac{dC_i(t)}{dt} = \langle i|F|f\rangle e^{-i\nu t} C_f(t) \tag{9}$$

Next we solve these equations exactly with the initial conditions $C_i(0) = 1, C_f(0) = 0$. The probability of transition from the initial level E_i to the final level E_f at time t is then given by

$$\boxed{P_{i\to f}(t) = \frac{2|\langle f|F|i\rangle|^2}{\hbar^2\Omega^2}|\{1-\cos\Omega t\}} \tag{10}$$

where

$$\Omega^2 = \frac{\hbar^2\nu^2 + |\langle f|F|i\rangle|^2}{\hbar^2} \tag{11}$$

It is to noted that the transition probability is periodic in time with the period $2\pi/\Omega$ and its varies from 0 to a maximum value

$$\frac{2|\langle f|F|i\rangle|^2}{\hbar^2\nu^2 + 4|\langle f|F|i\rangle|^2} \tag{12}$$

For the exact resonance $\nu = \frac{E_f - E_i - \hbar\omega}{\hbar} = 0$ and and we get the transition probability to be

$$\boxed{P_{i\to f}(t) = \frac{1}{2}\big(1 - \cos 2|\langle f|F|i\rangle|t/\hbar\big)} \tag{13}$$

and the system makes periodic transitions between the levels i and f with the period $\pi\hbar/|\langle f|F|i\rangle|$

§2 Details of solution

For the resonance transitions the equations satisfied by the coefficients C_i and C_f, Eq.(8) and Eq.(9), are

$$i\hbar\frac{dC_f(t)}{dt} = \langle f|F^\dagger|i\rangle e^{i\nu t} C_i(t) \tag{14}$$

$$i\hbar\frac{dC_i(t)}{dt} = \langle i|F|f\rangle e^{-i\nu t} C_f(t) \tag{15}$$

In this section we solve these equations exactly and obtain expressions for $C_i(t)$ and $C_f(t)$. To solve we define

$$b_f = C_f \exp(-i\epsilon t) \tag{16}$$

so that

$$\begin{aligned} \frac{d}{dt}C_f(t) &= \frac{d}{dt}\Big(b_f e^{i\epsilon t}\Big) && (17)\\ &= \Big(\frac{d}{dt}b_f + i\epsilon b_f\Big)e^{i\epsilon t} && (18)\end{aligned}$$

Eliminating C_fEq.(14) and Eq.(15), using Eq.(16) and Eq.(17), we get

$$\dot{C}_i = \frac{1}{i\hbar}\langle i|F|f\rangle b_f \tag{19}$$

and

$$\begin{aligned} \dot{b}_f + i\epsilon b_f &= \frac{1}{i\hbar}\langle f|F^\dagger|i\rangle C_i \\ &= \frac{1}{i\hbar}\langle f|F|i\rangle^* C_i && (20)\end{aligned}$$

Eliminating C_i from Eq.(18) and Eq.(20) we get

$$\begin{aligned} \ddot{b}_f + i\epsilon\dot{b}_f &= \frac{1}{i\hbar}\langle f|F^\dagger|i\rangle \dot{C}_i \\ &= -\frac{|F_{fi}|^2}{\hbar^2}b_f && (21)\end{aligned}$$

Therefore, we have

$$\ddot{b}_f + i\epsilon\dot{b}_f + \frac{|F_{if}|^2}{\hbar^2}\dot{b}_f = 0 \tag{22}$$

This is a linear differential equation with constant coefficient and can be solved exactly. The solutions of Eq.(22) have the form

$$b_f(t) = \exp(i\alpha t) \tag{23}$$

where α satisfies the equation

$$\alpha^2 + \epsilon\alpha - \frac{|F_{if}|^2}{\hbar^2} \tag{24}$$

The two roots of this equation are $\alpha_\pm$ where

$$\alpha_\pm = -\frac{\epsilon}{2} \pm \Delta \tag{25}$$

where Δ is given by

$$\Delta^2 = \frac{\epsilon^2}{4} + \frac{|F_{if}|^2}{\hbar^2} \tag{26}$$

Substituting back in Eq.(23) the general solution for b_f becomes

$$b_f(t) = A\exp(i\alpha_+ t) + B\exp(i\alpha_- t) \tag{27}$$

and hence

$$C_f(t) = \Big[A\exp(i\alpha_+ t) + B\exp(i\alpha_- t)\Big]\exp(i\epsilon t) \tag{28}$$

We then get, from Eq.(15),

$$\begin{aligned} C_i(t) &= \left(\frac{i\hbar}{F^*_{if}}\right)\big[iA\alpha_+\exp(i\alpha_+ t) + i\alpha_- B\exp(i\alpha_- t) \\ &\quad + i\epsilon A\exp(i\alpha_+ t) + i\epsilon B\exp(i\alpha_- t)\big] && (29)\end{aligned}$$

At time $t = 0$, the initial conditions are $C_i(0) = 1$ and $C_f(0) = 0$ giving

$$\begin{aligned} iA\alpha_+ + iB\alpha_- + i\epsilon(A+B) &= F^*_{if}/\hbar && (30)\\ A + B &= 0 && (31)\end{aligned}$$

Using Eq.(29) and Eq.(30) we get

$$A(\epsilon/2 + \Delta) + B(\epsilon/2 - \Delta) = -\frac{F^*_{if}}{\hbar} \tag{32}$$

or

$$2A\Delta = -\frac{F_{if}}{\hbar} \quad (33)$$

$$A = -\frac{F_{if}}{2\Delta\hbar} \quad (34)$$

$$B = \frac{F^*_{if}}{2\hbar\Delta} \quad (35)$$

Rearranging Eq.(29) and using $B = -A$ we get

$$C_i(t) = \left(\frac{i\hbar}{F^*_{if}}\right)\Big[iA(\epsilon+\alpha_+)\exp(i\alpha_+ t) + iB(\epsilon+\alpha_-)\exp(i\alpha_- t)\Big] \quad (36)$$

$$= \left(\frac{i\hbar}{F^*_{if}}\right)(iA)\Big[(\epsilon+\alpha_+)\exp(i\alpha_+ t) - (\epsilon+\alpha_-)\exp(i\alpha_- t)\Big] \quad (37)$$

Substituting for $\alpha_\pm$ from Eq.(25) we get

$$C_i(t) = \left(\frac{i\hbar}{F^*_{if}}\right)\left(\frac{-iF^*_{if}}{2\Delta\hbar}\right) \times \exp(-i\epsilon t/2) \times\Big[(\epsilon/2+\Delta)e^{i\alpha_+ t} - (\epsilon/2+\Delta)e^{i\alpha_- t}\Big] \quad (38)$$

$$= \frac{1}{2\Delta}\exp(-i\epsilon t/2)\Big[2\Delta\cos(\Delta t) + i\epsilon\sin(\Delta t)\Big] \quad (39)$$

and $C_i(t)$ is given by

$$C_i(t) = e^{-i\frac{\epsilon t}{2}}\left(\cos\Delta t + i\frac{\epsilon}{2\Delta}\sin\Delta t\right) \quad (40)$$

Also Eq.(28) with $B = -A$ gives

$$C_f(t) = A\exp(i\epsilon t)\big[\exp(i\alpha_+ t) - \exp(i\alpha_- t)\big] \quad (41)$$

$$= 2iA\exp(i\epsilon t/2)\sin\Delta t \quad (42)$$

$$= -\left(\frac{iF^*_{if}}{\Delta\hbar}\right)\sin\Delta t \quad (43)$$

Hence the probability o finding the system in the state f at time t is

$$|C_f(t)|^2 = \frac{|F_{if}|^2}{\Delta^2\hbar^2}\sin^2\Delta t \quad (44)$$

$$= \frac{|F_{if}|^2}{\Delta^2\hbar^2}\sin^2\left(\frac{\epsilon^2}{4} + \frac{|F_{if}|^2}{\hbar^2}\right)^{1/2} t \quad (45)$$

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