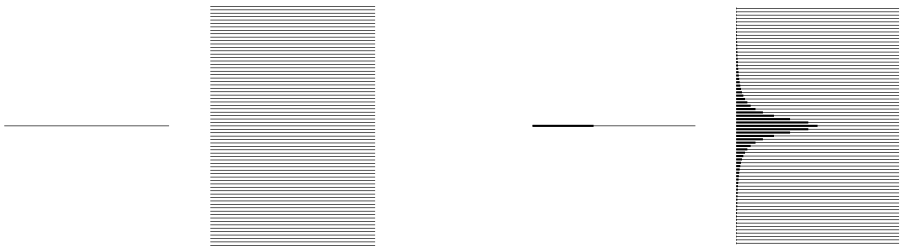
Light - Atom Interaction



PHYS261 autumn 2011

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Version 24.11.2011

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Time dep. QM- two-well problem
One level in continuum
Time-Dependent Schrödinger Equation
Perturbation theory for TDSE
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Fermi Golden Rule
Constant rate and exponent. decay
Line width from exponential decay

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Overview

1. Time dependent quantum mechanics:

   two isolated states, contrasted to

   one isolated level

   energetically embedded in (quasi-) continuum of states

2. derivation and understanding of the transition rate (probability change per time unit)

3. Time dependent perturbation theory

4. Fermi Golden rule derivation

5. The delta function (often mentioned as energy conservation; that is not precise).

6. In contrast to the delta function, the Lorentzian shape; finite line width (also known as Breit-Wigner formula or shape)

7. Electromagnetic field is an extended (actually continuous) system, therefore we must learn how to understeand eigenmodes of large system. Coupled oscillators transformed to a system of independent, de-coupled eigenmodes.

8. Any harmonic oscillator can be described by so called creation and anihilation operators. Harmonic oscillator via the algebraic method.

9. Follows quantization of the radiation field; **photons**

10. Evaluation of the transmissin rate for the emission proces

11. Spontaneous and Stimulated Emission

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1 Time dependent Q.M. illustrated on the two-well problem

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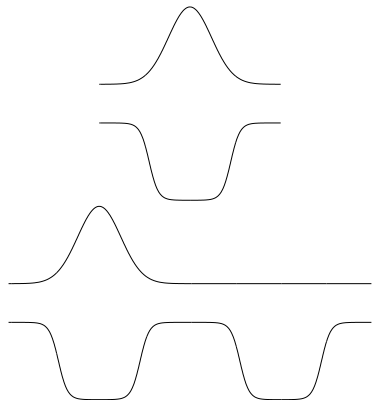


Figure 1: Above: Well with 1 bound state; Below: Two wells. System (particle) placed in a state which is not an eigenstate

The two eigenstates in each of the isolated wells are φ_1 and φ_2.

The static eigenstates of the particle confined to both of the wells are approximated by

$$\psi_+ = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$

$$\psi_- = \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$$

clearly,

$$\varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

$$\varphi_2 = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)$$

The states ψ_+, ψ_- are eigenstates of the Hamiltonian, but φ_1, φ_2 are not, they are eigenstates for each isolated well. Go to list of topics

If at $t = 0$ the system is brought into the state φ_1,

$$\Psi(t = 0) = \varphi_1 = \frac{1}{\sqrt{2}} (\psi_+ + \psi_-)$$

then at any other later time

$$\Psi(t) = \frac{1}{\sqrt{2}} \left(\psi_+ e^{iE_+ t/\hbar} + \psi_- e^{iE_- t/\hbar} \right)$$

This can be rewritten schematically as

$$\Psi(t) = C(t) \left(\psi_+ + \psi_- e^{i\omega t} \right)$$

so that we can see immediately that for

$$t_n = n \frac{\pi}{\omega}$$

the $\Psi(t_n)$ will be a multiple of φ_1,i.e.concentrated to the left, for even n, and a multiple of φ_2,i.e.concentrated to the right, for odd n. At general times there would be a continuously changing distribution between the two regions. List of topics

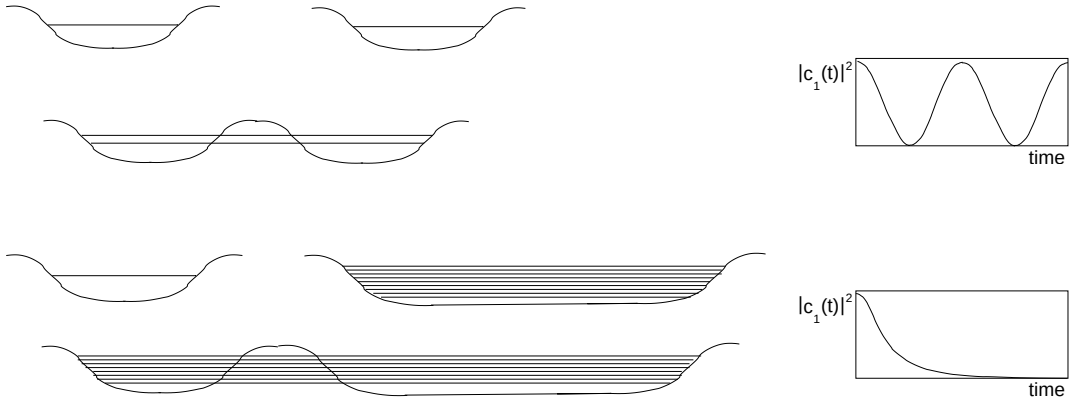
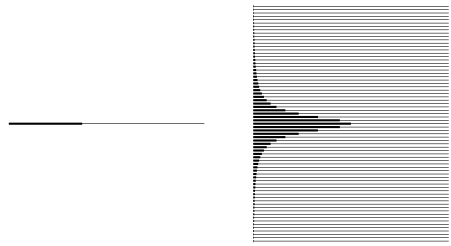


Figure 2: Above: 2 isolated states in two equal potential wells ; starting in left well - oscillations. Below: Many states in two potential wells; starting in left well - decay Go to list of topics



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2 Time-Dependent Schrödinger Equation

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The time-dependent Schrödinger equation

$$i\,\hbar\,\frac{\partial}{\partial \mathrm{t}}\,|\,\psi(t)\,\rangle = H(t)\;\;|\,\psi(t)\,\rangle \tag{3}$$

is very often solved via a transformation to the matrix formulation. The matrix formulation arises from expansion of the unknown wavefunction $|\,\psi(t)\,\rangle$ in a set of basis functions $|\,\phi_i\,\rangle$, much in analogy with Fourier series or expansions using orthogonal polynomials

$$|\,\psi(t)\,\rangle = \sum \alpha_i(t)\,|\,\phi_i\,\rangle \tag{4}$$

The unknown quantities to be found are the expansion coefficients, which form a vector. In this formulation, the time-dependent Schrödinger equation (eq. (3) above) is replaced by a set of coupled differential equations.

The system of coupled equations is conveniently expressed by matrix notation

$$i\,\hbar\,\frac{\mathrm{d}}{\mathrm{dt}}\begin{bmatrix}\alpha_1\\ \alpha_2\\ .\\ \alpha_n\end{bmatrix} = \begin{bmatrix}H_{11}(t) & H_{12}(t) & ... & H_{1n}(t)\\ H_{21}(t) & H_{22}(t) & ... & H_{2n}(t)\\ ... & ... & ... & ...\\ H_{n1}(t) & H_{n2}(t) & ... & H_{nn}(t)\end{bmatrix}\begin{bmatrix}\alpha_1\\ \alpha_2\\ .\\ \alpha_n\end{bmatrix}$$

where

$$H_{ij}(t) \;=\; \langle\ \phi_i\ \mid H(t) \mid\ \phi_j\ \rangle$$

This can also be written as

$$i\,\hbar\begin{bmatrix}\dot{\alpha}_1\\ \dot{\alpha}_2\\ .\\ \dot{\alpha}_n\end{bmatrix} = \begin{bmatrix}H_{11}(t) & H_{12}(t) & ... & H_{1n}(t)\\ H_{21}(t) & H_{22}(t) & ... & H_{2n}(t)\\ ... & ... & ... & ...\\ H_{n1}(t) & H_{n2}(t) & ... & H_{nn}(t)\end{bmatrix}\begin{bmatrix}\alpha_1\\ \alpha_2\\ .\\ \alpha_n\end{bmatrix}$$

which is a short-hand notation for

$$i\,\hbar\,\dot{\alpha}_k = \sum_i\ H_{ki}(t)\ \alpha_i$$

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3 Perturbation theory for the Time-dependent Schrödinger Equation

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To apply the perturbation theory, we must identify the small additional energy. It is usually a Hamiltonian $H(t)$, which differs only slightly from well known Hamiltonian H^0

$$H(t) \;=\; H^0 \;+\; H'(t) \tag{5}$$

If the $H'(t)$ were not present, and chosing then as $\mid \phi_k \rangle$ the eigensolutions of

$$H^0 \mid \phi_k \rangle = E_k \mid \phi_k \rangle \tag{6}$$

the matrix for $H(t) \rightarrow H^0$ would be diagonal with the eigenenergies E_k on the diagonal. The solutions for the the $\alpha_k(t)$ would be then very simply

$$\alpha_k(t) = e^{-iE_k t/\hbar} \tag{7}$$

and for usual stationary states only one of the $\alpha_k(t)$ would be different from zero. Since the probability P_a of the system being in a state a is

$$P_a(t) = |\alpha_a(t)|^2$$

it means that the system with probability 1 is in that state a, and with 0 in any other state, i.e.

$$|\alpha_k(t=0)| = \delta_{ka} \tag{8}$$

If the perturbation really is small, the $|\alpha_a(t)|$ remains ≈ 1 for all times t, while all others remain close to zero.

We will thus use the so called perturbation theory, an approximate method to solve the system of equations

$$i\,\hbar\,\dot{\alpha}_k = \sum_i H_{ki}(t)\;\alpha_i$$

while keeping

$$|\alpha_a(t)| \approx 1 \qquad\qquad \longrightarrow \alpha_a(t) = 1$$

and preserving

Go to list of topics

$$|\alpha_k(t=0)| = \delta_{ka} \qquad\longrightarrow\qquad |\alpha_k(t>0)| \approx 0 \quad \text{for} \quad k \neq a$$

To work with these assumptions we make a substitution $\alpha_k(t) \rightarrow c_k(t)\exp(-i\frac{E_k}{\hbar}t)$. Inserting this into the last equation

$$i\ \hbar\ \dot{\alpha}_k = \sum_i\ H_{ki}(t)\ \alpha_i$$

we get (using $d/dt(c\exp(-iEt)) = \dot{c}\exp(-iEt) + -iE\ c\exp(-iEt)$)

$$(i\ \hbar\ \dot{c}_k\ +\ E_k\ c_k)\exp(-i\frac{E_k}{\hbar}t)\ =\ \sum_i\ H^0_{ki}\ c_i\exp(-i\frac{E_i}{\hbar}t) + \sum_i\ H_{ki}(t)\ c_i\exp(-i\frac{E_i}{\hbar}t)$$

$$\text{With}\quad H^0_{ki} = E_k\delta_{ki} \qquad\qquad \omega_{ka} = \frac{E_k - E_a}{\hbar} \qquad (9)$$

$$i\ \hbar\ \dot{c}_k\ +\ E_k\ c_k\ =\ E_k\ c_k\ +\ \sum_i\ H'_{ki}(t)\ c_i\exp(i\frac{E_k - E_i}{\hbar}t)$$

$$i\ \hbar \begin{bmatrix} \dot{c}_1 \\ \dot{c}_2 \\ . \\ \dot{c}_n \end{bmatrix} = \begin{bmatrix} H'_{11}(t) & H'_{12}(t)e^{i\omega_{12}t} & ... & H'_{1n}(t)e^{i\omega_{13}t} \\ H'_{21}(t)e^{i\omega_{21}t} & H'_{22}(t) & ... & H'_{2n}(t)e^{i\omega_{2n}t} \\ ... & ... & ... & ... \\ H'_{n1}(t)e^{i\omega_{n1}t} & H'_{n2}(t)e^{i\omega_{n2}t} & ... & H'_{nn}(t) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ . \\ c_n \end{bmatrix}$$

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Taking the perturbation theory assumptions

$$||\alpha_a(t)| \approx 1|\alpha_{k\neq a}(t>0)| \approx 0 \qquad \longrightarrow \qquad \alpha_k(t=0)| = \delta_{ka}$$

the above matrix system of coupled equations decouple - we get independent equations for each $c_k(t)$

$$i\ \hbar\ \frac{d}{dt}c_k(t) = H_{ka}(t)e^{i\omega_{ka}t} \tag{10}$$

where we made a substitution $\alpha_k(t) \to c_k(t)\exp(-i\frac{E_k}{\hbar}t)$.

We say that the original assumption about the coefficients is a *'zero-th order* approximation, thus the superscript (0),

$$c_k^{(0)} = \delta_{ka} \qquad (\delta_{(k-a)}) \tag{11}$$

while the above equation is the first order, thus we rewrite it

$$\dot{c}_b^{(1)} = \frac{1}{i\hbar}H' e^{(i\omega_{ba}t)} \tag{12}$$

A detailed description of perturbation theory pictures it as an iterative process. Each order is obtained by applying the preceeding order of the approximation.
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Equation of the form $\dot{c} = f(t)$ is easily solved by integration

$$c_b^{(1)}(t) = \frac{1}{i\hbar}\int_{t_b}^{t} H' e^{(i\omega_{ba}t')} dt' \qquad H'(t) \equiv H' \tag{13}$$

So the transition probability for going from a state 'a' to a state 'b' is defined like Go to list of topics

$$P_{ba}(t) = |c_b^{(1)}(t)|^2 \tag{14}$$

Now we evaluate the integral in eq.(13), which is elementary for a constant potential: Go to list of topics

$$\begin{aligned} c_b^{(1)}(t) &= H'_{ba}\frac{1}{i\hbar}\int_{t_0}^{t} e^{i\omega_{ba}t} dt \quad ; \quad t_0 = 0 \\ &= H'_{ba}\frac{1}{i\hbar}\frac{1}{i\omega_{ba}}(e^{i\omega_{ba}t} - 1) \\ &= -\frac{H'_{ba}}{\hbar\omega_{ba}}(e^{i\omega_{ba}t} - 1) \end{aligned} \tag{15}$$

and rearrange $(e^{i\omega t} - 1)$ (in the following: $\omega_{ba} \longrightarrow \omega$)

$$\begin{aligned} e^{(i\omega t)} - 1 &= e^{(i\frac{\omega t}{2})}\left[e^{(i\frac{\omega t}{2})} - e^{(-i\frac{\omega t}{2})}\right] \\ &= 2ie^{(i\frac{\omega t}{2})}\sin\frac{\omega t}{2} \end{aligned}$$

Inserting this back into eq.(13)

$$c_b^{(1)}(t) = \frac{1}{i\hbar}\int_{t_0}^{t} H' e^{i\omega t'} dt' \tag{16}$$

$$|c_b^{(1)}(t)|^2 = \frac{1}{\hbar^2}|H'_{ba}|^2 F(t,\omega) \tag{17}$$

where the phase factor reduces to its absolute value one.

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4 Dirac delta-function

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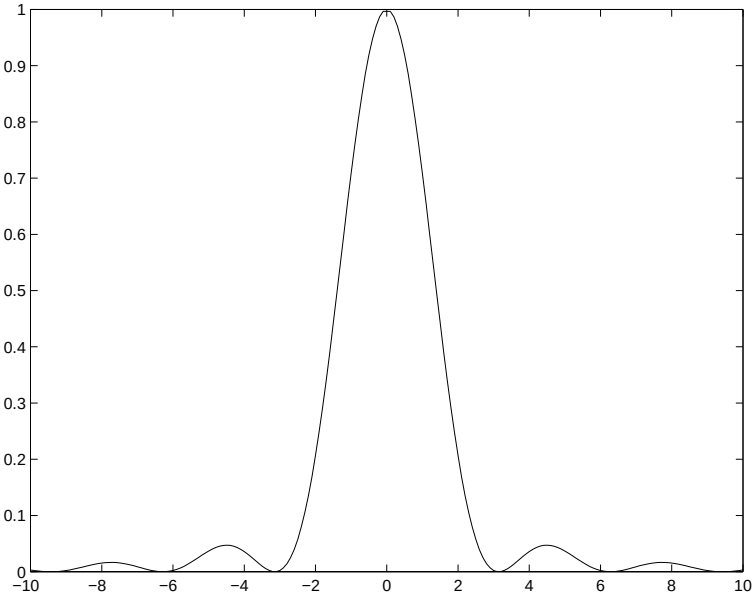
It is easy to find that the 'F' is a function of t and ω, and for each time 't' it is equal to

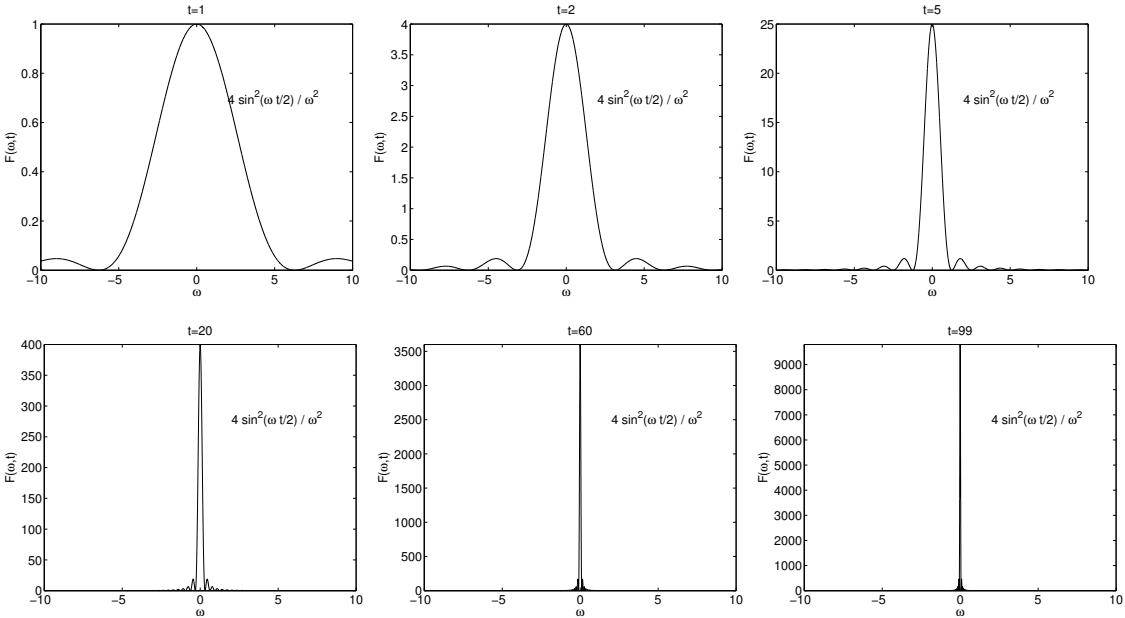
$$\begin{aligned} F(t,\omega) &= 4 \cdot \frac{\sin^2 \frac{\omega t}{2}}{\omega^2} \\ &= 4 \cdot \frac{t^2}{4} \cdot \frac{\sin^2 \frac{\omega t}{2}}{\frac{\omega^2 t^2}{4}} \\ &= t^2 \cdot \frac{\sin^2 x}{x^2} \quad ; \quad x = \frac{\omega t}{2} \end{aligned} \tag{18}$$

It can be seen that the function $F(\omega, t)$ for larger and larger t approaches the shape of the Dirac delta-function, (see the drawing). (Animated on the www)



Plot of the function

$$\frac{\sin^2 x}{x^2}$$



Approaching the δ-function with increasing t: Go to list of topics

$$F(\omega, t) = 4 \cdot \frac{\sin^2 \frac{\omega t}{2}}{\omega^2}$$

Trying to integrate the function 'F' over ω shows this

$$\begin{aligned} t^2 \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} d\omega &= 2t \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} \cdot d(\frac{\omega t}{2}) \\ &= 2t \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx \\ &= 2\pi t \end{aligned} \tag{19}$$

that for large t it really behaves as

$$F(t,\omega) = \frac{\sin^2 \frac{\omega t}{2}}{(\frac{\omega}{2})^2} \longrightarrow 2\pi t \delta(\omega) \tag{20}$$

The summation over all the states used for the expansion can be assumed to be replaced by the integration over ω or the energy $E = \hbar\omega$. This however needs to determine the factor $\rho(E)$ which accounts for the density of states. Since the 'F' approaches delta-function, we only need the density of states close to the final state b:

$$\bar{P}_{ba}(t) = \frac{1}{\hbar^2} \int_{E_b-\eta}^{E_b+\eta} |H'_{ba}|^2 F(t,\omega)\rho(E)dE \tag{21}$$

and also integration over $d\omega$ gives

$$\begin{aligned} \int \delta(\omega)d\omega &= \int \delta(E)dE \\ \delta(\omega) &= \delta(E) \cdot \frac{dE}{d\omega} \\ &= \hbar\delta(E - E_b) \end{aligned} \tag{22}$$

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5 Fermi Golden Rule

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The final result is

$$\begin{aligned} P_{ba}(t) &= \frac{1}{\hbar}\int_{E_b-\eta}^{E_b+\eta} 2\pi t|H'_{ba}|^2\delta(E-E_b)\rho(E)dE \\ &= \frac{2\pi}{\hbar}t|<b|H'|a>|^2\rho(E_b) \end{aligned} \tag{23}$$

The derivation of the above formula has been based on the assumption of a small perturbation. It shows that the probability of transition to the state b or states close to b increases linearly with time. Thus the rate of probability change per time is given by

$$\frac{dP_{ba}}{dt} = W_{ba} = \frac{2\pi}{\hbar}|<b|H'|a>|^2\rho(E_b) \tag{24}$$

This result is known as *Golden Rule* formula or *Fermi Golden Rule*.

6 Constant rate and exponential decay

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Fermi golden rule gives a constant rate

$$\frac{dP_f}{dt} = w \tag{25}$$

or if we consider the probability decrease to find the system in the original state,

$$\frac{dP_i}{dt} = -w \tag{26}$$

If this, instead of a definition, is taken as a differential equation

$$P_i = P_0 - wt \tag{27}$$

can quickly become negative.However, one can quite easily realize that the correct differential equation must be

$$\frac{dP_i}{dt} = -wP_i \tag{28}$$

since the loss of probability must be proportional to 'how much is left', i.e. the P_i itself.It can also be guessed from the differential equations of Q.M. (leading to the$\frac{dP_f}{dt}$) , since they contained the amplitude, which we replaced by 1.

The last differential equation leads to the well known exponential decay, since its solution is

$$P_i = e^{-wt} \tag{29}$$

since $P_i(t = 0) = 1$

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7 Line width from exponential decay

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In the equation (10) the expansion coefficient of the initial state $\alpha_0(t) \to 1$ for all times leads to the delta function for energy (frequency). In order to take into account the flow of probability from the initial state 0, the relation

$$\alpha_k(t) = \delta_{ka}$$

when working with the time dependent problem must be changed to

$$|\alpha_k(t)| = \delta_{ka} \exp(-\frac{w}{2}t)$$

where w is the constant rate factor obtained in the perturbation theory.

If we take into account the result of previous section 6, we have $|c_0(t)| \to \exp(-wt/2)$. Inserting this into equation (10), the integrals can still be performed, but the expressions which were found to converge to the δ-function in frequency (energy) for time going to infinity are not obtained. The term

$$\int V_{ba} e^{i\omega_{ba}t} dt$$

leading to

$$-V_{ba}\frac{1}{\omega_{ba}}(e^{i\omega_{ba}t}-1)$$

which has been shown to lead to δ-function like behaviour when integrated over ω is now replaced by

$$\frac{e^{i(\omega-\omega_{ba})t}e^{-wt/2}-1}{i(\omega-\omega_{ba})-\frac{w}{2}}$$

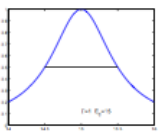
at large times t this leads to

$$\left|\frac{1}{i(\omega-\omega_{ba})-\frac{w}{2}}\right|^2=\frac{1}{(\omega-\omega_{ba})^2+\frac{1}{4}w^2}$$

The rate, which has the dimension of frequency becomes the energy width

$$\Gamma=\hbar w$$

when multiplied by $\hbar$. the so called Lorentz shape of the line,



$$I(E)\approx I_0\frac{\left(\frac{\Gamma}{2}\right)^2}{\left(E-E_0\right)^2+\left(\frac{\Gamma}{2}\right)^2} \qquad (30)$$

Thus a more realistic treatment than the perturbation theory with constant decay rate leads to the natural width of the energy spectrum of the ejeced photons as observed. This behaviour has been illustrated in our Golden Rule Simulator program

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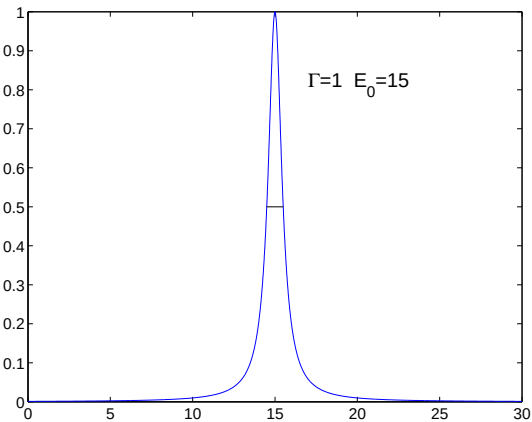

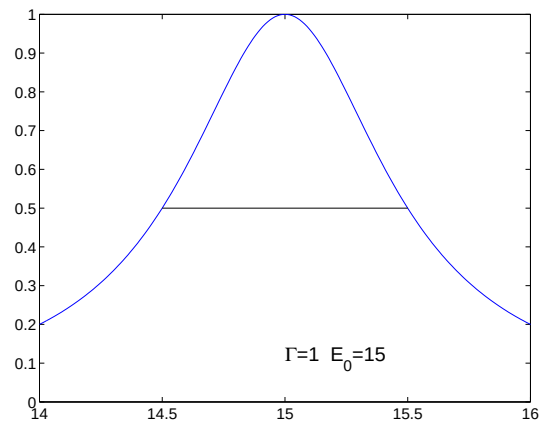

$$I(E) \approx I_0 \frac{\left(\frac{\Gamma}{2}\right)^2}{(E - E_0)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

8 Generally on quantum treatment of extended systems - fields.

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The system to be considered consists of an atom and the electromagnetic field.

The field has in principle infinitely many degrees of freedom, i.e. the values of field variables in each point of space.

The electromagnetic field can be treated by wave equations, it is thus a sort of harmonic system. The energy of a *finite* harmonic system can always be transformed to a sum of independent harmonic oscillators, each of them is in fact the eigenmode.

Each harmonic oscillator can be then described using the equations for harmonic oscillator, with the algebraic method and number of quanta states - The creation and annihilation operators - click 10.

The normal modes or eigenmodes for a general harmonic system are discussed in the section 9.

The prescription

1. identify the eigenmodes
2. quantize each of the modes as independent harmonic oscillator
3. use quanta of eigenmodes
4. express the general coordinates of the system using the eigenmode coordinates (inverse transformations to those discussed in section 9. Each coordinate χ_i will then be replaced by its combination of the creation and annihilation operators as discussed in section 10.

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9 Normal Coordinates for coupled harmonic vibrations.

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Transformation to normal coordinates can be described as follows:

Take the total energy, x represents the vector of all coordinates, x^{T} represents the transposed vctor, $\mathbf{M}$ is the mass matrix, $\mathbf{V}$ is the matrix which gives the potential energy, including the couplings.

Note that the mass matrix is written in a very general form, most often this matrix would be diagonal.

$$E = \frac{1}{2}\dot{\mathrm{x}}^{\mathrm{T}}\mathbf{M}\dot{\mathrm{x}} + \frac{1}{2}\mathrm{x}^{\mathrm{T}}\mathbf{V}\mathrm{x}$$

First we transform the kinetic energy to a "*spherical*" form

$$\frac{1}{2}\dot{\mathrm{x}}^T\mathbf{M}\dot{\mathrm{x}} = \frac{1}{2}\dot{\eta}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}\mathbf{M}\mathbf{S}\dot{\eta} = \frac{1}{2}\dot{\eta}^{\mathrm{T}}\dot{\eta}$$

This transformation does not conserve the lengths. The N-dimensional ellipsoid is transformed to an N-dim. sphere.

$$\mathbf{S}^{\mathrm{T}}\mathbf{M}\mathbf{S} = \mathbf{1}$$

If $\mathbf{M}_{ij} = m_{\mathrm{j}}\delta_{\mathrm{ij}}$, it is quite easy to find $\mathbf{S}_{ij} = {m_{\mathrm{j}}}^{-1/2}\delta_{\mathrm{ij}}$, Transformation $\mathbf{S}$ simplifies the kinetic energy, but the potential remains complicated. Therefore we use one more, from η to χ,

$$\frac{1}{2}\mathrm{x}^T\mathbf{V}\mathrm{x} = \frac{1}{2}\eta^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}\mathbf{V}\mathbf{S}\eta = \frac{1}{2}\chi^{\mathrm{T}}\mathbf{U}^{-1}\mathbf{S}^{\mathrm{T}}\mathbf{V}\mathbf{S}\mathbf{U}\chi$$

Transformation $\eta = \mathbf{U}\chi$ is a simple rotation obtained by diagonalizing the matrix of potential energy: Go to list of topics

$$\left(\mathbf{U}^{-1}\mathbf{S}^{\mathrm{T}}\mathbf{V}\mathbf{S}\mathbf{U}\right)_{\mathrm{ij}} = \Omega_{\mathrm{j}}^2\delta_{\mathrm{ij}} = \mathbf{W}_{\mathrm{ij}}$$

Therefore we took $\mathbf{U}^{-1} = \mathbf{U}^T$. We can see that the " *length* " is conserved.

$$\frac{1}{2}\dot{\eta}^T\dot{\eta} = \frac{1}{2}\dot{\chi}^T\mathbf{U}^{-1}\mathbf{U}\dot{\chi} = \frac{1}{2}\dot{\chi}^T\dot{\chi}$$

$$E = \frac{1}{2}\dot{\mathrm{x}}^{\mathrm{T}}\mathbf{M}\dot{\mathrm{x}} + \frac{1}{2}\mathrm{x}^{\mathrm{T}}\mathbf{V}\mathrm{x} = \frac{1}{2}\dot{\chi}^{\mathrm{T}}\dot{\chi} + \frac{1}{2}\chi^{\mathrm{T}}\mathbf{W}\chi$$

This expression however is a sum over the new mutually independent degrees of freedom, since $\mathbf{W}$ is diagonal.

$$\frac{1}{2}\dot{\chi}^T\dot{\chi} + \frac{1}{2}\chi^{\mathrm{T}}\mathbf{W}\chi = \sum_{i=1}^{N}\left(\frac{1}{2}\dot{\chi}_{\mathrm{i}}^2 + \frac{1}{2}\Omega_{\mathrm{i}}^2\chi_{\mathrm{i}}^2\right)$$

$$\sum_{i=1}^{N}\frac{1}{2}m_{\mathrm{i}}\dot{\mathrm{x}}_{\mathrm{i}}^2 + \frac{1}{2}\sum_{i,j=1}^{N}\mathrm{V}_{\mathrm{ij}}\mathrm{x}_{\mathrm{i}}\mathrm{x}_{\mathrm{j}} \rightarrow \sum_{i=1}^{N}\left(\frac{1}{2}\dot{\chi}_{\mathrm{i}}^2 + \frac{1}{2}\Omega_{\mathrm{i}}^2\chi_{\mathrm{i}}^2\right)$$

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Example Go to list of topics

A string of balls of mass m connected by springs of equal spring constant is described by displacements u_i. We can label the displacements $u_i = u(x_i)$ where x_i is the equilibrium position of the i-th ball. In the limit of infinitisemal small balls and short springs this would then lead to a "wave equations" for a continuous elastic string, with continuously observed displacement $u(x)$.

The total energy is:

$$\frac{1}{2}\sum_i m\left(\dot{u}(x_i)\right)^2 + \frac{1}{2}k\sum_i (u(x_i) - u(x_i+1))^2 + \frac{1}{2}ku(x_1)^2 + \frac{1}{2}ku(x_N)^2$$

The last two terms represent the fixed end springs. The matrix M is simply a diagonal matrix with m as all diagonal elements. The matrix V is a band matrix (below).

The transformation from $u(x_i)$ to χ_i can also be reversed. The reversed transformation in this case simply consists of eigenvectors of the matrix V, so that each of the eigenmodes is simply given by a function of time

$$\chi_k(t) = \chi_{k0}e^{i\Omega_k t}$$

where χ_{k0} is the amplitude, and the actual displacements for the k-th mode can be written as

$$u_k(x_i) = S_i^k \chi_k(t) = S_i^k \chi_{k0} e^{i\Omega_k t}$$

where S_i^k is the i-th component of the k-th eigenmode with the frequency Ω_k

The matrix V has the form

$$\begin{bmatrix} \mathbf{+2} & \mathbf{-1} & 0 & 0 & 0 & ... & 0 \\ \mathbf{-1} & \mathbf{+2} & \mathbf{-1} & 0 & 0 & ... & 0 \\ 0 & \mathbf{-1} & \mathbf{+2} & \mathbf{-1} & 0 & ... & 0 \\ 0 & 0 & \mathbf{-1} & \mathbf{+2} & \mathbf{-1} & ... & 0 \\ 0 & ... & ... & ... & ... & ... & ... \\ 0 & ... & ... & ... & \mathbf{+2} & \mathbf{-1} & 0 \\ 0 & ... & ... & ... & \mathbf{-1} & \mathbf{+2} & \mathbf{-1} \\ 0 & ... & ... & ... & 0 & \mathbf{-1} & \mathbf{+2} \end{bmatrix}$$

The eigenvectors - giving the eigenmodes - are eigenvectors of this band matrix. The modes are "standing waves", in the string limit. For infinite system - traveling waves. **leads to Fourier expansions for fields**) see (link) A(r) expressed in eigenmodes Go to list of topics

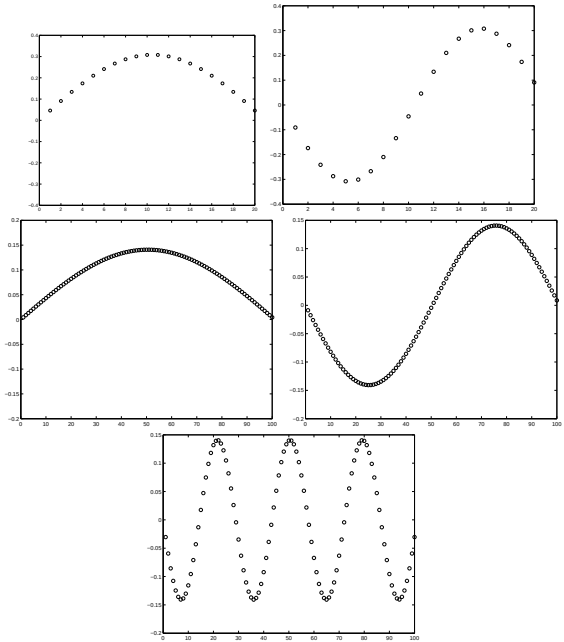

Figure 3: Components of eigenmodes at positions x_i. For $N = 20$ first and second node, fo $N = 100$ nodes 1,2, and 6. Go to list of topics

10 Algebraic Method for Harmonic Oscillator.

Go to list of topics

In this section we show how one can work with the harmonic oscillator introducing so called ladder operators which move from state to state, the states being separated by the same 'quantum of energy'.

The classical hamiltonian can be transformed:

$$\frac{1}{2m}\,p^2 + \frac{m\omega^2}{2}\,q^2 \qquad \text{transforms to} \qquad \frac{\hbar\omega}{2}\left(P^2 + Q^2\right)$$

$$P = \sqrt{\frac{1}{\hbar\, m\, \omega}}\,p \qquad\qquad Q = \sqrt{\frac{m\,\omega}{\hbar}}\,q$$

With this the commutator

$$[\,q, p\,] = i\hbar$$

becomes

$$[\,Q, P\,] = i$$

This simplifies the equation and brings it into a form where the energy is expressed in $\hbar\omega$.

The main transformation, however, is to go over to linear combinations of P and Q

$$a \;=\; \frac{1}{\sqrt{2}}\,Q \;+\; \frac{i}{\sqrt{2}}\,P \qquad \text{and} \qquad a^{+} \;=\; \frac{1}{\sqrt{2}}\,Q \;-\; \frac{i}{\sqrt{2}}\,P$$

By a very simple algebra we find that for their commutator

$$\left[\,a, a^{+}\,\right] = 1$$

and the energy is transferred to Go to list of topics

$$\frac{\hbar\omega}{2}\left(P^2 + Q^2\right) \quad \rightarrow \quad \frac{\hbar\omega}{2}\left(a\;a^{+} \;+\; a^{+}a\right)$$

Using the commutator $a\;a^{+} \;- a^{+}a = 1$ we finally get

$$H \;=\; \hbar\omega \;\; a^{+}a \;+ \frac{\hbar\omega}{2} \;=\; \hbar\omega \;\; N + \frac{\hbar\omega}{2}$$

where we already include that

$$N \;=\; a^{+}a$$

will be a *number* operator.

Why number? Let us play with $[\,a, a^{+}\,] = 1$ or alternatively $\quad a\,a^{+} - a^{+}a = 1$ and the operator N. We quickly derive that

$$\left[\,N,\; a^{+}\,\right] = \;a^{+} \qquad \text{and} \qquad [\,N,\; a\,] = \;-a$$

This is done simply by writing out Go to list of topics

$$\left[N,\; a^{+}\right] \;=\; Na^{+} - a^{+}N = (a^{+}a)\,a^{+} - a^{+}(a^{+}a) = a^{+}(a\,a^{+} - a^{+}a) = a^{+}\left[\,a, a^{+}\,\right] = a^{+}$$

Since $H = \;\hbar\omega\;\; N + \frac{\hbar\omega}{2}$ we also have

$$\left[\,H,\; a^{+}\,\right] = \;\hbar\omega\; a^{+} \qquad \text{and} \qquad [\,H,\; a\,] = \;-\;\hbar\omega\; a$$

These are the last equations which bring the physical interpretation.

If there is a Q.M. state $\psi(q) \to |\psi\rangle$ such that

$$H\;|\psi\rangle \;=\; E\;|\psi\rangle$$

then

$$H\,(a\,|\psi\rangle\,)\;=\;a\,H\,|\psi\rangle - \hbar\omega\,a\,|\,\psi\rangle\;=\;a\,E\,|\psi\rangle - \hbar\omega\,a\,|\,\psi\rangle\;=\;(E-\hbar\omega\,)\,(a\,|\psi\rangle\,)$$

that means that $(a\,|\psi\rangle\,)$ is also an eigenstate. It has energy lower by $\hbar\omega$. This we can continue again and again, getting eigenstates for

$$E\;-\;\hbar\omega\,, E\;-\;2\,\hbar\omega\,, E\;-\;3\,\hbar\omega\,, E\;-\;4\,\hbar\omega\,, E\;-\;5\hbar\omega\;.....$$

Since this cannot go on infinitely, we get finally a state such that

$$a\,|\psi_0\,\rangle\;=\;0$$

We quickly verify that this state has Go to list of topics

$$E_0\;=\;\frac{\hbar\omega}{2}$$

further that the same thing is possible with a^+ only with opposite sign, so that we get energies

$$E_0\,, E_0\;+\hbar\omega\,, E_0\;+\;2\,\hbar\omega\,, E_0\;+\;3\,\hbar\omega\,, E_0\;+\;4\,\hbar\omega\,, E_0\;+\;5\hbar\omega\;.....$$

Each of the eigenstates is an eigenstate of both H and N with obvious number of quanta. Therefore we call a^+ and *a creation and annihilation* operators. They make states with one more ore one less *quantum* $\hbar\omega$

We can complete this treatment by a complete solution for the wavefunction:

$$a\,|\psi_0\,\rangle \;=\; 0 \qquad a \;=\; \frac{1}{\sqrt{2}}\,(Q \,+\, i\,P) \qquad P \;=-i\frac{\partial}{\partial Q}$$

Thus, writing $|\psi_0\,\rangle \;\longrightarrow\; \psi_0(Q)$

$$a\,|\psi_0\,\rangle \;=\; 0 \qquad \longrightarrow \qquad \left(Q \,+\, \frac{\partial}{\partial Q}\right)\psi_0(Q) \;=\; 0$$

The solution of 1. order differential eq. to the left is easy

$$\psi_0(Q) \;=\; C_0\; e^{-Q^2/2}$$

and using the expression for a^+ and the $|\psi_n\,\rangle$ Go to list of topics

$$\psi_1(Q) \;=\; C_1\left(Q \,-\, \frac{\partial}{\partial Q}\right)\,e^{-Q^2/2} \qquad \psi_2(Q) \;=\; C_2\left(Q \,-\, \frac{\partial}{\partial Q}\right)\left(Q \,-\, \frac{\partial}{\partial Q}\right)\,e^{-Q^2/2}$$

and n times for general $|\psi_n\,\rangle$. cf. recursion relations for Hermite polynomials.

11 Electromagnetic fields

Go to list of topics

In atomic physics we prefer to work in Gaussian units, where the strengths of the fields have the same physical dimension. In vacuum $\vec{D} = \vec{E}$ and $\vec{H} = \vec{B}$

The classical electromagnetic field is described by electric and magnetic field vectors $\vec{E}$ and $\vec{B}$, which satisfy Maxwell's equations:

$$\nabla \cdot \vec{E} = 4\pi\rho \tag{31}$$

$$\nabla \cdot \vec{B} = 0 \tag{32}$$

$$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \tag{33}$$

$$\nabla \times \vec{B} = \frac{1}{c}\left(\frac{\partial \vec{E}}{\partial t} + 4\pi\vec{J}\right) \tag{34}$$

The electric field $\vec{E}$ and magnetic field $\vec{B}$ can be generated from scalar and vector potentials ϕ and $\vec{A}$ by

$$\vec{E}(\vec{r},t) = -\nabla\phi(\vec{r},t) - \frac{1}{c}\frac{\partial}{\partial t}\vec{A}(\vec{r},t) \tag{35}$$

$$\vec{B}(\vec{r},t) = \nabla \times \vec{A}(\vec{r},t) \tag{36}$$

The potentials are not unique, observable field strengths $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$ remain the same when the potentials are changed by

$$\vec{A}(\vec{r},t) \to \vec{A}(\vec{r},t) + \nabla\lambda(\vec{r},t)$$

$$\phi(\vec{r},t) \to \phi(\vec{r},t) - \frac{\partial\lambda(\vec{r},t)}{\partial t}$$

where $\lambda(\vec{r},t)$ is any scalar field. Go to list of topics

This property is called gauge invariance. It allows us to choose $\vec{A}$ so that

$$\nabla \cdot \vec{A} = 0 \tag{37}$$

When $\vec{A}$ satisfies this condition, we are using the "Coulomb Gauge". From Maxwell's equations (without sources) we can show that $\vec{A}$ satisfies the wave equation

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0 \tag{38}$$

Also ϕ, $\vec{B}$ and $\vec{E}$ satisfy wave equations, but for radiation problems in empty space (vacuum) we have the potential $\phi = 0$ since there are no charges there.

The energy stored or contained in the electromagnetic field is given by the formula

$$H_{field} = \frac{1}{8\pi}\int d^3\mathbf{r}\,(\mathbf{E}\cdot\mathbf{E} + \mathbf{B}\cdot\mathbf{B}) \tag{39}$$

Eigenmode in "infinite box" - a plane wave solution of equations (37) and (38) , with angular frequency ω (i.e. the frequency $\nu = \omega/2\pi$) is given by the vector potential $\vec{A}$ Go to list of topics

$$\begin{aligned} \vec{A}(\omega; r, t) &= 2\vec{A}_0(\omega)\cos(k\cdot r - \omega t + \delta_\omega) \\ &= \vec{A}_0(\omega)\,[exp[i(k\cdot r - \omega t + \delta_\omega)] + c.c.] \end{aligned} \tag{40}$$

12 The Quantum Theory of Electromagnetic Field

Go to list of topics

The energy stored or contained in the electromagnetic field is given by the formula

$$H_{field} = \frac{1}{8\pi} \int d^3\mathbf{r} \, (\mathbf{E} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{B}) \tag{41}$$

Gaussian units, the electric and magnetic field strengths have the same physical dimension.

The energy of extended system can be written as a sum of energies in eigenmodes. The eigenmodes in "infinite box" are the plane waves.

The sum over plane waves gives the form of Fourier series - for the operator of the vector potential $\vec{A}(\vec{r})$

$$\vec{A}(\vec{r}) = \sum_{\vec{k}\lambda} \sqrt{\frac{2\pi\hbar c^2}{V\omega_k}} \widehat{e}_{\vec{k}\lambda} \left(a_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{r}} + a^{\dagger}_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{r}} \right) \tag{42}$$

The sum includes all the possible values of the propagation vector $\vec{k}$ and also the two possible polarizations $\lambda = 1, 2$.In a *finite box* the boundary conditions lead to quantization of $\vec{k}$ as discussed in "Density of states" section. Periodicity on the box walls gives allowed values $(n_x, n_y, n_z)\frac{2\pi}{L}$ where n_i are integers.

The dimensional factor

$$\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}$$

is determined by the necessity that Go to list of topics

$$\langle\Phi| H_{rad} |\Phi\rangle = \langle\Phi| \int_V \mathcal{H}\, dV\, |\Phi\rangle = \langle\Phi| \int_V \frac{(E^2 + B^2)}{8\pi}\, dV\, |\Phi\rangle \tag{43}$$

must give the total energy of the electromagnetic field inside the box, when written as sum over quantized eigenmodes

$$\langle\Phi| H_{rad} |\Phi\rangle = \langle\Phi| \sum_{\vec{k}\lambda} H_{\vec{k}\lambda} |\Phi\rangle = \langle\Phi| \sum_{\vec{k}\lambda} \hbar\omega_k a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda} |\Phi\rangle \tag{44}$$

This is done using

$$\vec{B}(\vec{r}) = i\vec{k} \times \vec{A}(\vec{r}) \qquad \vec{E}(\vec{r}) = i\frac{\omega_k}{c}\vec{A}(\vec{r}) \qquad \omega_k = kc$$

The operators $a_{\vec{k}\lambda}$, $a^{\dagger}_{\vec{k}\lambda}$ and $N_{\vec{k}\lambda}$ are "*annihilation*", is called "*creation*" and number operators for photons in each eigenmode.

One ignores the term $\frac{1}{2}\sum_{\vec{k}\lambda}\hbar\omega_k$ that refers to "zero point energy" (infinite number of modes - Casimir effect).

The state of the field can be written as a *direct product* of the vector states for each of the oscillators Go to list of topics

$$|\Phi\rangle \to \left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle = |\cdots\rangle\cdots\left|n_{\vec{k}\lambda}\right\rangle\cdots\left|n_{\vec{k}'\lambda'}\right\rangle\cdots \tag{45}$$

For such state vectors:

$$a_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle = \sqrt{n_{\vec{k}\lambda}}\left|\cdots n_{\vec{k}\lambda}-1\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle \tag{46}$$

$$a^{\dagger}_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle = \sqrt{n_{\vec{k}\lambda}+1}\left|\cdots n_{\vec{k}\lambda}+1\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle \tag{47}$$

$$N_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle = n_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle \tag{48}$$

$$H_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle = \hbar\omega_k n_{\vec{k}\lambda}\left|\cdots n_{\vec{k}\lambda}\cdots n_{\vec{k}'\lambda'}\cdots\right\rangle \tag{49}$$

where

$n_{\vec{k}\lambda} = 0, 1, 2, 3, \ldots, \infty$

13 Density of States

Go to list of topics

We consider the electromagnetic field enclosed in a box with volume V. For a finite volume there is a discrete number of modes satisfying the imposed boundary conditions. Therefore the sum over final states is an ordinary sum. As this volume approaches infinite size, the summation over $\vec{k}$, will be approaching an integral.

The density of states factor is found from performing such a limiting process, using following relations.

The summation will be replaced by an integral

$$\sum_{\vec{k}} \longrightarrow \int \rho(\vec{k})\, d\vec{k} \tag{50}$$

$\rho(\vec{k})$ is the density of states in the K-space.

The allowed discrete values of $\vec{k}$ are obtained by combinations of components

$$k_x^{(n_x)} = \frac{2\pi}{L}\, n_x \qquad k_y^{(n_y)} = \frac{2\pi}{L}\, n_y \qquad k_z^{(n_z)} = \frac{2\pi}{L}\, n_z \tag{51}$$

where the numbers n_x,n_y,n_z are positive and negative integers. It means that each of the allowed vectors $\vec{k}$ occupies a small volume of the K-space

$$\Delta k_x \Delta k_y \Delta k_z = \left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{V} \tag{52}$$

The density of states in the K-space is thus a constant (i.e. one per the above small k-space volume), and the above relation can be written as

$$\sum_{\vec{k}} \longrightarrow \frac{V}{(2\pi)^3} \int d\vec{k} \tag{53}$$

Since the derivation of the golden rule assumes integration over frequencies, or energies, we shall transform this integral over momenta (i.e. wave numbers k) to integral over energy, Go to list of topics

$$\frac{V}{(2\pi)^3} \int d\vec{k} \longrightarrow \int \rho(E) dE$$

$$\frac{V}{(2\pi)^3} \int d\vec{k} = \frac{V}{(2\pi)^3} \int_{\Omega_k} d\Omega_k \int k^2 \, dk = \int_{\Omega_k} \int \left[\frac{V}{(2\pi)^3} k^2 \frac{dk}{dE} d\Omega_k\right] dE \tag{54}$$

so that the $\rho(E)$ can be identified as

$$\frac{V}{(2\pi)^3} k^2 \frac{dk}{dE} \int_{\Omega_k} d\Omega_k \tag{55}$$

If the processes depend on the direction of the wave vector, which is true in photon emission case, we must keep the angular information inside of the density of states, and perform the angular integration afterwards.

We must now evaluate the above density of states in terms of energy only, using

$$k = \frac{\omega}{c} \qquad E = \hbar k c$$

Setting these relations of k and E, we obtain the expression for $\rho(E)$

$$\rho(E) \;=\; \frac{V}{(2\pi)^3} \cdot \frac{E^2}{(\hbar c)^3}\, d\Omega_k \;=\; \frac{V}{(2\pi)^3} \cdot \frac{1}{\hbar} \cdot \frac{\omega^2}{c^3}\, d\Omega_k \tag{56}$$

Go to list of topics

14 Charged Particles In an Electromagnetic Field

Go to list of topics

The Hamiltonian of a spinless particle q and mass m in an electromagnetic field is

$$H = \frac{1}{2m}(\vec{p} - \frac{q}{c}\vec{A})^2 + q\phi \tag{57}$$

where p is the generalized momentum of the particle. The Hamiltonian of an electron of mass m in an electromagnetic field is given by the above equation, with $q = -e$. In order to describe a hydrogenic atom, as an example, in an electromagnetic field we must also take into account the presence of the nucleus, of charge Ze and mass M . We must include in the Hamiltonian the electrostatic Coulomb potential $-\frac{Ze^2}{r}$ between the electron and the nucleus. This electrostatic interaction is an additional potential energy term, while the radiation field which perturbs the atom is described in terms of a vector potential $\vec{A}$ alone

The time dependent Schrödinger equation for a hydrogenic atom in an electromagnetic field then reads

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = \left[1/2m(-i\hbar\nabla + e\vec{A})^2 - \frac{Ze^2}{(4\pi\varepsilon_0)r}\right]\psi(r,t) \tag{58}$$

where we have written $p = -i\hbar\nabla$. Because of the gauge condition $\nabla\cdot\vec{A} = 0$, we have

$$\nabla\cdot(\vec{A}\psi) = \vec{A}\cdot(\nabla\psi) + \underbrace{(\nabla\cdot\vec{A})}_{0}\psi = \vec{A}\cdot(\nabla\psi) \tag{59}$$

so that ∇ and $\vec{A}$ effectively commute. Then

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = \left[\frac{-\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} - \frac{i\hbar e}{m}\vec{A}\cdot\nabla + \frac{e^2}{2m}\vec{A}^2\right]\psi(r,t) \tag{60}$$

In "weak field case" the term with $\vec{A}^2$ is small compared with the linear term $\vec{A}$.

Go to list of topics

15 The Hamiltonian of Interaction

Go to list of topics

Now, we study the interaction between radiation and atomic system. In this case the total Hamiltonian of the system is written as

$$\begin{aligned} H &= H_{atom} + H_{rad} + H_I \\ &= H^0 + H_I \end{aligned} \tag{61}$$

H_{atom} is the Hamiltonian of the atomic system and H_{rad} is the Hamiltonian of the free radiation field. H_I shows the Hamiltonian of the interaction effect between two previous systems. By replacing H_I, we replace $\vec{p}$ by $\vec{p} + e/c\vec{A}$ in H_{atom} we can construct H_I as

$$H_I = \frac{e}{mc}\vec{p}\cdot\vec{A} + \frac{e^2}{2mc^2}\vec{A}^2 \qquad H_I \to \frac{e}{mc}\vec{p}\cdot\vec{A} \tag{62}$$

As we see the first term of the eq.(62), is proportional to $\vec{A}$ that contributes in the transitions involving the emission or absorption of a single photon and the

next term that's proportional to $\vec{A}^2$ contributes in the transitions involving the emission or absorption of two photons. We can also see that the first term; $\vec{A}$; contains just one creation or annihilation operator, but $\vec{A}^2$ contains the terms as : $a_{\vec{k}\lambda}a_{\vec{k}\lambda}$, $a^\dagger_{\vec{k}\lambda}a^\dagger_{\vec{k}\lambda}$, $a_{\vec{k}\lambda}a^\dagger_{\vec{k}\lambda}$, $a^\dagger_{\vec{k}\lambda}a_{\vec{k}\lambda}$ which correspond to absorption of two photons; emission of two photons. Here we study the first term. The probability for a transition involving two photons contains e^4 while this probability for one photon is proportional to e^2. This extra power of e^2 will lead to one more power of $\alpha \simeq 1/137$.

The eigenfunctions of the unperturbed Hamiltonian $H_\circ$ are direct products of the atomic and radiation wave functions

$$\psi_{atom}\psi_{rad} = |\psi_a; n_1, n_2, \ldots, n_i, \ldots\rangle \tag{63}$$

where ψ_a is the wave function of the atomic Hamiltonian, $n_i \equiv n_{\vec{k}_i\lambda_i}$ is the wave function describing the mode $\vec{k}_i\lambda_i$ in the radiation field.

Go to list of topics

16 Emission of Radiation By an Excited Atom:

Go to list of topics

Here we study the emission of a single photon by an excited atom, and we use the time-dependent perturbation theory to find the transition probability for atom.If we consider $|i\rangle$ as the initial state and $|f\rangle$ as the final state, then the probability per unit time for a transition by the emission of a single photon from the initial to final state is given by

$$W_{i\to f}(\vec{k},\lambda) = \frac{2\pi}{\hbar}\left|\langle f|H_p|i\rangle\right|^2 \rho(E_f) \tag{64}$$

where $\hbar\vec{k}$ denotes the momentum and λ denotes the polarization, and H_p is the perturbing Hamiltonian. This equation is known as *Fermi's Golden Rule.*

The perturbing Hamiltonian for this process is

$$H_p = -\frac{e}{mc}\vec{p}\cdot\vec{A} \tag{65}$$

by referring to the eq.(42), we have

$$H_p = -\frac{e}{mc}\sum_{\vec{k}\lambda}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\vec{p}\cdot\hat{e}_{\vec{k}\lambda}\left(a_{\vec{k}\lambda}e^{i\vec{k}\cdot\vec{r}} + a^{\dagger}_{\vec{k}\lambda}e^{-i\vec{k}\cdot\vec{r}-}\right) \tag{66}$$

The initial and final states $|i\rangle$; $|f\rangle$;, i.e. the unperturbed wavefunctions before and after the emission of one photon is

$$|i\rangle = |a\rangle\left|\cdots n_{\vec{k}\lambda}\cdots\right\rangle \tag{67}$$

$$|f\rangle = |b\rangle\left|\cdots n_{\vec{k}\lambda}+1\cdots\right\rangle \tag{68}$$

The energy difference of these two states is

$$E_f - E_i = \left(E_b + n_{\vec{k}\lambda}\hbar\omega_k + \hbar\omega_k\right) - \left(E_a + n_{\vec{k}\lambda}\hbar\omega_k\right) = E_b - E_a + \hbar\omega_k \tag{69}$$

For spontaneous emission, no photon is present in the initial state: $n_{\vec{k}} \to 0$ and $(n_{\vec{k}}+1) \to 1$

Go to list of topics

17 The matrix element reduction

Go to list of topics

Inserting the final and initial states and the Hamiltonian into the matrix element, we obtain

$$\langle f\,|H_p|\,i\rangle = -\frac{e}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\left\langle b\left|\vec{p}\cdot\widehat{e}_{\vec{k}\lambda}e^{-i\vec{k}\cdot\vec{r}}\right|a\right\rangle\sqrt{n_{\vec{k}\lambda}+1} \tag{70}$$

For spontaneous emission, no photon is present in the initial state: $n_{\vec{k}} \to 0$ and $(n_{\vec{k}}+1) \to 1$

By considering the eq.(70) we can transform the Golden Rule formula eq.(64) for spontaneous emission

$$W_{i\to f}(\vec{k},\lambda) = \frac{2\pi}{\hbar}\left(\frac{e}{mc}\right)^2\left(\frac{2\pi\hbar c^2}{V\omega_k}\right)\left|\left\langle b\left|\vec{p}\cdot\widehat{e}_{\vec{k}\lambda}e^{-i\vec{k}\cdot\vec{r}}\right|a\right\rangle\right|^2\rho(E_f) \tag{71}$$

$$\langle \Psi_{fin} | \quad H_I \quad | \Psi_{init} \rangle \qquad H_I \rightarrow \frac{e}{m\,c}\,\vec{p}\cdot\vec{A}$$

$$\langle \Psi_{fin} | \ \frac{e}{m\,c}\,\mathbf{p}\cdot\mathbf{A} \ | \Psi_{init} \rangle \qquad | \Psi_{init} \rangle \rightarrow |0_{photon}\rangle |\ \varphi_{EXC}\rangle$$

$$\langle \Psi_{fin} | \rightarrow \langle \varphi_{GS}| \langle \hbar\,\omega|$$

$$\langle \varphi_{GS}| \langle \hbar\,\omega| \ \frac{e}{m\,c}\ \vec{p}\cdot\vec{A}\ |0_{photon}\rangle |\ \varphi_{EXC}\rangle$$

$$\vec{A} \rightarrow \sum_{\vec{\varepsilon}_k k} \vec{\varepsilon}_k \sqrt{\frac{2\pi\hbar c^2}{\omega_k V}}\ e^{i\,k\,\mathbf{r}}\,a^{+} \qquad \vec{p}\cdot\vec{A} \rightarrow \sum \vec{p}\cdot\vec{\varepsilon} \sqrt{\frac{2\pi\hbar c^2}{\omega\,V}}\ e^{i\,k\,\mathbf{r}}\,a^{+}$$

$$\langle \varphi_{GS}| \langle \hbar\,\omega| \ \frac{e}{m\,c} \sum \vec{p}\cdot\vec{\varepsilon} \sqrt{\frac{2\pi\hbar c^2}{\omega\,V}}\ e^{i\,k\,\mathbf{r}}\,a^{+} |0_{photon}\rangle |\ \varphi_{EXC}\rangle$$

$$\frac{e}{m\,c} \sqrt{\frac{2\pi\hbar c^2}{\omega\,V}}\ \langle \varphi_{GS}|\ \vec{p}\cdot\vec{\varepsilon}\ e^{i\,k\,\mathbf{r}} |\ \varphi_{EXC}\rangle \langle \hbar\,\omega|\ a^{+}\ |0_{photon}\rangle$$

18 Dipole Approximation

Go to list of topics

An important simplification is obtained by applying the so called dipole approximation, considering the case $kr \ll 1$. This means that the wavelength of the emitted photon is much larger than atomic dimension. The electric dipole approximation is obtained by replacing, to a good approximation,

$$e^{i\vec{k}\cdot r} \approx 1$$

i.e.

$$\langle b \left| \vec{p} e^{-i\vec{k}\cdot\vec{r}} \right| a \rangle \;\rightarrow\; \langle b \left| \vec{p} \right| a \rangle$$

This approximation is limited by these requirements:

$$\lambda \gg 1\text{Å} \qquad \text{and} \qquad \hbar\omega \ll 10 \text{ keV}.$$

Here we also derive the relation between matrix element of momentum and coordinate using the following commutation relations

$$\left[r, p^2\right] = p\ [r,p] + [r,p]\ p = 2i\hbar p \tag{72}$$

$$[\vec{r}, H_{atom}] = \frac{i\hbar}{m}\,\vec{p} \tag{73}$$

we change the matrix element of the momentum to a matrix element of the special coordinate of the atomic electron

$$\begin{aligned} \langle b\,|\,\vec{p}\,|\,a\rangle &= \frac{m}{i\hbar}\,\langle b\,|[\vec{r}, H_{atom}]|\,a\rangle \\ &= \frac{im}{\hbar}\,(E_a - E_b)\;\langle b\,|\,\vec{r}\,|\,a\rangle \\ &= im\omega_{ab}\;\langle b\,|\,\vec{r}\,|\,a\rangle \end{aligned} \tag{74}$$

Go to list of topics

19 Detailed Evaluation of Emission rate

Go to list of topics

For *spontaneous emission*is that, we first perform the summation over the two possible polarizations by considering the following figure, fig.4. The figure shows that placing for a moment the z-axis in the direction of the wavevector $\vec{k}$, the directions of the polarization vectors $\widehat{e}_{\vec{k}\lambda}$, for $\lambda = 1, 2$ can then define the x- and y-axes, so that

$$\begin{aligned}\sum_{\lambda=1,2} \left|\left\langle b \left| \vec{p}\cdot\widehat{e}_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{r}} \right| a \right\rangle\right|^2 &= \left|\left\langle b \left| \vec{p} e^{-i\vec{k}\cdot\vec{r}} \right| a \right\rangle\right|^2 (sin^2\theta cos^2\phi + sin^2\theta sin^2\phi) \\ &= \left|\left\langle b \left| \vec{p} e^{-i\vec{k}\cdot\vec{r}} \right| a \right\rangle\right|^2 (sin^2\theta) \qquad (75)\end{aligned}$$

where the angle θ is the angle between the wave number $\vec{k}$ and the momentum vector of the electron (if it were classically defined). Conversely, after performing this reduction, we can think that our z-axis is always placed along the direction of $\vec{p}$, so that we can identify the angle θ with the polar angle of the photon emission to be integrated over.

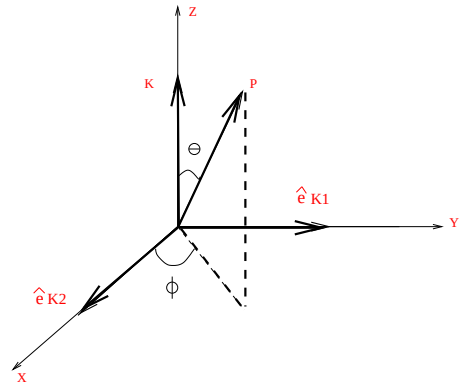

Figure 4: As the z-axis is for the moment in the direction of the wavevector $\vec{k}$, the directions of the polarization vectors $\widehat{e}_{\vec{k}\lambda}$ (perpendicular to each other and to the vector $\vec{k}$, can then define the x- and y-axes. The angle θ is the angle between the wave number $\vec{k}$ and the momentum vector of the electron $\vec{p}$.

Go to list of topics

By using the eq.(55) and dipole approximation discussed above, we can evaluate the integral over all emission angles Ω_k,

$$\left(\frac{1}{\tau}\right)_{a\to b} = \frac{e^2}{2\pi m^2}\frac{\omega_k}{\hbar c^3}\int |\langle b\,|\,\vec{p}\,|\,a\rangle|^2\, sin^2\theta\, d\Omega_k \tag{76}$$

where the integration angular variables are

$$d\Omega_k = \sin\theta\, d\theta\, d\phi \tag{77}$$

Note that in the above evaluations the volume V in $\rho[E_f]$ cancels the volume in the field normalization factor

$$\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}$$

in equation (42).

The last equation eq.(76) then becomes Go to list of topics

$$\left(\frac{1}{\tau}\right)_{a\to b} = \frac{e^2}{2\pi m^2}\frac{\omega_k}{\hbar c^3}\,|\langle b|\,\vec{p}\,|a\rangle|^2\int d\phi\int \sin^2\theta\,\sin\theta\, d\theta \tag{78}$$

The angular integration is easily seen to yield a factor $8\pi/3$, so that finally

$$\left(\frac{1}{\tau}\right)_{a\to b} = \frac{4\omega_{ab}e^2}{3\hbar m^2c^3}\,|\langle b|\,\vec{p}\,|a\rangle|^2 \tag{79}$$

Further we use the relation between matrix element of momentum and coordinate eq. (74) in section 18 $\langle b\,|\,\vec{p}\,|\,a\rangle = im\omega_{ab}\,\langle b\,|\,\vec{r}\,|\,a\rangle$ and thus eq.(79) becomes

$$W_{sp.\,em.} = \left(\frac{1}{\tau}\right)_{a\to b} \tag{80}$$

$$= \frac{4e^2\omega_{ab}^3}{3\hbar c^3}\,|\langle b\,|\,\vec{r}\,|\,a\rangle|^2 \tag{81}$$

$$= \frac{4}{3}\left(\frac{\varepsilon_\circ}{\hbar}\right)\left(\frac{\hbar\omega_{ab}}{\varepsilon_\circ}\right)^3\alpha^3\left|\left\langle b\left|\frac{\vec{r}}{a_\circ}\right|a\right\rangle\right|^2 \tag{82}$$

$a_\circ = \hbar^2/me^2$ $\qquad$ $\varepsilon_\circ = 2\,Ryd = e^2/a_\circ = 27.21\,eV$ Go to list of topics

$\alpha = e^2/\hbar c = 1/137.04$, the fine structure constant .

For one-electron hydrogenlike atoms (or ions), the life time of the transition of $2p \longrightarrow 1s$ of one photon is given by

$$\left(\frac{1}{\tau}\right)_{2p\longrightarrow 1s} = 0.6\times 10^9\,Z^4\,sec^{-1} \tag{83}$$

20 Stimulated emission

Go to list of topics

For the case of *stimulated emission*, that is dependent on the number of photons in the field (intensity), we must keep the $\sqrt{n_{\vec{k}\lambda}+1}$ term of the $n_{\vec{k}\lambda}$ initial photon state and start from

$$W_{i\to f}(\vec{k},\lambda) = \frac{2\pi}{\hbar}\left(\frac{e}{mc}\right)^2\left(\frac{2\pi\hbar c^2}{V\omega_k}\right)(n_{\vec{k}\lambda}+1)\left|\left\langle b\left|\vec{p}\cdot\hat{e}_{\vec{k}\lambda}e^{-i\vec{k}\cdot\vec{r}}\right|a\right\rangle\right|^2\rho(E_f) \quad (84)$$

The emission rate then becomes

$$W_{st.\,em.} = \left(\frac{1}{\tau}\right)_{a\to b} \quad (85)$$

$$= \frac{4}{3}\left(\frac{\varepsilon_\circ}{\hbar}\right)\left(\frac{\hbar\omega_{ab}}{\varepsilon_\circ}\right)^3\alpha^3\,(n_\omega\ +1)\left|\left\langle b\left|\frac{\vec{r}}{a_\circ}\right|a\right\rangle\right|^2 \quad (86)$$

where n_ω represents the number of photons in the field, with the energy of $E_\omega = \hbar\omega$.

The last equation can be considered as a sum of two terms; one is proportional to the number of photons in the field $n_{\vec{k}\lambda}$, so it's radiation field intensity-dependent, and describes the stimulated emission; the other one (expressed by number one in the paranthesis) is independent of the field intensity.

The term with is the said to account for the *spontaneous emission* contribution.

Go to list of topics

21 Fermi Golden Rule Simulation

——— Go to list of topics ——— Time dependent wavefunction ——— Model realization ——— The Hamiltonian of the model ———

The physical problem: solve the time-dependent Schrödinger equation with hamiltonian as in the derivations of the Fermi Golden Rule.

continuum of textbook derivation $\longrightarrow$ *quasicontinuum* here, i.e. a set of many equidistantly closely spaced levels.

The idea is to demonstrate how the line width is proportional to the density of states and the strength of the coupling.

Only the couplings from the discrete states to continuum and back are nonzero, have a constant value.

22 Realization of the model

Start of the simulator part — Go to list of topics

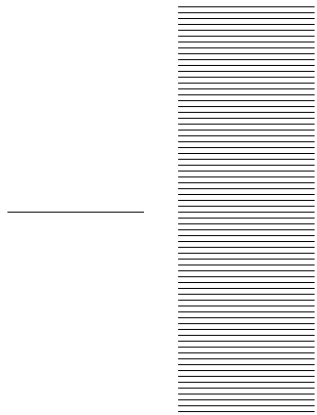

Figure 5: Schematic representation of the Energy levels

The figure 5 shows the energy levels: the single discrete level and the two quasicontinua. Note that each has a different density of levels.

The Hamilton operator matrix - see figure 7

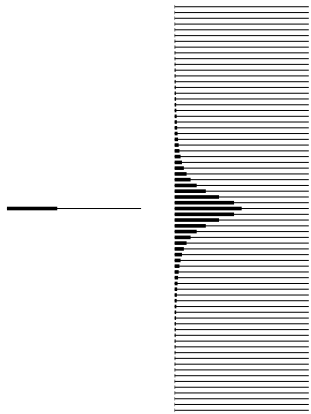

Figure 6: Schematic representation of the population probabilities, drawn at the energy levels

23 The time-dependent wavefunction

——— Start of the simulator part ——— Go to list of topics ———

The time-dependent wavefunction $\Psi(t)$ is expanded in terms of the model states $\varphi_i(t)$ as

$$\Psi(t) \;=\; \sum_i \; c_i(t) \; \varphi_i(t)$$

with the initial condition

$$c_1(0) = 1, \;\; c_2(0) = 0, \;\; c_3(0) = 0, \;\; \cdots\cdots$$

and inserted in the Schrödinger equation

$$i\hbar \; \frac{\partial}{\partial t} \Psi(t) \;= H \; \Psi(t)$$

In the usual way this results in a set of coupled equations. The populations of the states, i.e. the absolute value squared of the expansion coefficients $c_i(t)$ is shown in fig. 6.

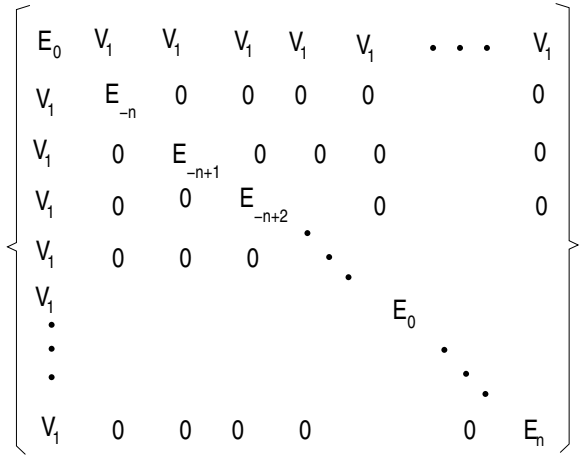

Figure 7: Schematic representation of Hamiltonian Matrix

Go to list of topics

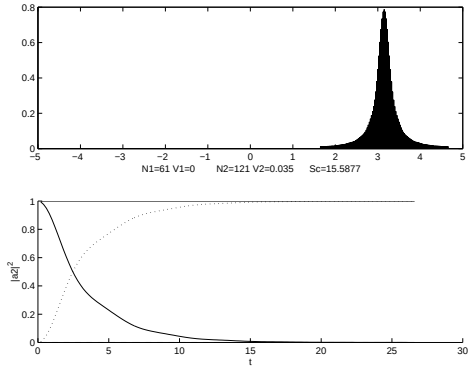

Figure 8: Decay in the simulator

Start of the simulator part — Go to list of topics

Overview of the topics

Time dependent QM- two-well problem
Perturbation theory for TDSE
Fermi Golden Rule
Line width from exponential decay
Eigenmodes for coupled vibrations.
Electromagnetic fields
Density of States
The Hamiltonian of Interaction
The matrix element reduction
Detailed Evaluation of Emission rate
Golden Rule Simulator part

One level in continuum
Final $W = 1/\tau$ result

Time-Dependent Schrödinger Equation
Dirac delta-function
Constant rate and exponential decay
Quantum theory of extended systems - fields
Algebraic Method for Harmonic Oscillator.
The Quantum Theory of Electromag. Field
Charged Particles In an Electromag. Field
Emission of Radiation by an Excited Atom
Dipole Approximation
Stimulated emission
Time-Dependent Schrödinger
Equation in Simulator