FS-5323: Quantum Mechanics III

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Chapter 1

Time Independent Perturbation Theory

Perturbation theory is a technique usually used to study the spectra of Hamiltonians that cannot be exactly solved by analytical methods. That is, for example, the case of the hydrogen atom when we include corrections for the relativistic motion of the electron or when we include the magnetic interaction between the electron's orbit around the proton and the electron's spin magnetic moment[1]. Another example where perturbation theory is used is in the calculation of some corrections for multielectronic atoms.

To be honest, we must state that nowadays, the tool kit of the trade of solving real problems is typically numerical analysis, i.e. attacking them with powerful computers and sophisticated algorithms, but it is not rare to see this approach combined with analytical techniques derived from perturbation theory.

In this chapter we will be interested in the approximation method called *stationary perturbation theory* which, as we shall see, gives us approximate analytical solutions to the spectral problem for the Hamiltonian.

[1] This is called *spin orbit coupling*.

1.1 Description of the method

1.1.1 Motivation

Imagine a two level system with Hamiltonian

$$\mathbf{H} = \begin{pmatrix} E_1 + \varepsilon e_{11} & \varepsilon e_{12} \\ \varepsilon e_{12} & E_2 + \varepsilon e_{22} \end{pmatrix} , \tag{1.1}$$

where $\varepsilon << 1$ is a real adimensional quantity and e_{ij} has energy dimensions for all i, j. And let $|1\rangle$, $|2\rangle$ be the basis in which we are describing the system. It is clear that we may cast $\mathbf{H}$ as

$$\mathbf{H} = \mathbf{H}_0 + \varepsilon\, \mathbf{W} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \varepsilon \begin{pmatrix} e_{11} & e_{12} \\ e_{12} & e_{22} \end{pmatrix} , \tag{1.2}$$

and we may safely say that $|1\rangle$, $|2\rangle$ is the basis in which $\mathbf{H}_0$ is diagonal.

It is natural to ask two questions,

1. What are the energies of $\mathbf{H}$? and

2. What is the basis that diagonalizes $\mathbf{H}$?

To answer the first question we may write the characteristic polynomial of $\mathbf{H}$, namely

$$P(\lambda) = [(E_1 + \varepsilon\, e_{11}) - \lambda]\,[(E_2 + \varepsilon\, e_{22}) - \lambda] - \varepsilon^2\, e_{12}^2 \tag{1.3}$$

if we approximate to first order in ε we get

$$P(\lambda) \approx [(E_1 + \varepsilon\, e_{11}) - \lambda]\,[(E_2 + \varepsilon\, e_{22}) - \lambda] \ , \tag{1.4}$$

from where we obtain that the corrected energies are

$$\begin{aligned} \mathcal{E}_1 &= E_1 + E_1^{(1)} = E_1 + \varepsilon\, e_{11} \\ \mathcal{E}_2 &= E_2 + E_2^{(1)} = E_2 + \varepsilon\, e_{22} \end{aligned} , \tag{1.5}$$

which in turn implies that the first order correction to the energies are given by

$$\begin{aligned} E_1^{(1)} &= \varepsilon \langle 1|\mathbf{W}|1\rangle \\ E_2^{(1)} &= \varepsilon \langle 2|\mathbf{W}|2\rangle \end{aligned} . \tag{1.6}$$

1.1.2 Statement of the problem

Let us assume that we are studying a system whose Hamiltonian $\mathbf{H}$ can be split as:

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{W} , \tag{1.7}$$

where $\mathbf{H}_0$, called the *unperturbed Hamiltonian*, is a time independent Hamiltonian that we have already diagonalized, i.e. we have found its full spectrum, i.i. the sets of all its eigenvalues and associated eigenvectors, which in fact provide a basis for the state space. The second term $\mathbf{W}$ corresponds to the "perturbation", which is, in a sense, much smaller than $\mathbf{H}_0$.

When $\mathbf{W}$ is time independent (the subject of this chapter), we talk about "stationary perturbation". Our problem is to find the **modifications** produced in the energy levels of the system (eigenvalues) and in its stationary states (eigenstates) by the addition of the perturbation $\mathbf{W}$.

For reasons that will become clear as we play along, we introduce a dimensionless parameter λ and redefine $\mathbf{W}$ as

$$\mathbf{W} \equiv \lambda \hat{\mathbf{W}} \quad \text{with, } \lambda \ll 1 \tag{1.8}$$

where $\hat{\mathbf{W}}$ is an operator with matrix elements which might be comparable with those of $\mathbf{H}_0$. In these terms, we write the hamiltonian as

$$\mathbf{H} = \mathbf{H}_0 + \lambda \hat{\mathbf{W}} . \tag{1.9}$$

Under certain conditions, the eigenvalues and eigenstates of $\mathbf{H}$ happen to be analytic in λ. This means that we can expand them in powers of λ. In practice, we keep only a few terms, often the first one or two.

For the sake of clarity, we assume that the unperturbed energies of $\mathbf{H}_0$ form a discrete spectrum and we label them with the integral index "p"

$$E_p^{(0)} ,$$

the zero on top meaning that these correspond to order zero in λ. The corresponding eigenstates are denoted by

$$\left|\varphi_p^{i(0)}\right\rangle ,$$

where the index i is used if the states are degenerate.

Accordingly to the above comments,

$$\mathbf{H}_0 \left|\varphi_p^{i(0)}\right\rangle = E_p^{(0)} \left|\varphi_p^{i(0)}\right\rangle , \tag{1.10}$$

where we must recall that the eigenstates form an orthonormal basis of the state space, i.e.

$$\left\langle\varphi_p^{i(0)}\middle|\varphi_p^{i(0)}\right\rangle = \delta_{ii'}\delta_{pp'} , \tag{1.11}$$

$$\sum_p \sum_i \left|\varphi_p^{i(0)}\right\rangle \left\langle\varphi_p^{i(0)}\right| = \mathbf{1} . \tag{1.12}$$

Notice in particular that formula (1.11) states that energy degenerate eigenstates are orthonormal for a fixed energy eigenspace.

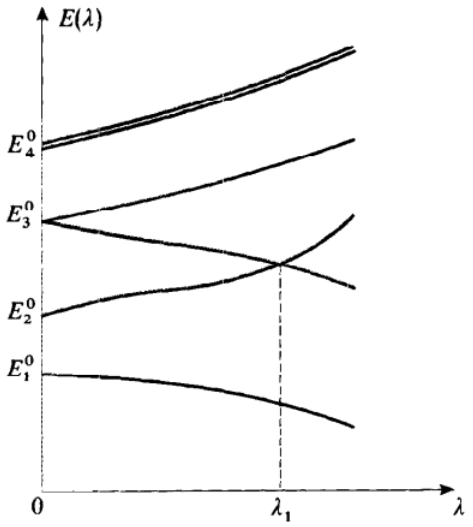

FIGURE 1

Variation of the eigenvalues $E(\lambda)$ of the Hamiltonian $H(\lambda) = H_0 + \lambda\hat{W}$ with respect to λ. Each curve corresponds to an eigenstate of $H(\lambda)$. For $\lambda = 0$, we obtain the spectrum of H_0. We have assumed here that the eigenvalues E_3^0 and E_4^0 are doubly degenerate; application of the perturbation $\lambda\hat{W}$ removes the degeneracy of E_3^0, but not that of E_4^0. An additional two-fold degeneracy appears for $\lambda = \lambda_1$.

Figure 1.1: We can see the bigger the λ the bigger the perturbation of the energies. Taken from Cohen-Tannoudji vol.2 [1].

Under the assumption of analyticity in λ, the energies $E_p(\lambda)$ and eigenstates $\left|\varphi_p^i(\lambda)\right\rangle$ can be expanded as

$$E_p(\lambda) = E_p^{(o)} + \lambda\, E_p^{(1)} + \cdots + \lambda^q\, E_p^{(q)} + \ldots , \tag{1.13}$$

$$|\varphi_p(\lambda)\rangle = \left|\Phi_p^{(0)}\right\rangle + \lambda \left|\Phi_p^{(1)}\right\rangle + \cdots + \lambda^q \left|\Phi_p^{(p)}\right\rangle + \dots \,. \tag{1.14}$$

Please note the following slight change, instead of using $|\varphi_n^i(\lambda)\rangle$we are writing $\left|\Phi_p^{(1)}\right\rangle$, the reason is relatively simple. In the case of degeneration of an energy level, all we know about -for instance- of the zero order in equation is that the right side of equation 1.14 is that $\left|\Phi_p^{(0)}\right\rangle$ belongs to the eigenspace associated to $E_n^{(0)}$ and is not necessarily one of the basis elements.

The expansions in λ must be substituted in the time independent Schrödinger equation

$$\mathbf{H}\,|\varphi_n(\lambda)\rangle = E_p(\lambda)\,|\varphi_n(\lambda)\rangle \ , \tag{1.15}$$

which leads to a series of identities which must be satisfied order by order in λ.

1.1.3 Perturbation of the Non-Degenerated Levels

In the case of non-degenerate states, the substitution yields

$$\begin{aligned}&(\mathbf{H}_0 + \lambda\hat{\mathbf{W}})\left(\left|\phi_n^{(0)}\right\rangle + \lambda\left|\phi_n^{(1)}\right\rangle + +\lambda^2\left|\phi_n^{(2)}\right\rangle + \dots\right) = \\ &(E_n^{(0)} + \lambda\, E_n^{(1)} + \dots)\left(\left|\phi_n^{(0)}\right\rangle + \lambda\left|\phi_n^{(1)}\right\rangle + +\lambda^2\left|\phi_n^{(2)}\right\rangle + \dots\right) \ .\end{aligned} \tag{1.16}$$

1.1.3.1 First Order Corrections to the energy

From equations (1.16) it is easy to arrive to the following pair of identities valid to order 1 in λ

$$\mathbf{H}_0\left|\phi_n^{(0)}\right\rangle = E_n^{(0)}\left|\phi_n^{(0)}\right\rangle \tag{1.17}$$

$$\lambda\left[\mathbf{H}_0\left|\phi_n^{(1)}\right\rangle + \hat{\mathbf{W}}\left|\phi_n^{(0)}\right\rangle\right] = \lambda\,\left[E_n^{(0)}\left|\phi_n^{(1)}\right\rangle + E_n^{(1)}\left|\phi_n^{(0)}\right\rangle\right] \ , \tag{1.18}$$

Multiplying the last formula to the left by $\langle\phi_n^{(0)}|$, the following is obtained:

$$\left\langle\phi_n^{(0)}\middle|\mathbf{H}_0\middle|\phi_n^{(1)}\right\rangle + \left\langle\phi_n^{(0)}\middle|\hat{\mathbf{W}}\middle|\phi_n^{(0)}\right\rangle = E_n^{(0)}\left\langle\phi_n^{(0)}\middle|\phi_n^{(1)}\right\rangle + E_n^{(1)}\left\langle\phi_n^{(0)}\middle|\phi_n^{(0)}\right\rangle \ . \tag{1.19}$$

Since $\mathbf{H}_0$ is hermitian, $\left\langle\phi_n^{(0)}\right|\mathbf{H}_0 = E_n^{(0)}\left\langle\phi_n^{(0)}\right|$, and therefore the first two terms in both sides of the equation are equal and cancel, whilst the orthonormality of the states imply that the last term of the RHS[2] is just $E_n^{(1)}$. We therefore have found that the first order correction to the energy is

[2]RHS: Standard accronym for 'right hand side'. Analologously, LHS stands for 'left hand side'.

given by

$$E_n^{(1)} = \left\langle \phi_n^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle . \tag{1.20}$$

1.1.3.2 First Order Corrections to the energy eigenstates

If instead of multiplying equation 1.18 to the left by $\langle \phi_n^{(0)}|$ as previously done, we do it by $\langle \phi_k^{(0)}|$ $(k \neq n)$, we get

$$\left\langle \phi_k^{(0)} \middle| \mathbf{H}_0 \middle| \phi_n^{(1)} \right\rangle + \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle = E_n^{(0)} \left\langle \phi_k^{(0)} \middle| \phi_n^{(1)} \right\rangle + E_n^{(1)} \left\langle \phi_k^{(0)} \middle| \phi_n^{(0)} \right\rangle , \tag{1.21}$$

i.e.

$$(E_k^{(0)} - E_n^{(0)}) \left\langle \phi_k^{(0)} \middle| \phi_n^{(1)} \right\rangle = +E_n^{(1)} \delta_{nk} - \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle . \tag{1.22}$$

since the set of all $\left|\phi_k^{(0)}\right\rangle$ is a basis for the state space,

$$\left|\phi_n^{(1)}\right\rangle = \sum_\ell c_\ell \left|\phi_k^{(0)}\right\rangle , \tag{1.23}$$

substitution in formula 1.22 yields

$$(E_k^{(0)} - E_n^{(0)}) \left\langle \phi_k^{(0)} \right| \left[\sum_\ell c_\ell \left|\phi_\ell^{(0)}\right\rangle \right] = - \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle . \tag{1.24}$$

from where

$$(E_k^{(0)} - E_n^{(0)})\, c_k = - \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle . \tag{1.25}$$

and from here we get the first order corrected ket, namely

$$|\phi_n\rangle = \left|\phi_n^{(0)}\right\rangle + \sum_{k \neq n} \left[\frac{\left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} \right] \left|\phi_k^{(0)}\right\rangle . \tag{1.26}$$

1.1.4 Second order corrections to the energy

Here we just quote the second order corrections and leave the proof as one of those calculations that everyone has to do at least once in her/his lifetime. ENJOY

$$E_n^{(2)} = \sum_{k \neq n} \frac{\left| \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle \right|^2}{E_n^{(0)} - E_k^{(0)}} \,. \tag{1.27}$$

1.1.5 Second order corrections to the energy eigenstates

$$\begin{aligned} \left|\phi_n^{(0)}\right\rangle = \sum_{m \neq n} \Bigg[\sum_{k \neq n} \frac{\left\langle \phi_m^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_k^{(0)} \right\rangle \left\langle \phi_k^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_m^{(0)})} - \\ - \frac{\left\langle \phi_m^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle \left\langle \phi_n^{(0)} \middle| \hat{\mathbf{W}} \middle| \phi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_m^{(0)})^2} \Bigg] \,. \end{aligned} \tag{1.28}$$

1.2 Perturbation theory for degenerate states

We just consider first order corrections. To that end we recall the recursions up to first order,

$$\mathbf{H}_0 \left|\varphi_n^{i(0)}\right\rangle = E_0^{(0)} \left|\varphi_n^{i(0)}\right\rangle \tag{1.29}$$

$$\left[\mathbf{H}_0 - E_n^{(0)}\right] \left|\Phi_n^{(0)}\right\rangle = \left[\hat{\mathbf{W}} - E_n^{(1)}\right] \left|\Phi_n^{i(0)}\right\rangle \,, \tag{1.30}$$

where we recall that the only thing we know about $\left|\Phi_n^{i(0)}\right\rangle$ is that it belongs to the g-dimensional eigenspace associated with the degenerate energy $E_n^{(0)}$. We now chose one and only one element of the basis of the degenerate eigenspace and project equation 1.30 on it, to get

$$\left\langle \varphi_n^{f(0)} \right| \left[\mathbf{H}_0 - E_n^{(0)}\right] \left|\Phi_n^{(0)}\right\rangle = \left\langle \varphi_n^{f(0)} \right| \left[\hat{\mathbf{W}} - E_n^{(1)}\right] \left|\Phi_n^{i(0)}\right\rangle \,, \tag{1.31}$$

clearly

$$\left[E_n^{(0)} - E_n^{(0)}\right] \left|\Phi_n^{(0)}\right\rangle = \left\langle \varphi_n^{f(0)} \right| \left[\hat{\mathbf{W}} - E_n^{(1)}\right] \left|\Phi_n^{i(0)}\right\rangle \,, \tag{1.32}$$

implying:

$$\left\langle \varphi_n^{f(0)} \right| \hat{\mathbf{W}} \left|\Phi_n^{i(0)}\right\rangle = E_n^{(1)} \left\langle \varphi_n^{f(0)} \middle| \Phi_n^{i(0)} \right\rangle \,, \tag{1.33}$$

we now conveniently insert the identity[3] in the l.h.s. of the above equation

$$\sum_{n'}\sum_{f'}\left\langle\varphi_n^{f(0)}\right|\hat{\mathbf{W}}\left|\varphi_{n'}^{f'(0)}\right\rangle\left\langle\varphi_{n'}^{f'(0)}\right|\left.\Phi_n^{i(0)}\right\rangle = E_n^{(1)}\left\langle\varphi_n^{f(0)}\right|\left.\Phi_n^{i(0)}\right\rangle\ , \tag{1.35}$$

now we note that the n eigenspace is orthogonal to the rest of the Hilbert space so

$$\sum_{f'}\left\langle\varphi_n^{f(0)}\right|\hat{\mathbf{W}}\left|\varphi_n^{f'(0)}\right\rangle\left\langle\varphi_n^{f'(0)}\right|\left.\Phi_n^{i(0)}\right\rangle = E_n^{(1)}\left\langle\varphi_n^{f(0)}\right|\left.\Phi_n^{i(0)}\right\rangle\ . \tag{1.36}$$

A little bit of inspection shows that the g^2 numbers

$$W^{f\,f'} = \left\langle\varphi_n^{f(0)}\right|\hat{\mathbf{W}}\left|\varphi_n^{f'(0)}\right\rangle\ , \tag{1.37}$$

are nothing but the entries of $\hat{\mathbf{W}}$ restricted to the eigenspace related to $E_n^{(0)}$. Once we realize this, we recognize eqn. 1.37 as the eigen problem:

$$\hat{\mathbf{W}}\left|\Phi_n^{i(0)}\right\rangle = E_n^{(1)}\left|\Phi_n^{i(0)}\right\rangle\ , \tag{1.38}$$

1.3 Problems

Problem 1.1. *Let the Hamiltonian of a two level system be*

$$\mathbf{H} = \begin{pmatrix} E & \varepsilon e_{12} \\ \varepsilon e_{12} & E \end{pmatrix}\ , \tag{1.39}$$

(a) What can you say about the unperturbed system?

(b) Show that in this case, the corrected energies are

$$E_{1,2} = E \pm \varepsilon e_{12} = E \pm \varepsilon\left\langle 1|\mathbf{W}|2\right\rangle\ .$$

Can you say something about the physics?

[3]
$$\sum_{n'}\sum_{f'}\left|\varphi_{n'}^{f'(0)}\right\rangle\left\langle\varphi_{n'}^{f'(0)}\right| = \mathbf{I} \tag{1.34}$$

Problem 1.2. *Use perturbation theory to solve the spectral problem of the self-adjoint matrix*

$$\mathbf{W} = \begin{bmatrix} 1.95 & -0.05 & 0 \\ -0.05 & 1 & 0 \\ 0 & 0 & 2.95 \end{bmatrix} \tag{1.40}$$

Problem 1.3. *Repeat problem 1.2 with the matrix:*

$$\mathbf{W} = \begin{bmatrix} 2 & -0.05 & 0 \\ -0.05 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \tag{1.41}$$

Problem 1.4. *Repeat problem 1.3 with the following matrix*

$$\mathbf{W} = \begin{bmatrix} 2 & 0.1 & 0 & 0 \\ 0.1 & 1 & 0 & 0 \\ 0 & 0 & 1.95 & -0.05 \\ 0 & 0 & -0.05 & 2.95 \end{bmatrix} \tag{1.42}$$

Problem 1.5. Problem taken from Schiff [2], as cited by Sakurai [3]. *A system that has three unperturbed states can be represented by the perturbed Hamiltonian matrix*

$$\begin{bmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{bmatrix},$$

where $E_2 > E_1$. The quantities a and b are to be regarded as perturbations that are both of the same order and small compared to $E_2 - E_1$.

(a) Use the second-order nondegenerate perturbation theory to calculate the perturbed eigenvalues. Is this procedure correct?

(b) Diagonalize the matrix and find the EXACT *eigenvalues.*

(c) Use the second-order degenerate perturbation theory.

(d) Compare the three previously obtained results.

Problem 1.6. *Consider a spinless particle of mass M trapped in an infinite square potential of width L. The energy well is modified by adding a small (square) bump of width δL ($\delta L << L$) and height $\mathcal{E}$ which is centered at the center of the well.*

(a) Find the first order correction to the ground state energy and eigenstate

(b) What difference does it make if we consider the first excited state.

Problem 1.7. *Consider the following natural generalization of problem 1.6: A spinless particle of mass M trapped in a rectangular cavity of sides $L_x \neq L_y$. This time, the bump has square shape of sides δL, its height still being $\mathcal{E}$*

(a) Find the first order perturbed eigenvalues and eigenfunctions.

(b) What happens with the lowest energy states if $L_x = L_y$?

Problem 1.8. Problem taken from Sakurai [3]. To solve this problem you must review Cohen-Tannoudji et al. [1], chapter 4.

A simple one-dimensional harmonic oscillator is subjected to a perturbation

$$\lambda\hat{\mathbf{W}} = \beta\mathbf{X}\,,$$

where β is a real constant.

(a) Calculate the energy shift of the ground state to lowest nonvanishing order.

(b) Solve this problem EXACTLY *and compare with your previously obtained result.*

Problem 1.9. *A classical charged particle moves along the x axis under the action of an uniform electric field $\vec{E} = \mathcal{E}\,\hat{\mathbf{e}}_x$, where $\mathcal{E}$ is a constant. Setting the interaction energy equal to zero at the origin, the potential energy associated with this interaction is $V(x) = -q\,x\,\mathcal{E}$.*

(a) What are the SI units of $\mathcal{E}$

(b) Imagine a harmonic oscillator of mass m and angular frequency ω moving along the x axis and let its equilibrium position be at the origin. Let the mass be charged an turn on a uniform electric field.

(i) Find the classical Hamiltonian

(ii) Solve the classical equations of motion. Do you find any differences between the motion in this case and the uncharged one?

(iii) Use the correspondence principle to find the quantum Hamiltonian for the system.

(iv) Solve the energy eigen problem EXACTLY, i.e. diagonalize the Hamiltonian. **HINT:** *There is a simple and lovely algebraic trick which requires watching the Hamiltonian very carefully.*

(v) Think of the potential due to the electric field as a perturbation to the harmonic oscilator. Use this fact to study the corrections to the energy and comment on your findings.

Problem 1.10. Problem taken from Merzbacher [4], as cited by Sakurai [3]. *Suppose the Hamiltonian of a rigid rotator in a magnetic field perpendicular to the axis is of the form*

$$\alpha \mathbf{L}^2 + \beta \mathbf{L}_z + \gamma \mathbf{L}_y$$

if quadratic terms in the field are neglected. Assuming $\beta \gg \gamma$, use perturbation theory to lowest non-vanishing order *to get approximate energy eigenvalues.*

Problem 1.11. *Review the angular-radial split of the time independent Schrödinger's equation for radial potentials, make sure that you understand that the eigenstates get the general form*

$$|\psi\rangle = |n\rangle|\ell, m\rangle\,, \tag{1.43}$$

where $|\ell, m\rangle$ are orbital angular momentum eigenstates.

Problem 1.12. Problem taken from Sakurai [3]. *Consider an isotropic two-dimensional harmonic oscillator subjected to a perturbation*

$$\lambda \hat{\mathbf{W}} = m\omega^2 \mathbf{XY}\,.$$

(a) What are the energies of the three lowest-lying states in the unperturbed case*? Is there any degeneracy?*

(b) Find the zeroth-order energy eigenvector and the corresponding energy to first order[4] *for each of the three lowest-lying states.*

[4] That is, the unperturbed energy obtained in (a) plus the first-order energy shift.

(c) Solve this problem EXACTLY *and compare with your previously obtained result.*

Problem 1.13. Problem taken from Cohen-Tannoudji et al., Complement H_{XI}, [1]. *A particle of mass m, constrained to move in the xOy plane, has a Hamiltonian corresponding to a two-dimensional isotropic harmonic oscillator. Consider the effect on this particle of a perturbation*

$$\mathbf{W} = \lambda_1 \hat{\mathbf{W}}_1 + \lambda_2 \hat{\mathbf{W}}_2 \,,$$

where λ_1 and λ_2 are constants, and

$$\hat{\mathbf{W}}_1 = m\omega^2 \mathbf{XY} \,, \quad \hat{\mathbf{W}}_2 = \hbar\omega \left(\frac{\mathbf{L}_z^2}{\hbar^2} - 2 \right) .$$

Considering only first order corrections for the energies and the second excited state of $\mathbf{H}_0$ of energy $3\hbar\omega$, which is three-fold degenerate, answer the following questions:

(a) Calculate the matrices representing the restrictions of $\hat{\mathbf{W}}_1$ and $\hat{\mathbf{W}}_2$ to the eigensubspace of the aforementioned energy level of $\mathbf{H}_0$.

*(b) Assume $\lambda_2 \ll \lambda_1 \ll 1$ and use the results obtained in problem **??** to study the effect of $\lambda_2 \hat{\mathbf{W}}_2$.*

(c) Assume $\lambda_1 = 0$ and calculate the effect of $\lambda_2 \hat{\mathbf{W}}_2$ on the second excited state of $\mathbf{H}_0$.

(d) Solve the previous case EXACTLY.

(e) Finally, assume that $\lambda_1 \ll \lambda_2 \ll 1$ and consider the previous result to be the new unperturbed situation and calculate the effect of $\lambda_1 \hat{\mathbf{W}}_1$.

Problem 1.14. Problem taken from Merzbacher [4], as cited by Sakurai [3]. *A slightly anisotropic three-dimensional harmonic oscillator has $\omega_z \approx \omega_x = \omega_y$. A charged particle moves in the field of this oscilator and is at the same time exposed to a uniform magnetic field in the x-direction. Assuming that the Zeeman splitting is comparable to the splitting produced by the anisotropy, but small compared to $\hbar\omega$, calculate to first order the energies of the first excited state. Discuss various limiting cases.*

Problem 1.15. Problem taken from Cohen-Tannoudji et al., Complement H_{XI}, [1]. *Consider a system formed by an electron spin $\mathbf{S}$ and two nuclear spins $\mathbf{I}_1$ and $\mathbf{I}_2$. Assume that*

$\mathbf{S}$, $\mathbf{I}_1$ *and* $\mathbf{I}_2$ *are all spin* $1/2$*'s. The state space of the three-spin system is spanned by the eight othonormal kets* $|\varepsilon_S, \varepsilon_1, \varepsilon_2\rangle$*, the common eigenvectors of* $\mathbf{S}$, $\mathbf{I}_1$ *and* $\mathbf{I}_2$*, with eigenvalues* $\varepsilon_i\hbar/2$ *and* $\varepsilon_i = \pm$ *for* $i \in \{S, 1, 2\}$.

(a) Neglect any coupling of the three spins and assume, however, that they are placed in a uniform magnetic field $\vec{\mathbf{B}} \parallel \hat{k}$*. Since the gyromagnetic ratios of* $\mathbf{I}_1$ *and* $\mathbf{I}_2$ *are equal, the Hamiltonian of the system can be written as*

$$\mathbf{H}_0 = \Omega\, \mathbf{S}_z + \omega \mathbf{I}_{1z} + \omega \mathbf{I}_{2z}\,,$$

where Ω *and* ω *are real, positive constants, proportional to* $|\vec{\mathbf{B}}|$*. Assume* $\Omega > 2\omega$*. What are the possible energies of the three-spin system and their degrees of degeneracy? Draw the energy diagram.*

(b) Now take into account the copuling of the spins, still neglecting the direct coupling of $\mathbf{I}_1$ *and* $\mathbf{I}_2$*, by adding the Hamiltonian*

$$\mathbf{W} = \beta\, [\mathbf{S}.\mathbf{I}_1 + \mathbf{S}.\mathbf{I}_2]\,,$$

where β *is a real, positive constant. What conditions must be satisfied by* $\varepsilon_S, \varepsilon_1, \varepsilon_2, \varepsilon'_S, \varepsilon'_1, \varepsilon'_2$ *for* $\beta\, \mathbf{S}.\mathbf{I}_1$ *to have non-zero matrix elements between* $|\varepsilon_S, \varepsilon_1, \varepsilon_2\rangle$ *and* $|\varepsilon'_S, \varepsilon'_1, \varepsilon'_2\rangle$*? Same question for* $\beta\, \mathbf{S}.\mathbf{I}_2$.

(c) Assume that $\beta\hbar^2 \ll \{\hbar\Omega, \hbar\omega\}$ *so that* $\mathbf{W}$ *can be treated as a perturbation with respect to* $\mathbf{H}_0$*. To first order in* $\mathbf{W}$*, what are the eigenvalues of the total Hamiltonian* $\mathbf{H}$ (1.7)*? To zeroeth order in* $\mathbf{W}$*, what are the eigenstates of* $\mathbf{H}$ (1.7)*? Draw the energy diagram.*

(d) Using the approximation of the preceding question, determine the Bohr frequencies which can appear in the evolution of $\langle \mathbf{S}_x \rangle$ *when the coupling* $\mathbf{W}$ *of the spins is taken into account.*

(e) Review what an EPR (Electronic Paramagnetic Resonance) experiment is and relate the frequencies of the resonance lines to the preceding Bohr frequencies. What is the shape of the EPR spectrum observed for the three-spin system? How can the coupling constant β *be determined from this spectrum?*

In what follows we shall learn a great deal about the physics of Hydrogen atom. You are expected to master Chapter XII of Cohen-Tannoudji et al. [1].

Problem 1.16. Hydrogen Atom, part I

(a) *Use a semiclassical argument (Bohr-Sommerfeld quantization conditions are enough for this) to show that the Bohr radius and Rydberg's constant appear naturally as a consequence of quantum mechanics.*

(b) *Look for the definiton of the fine structure constant α and find its numerical value.*

(c) *Make sure to review the Hydrogen atom as described in Cohen-Tannoudji et al. vol I [1] (unlees you find it necessary, don't go through the complements).*

Problem 1.17. Hydrogen Atom, part II. Relativistic correction to the Kinetic Energy You may find chapter 6 of Griffiths [5] very useful. Arfken [6] might also become handy.

The Hamiltonian for the Hydrogen atom is usually built using the correspondence principle and the non relativistic formula[5]

$$T = \frac{p^2}{2M} \tag{1.44}$$

to represent the kinetic energy operator of the electron.

(a) *Considering orders of magnitude, is this formula totally acceptable?*

(b) *In special relativity, the classical*[6] *kinetic energy of a particle of mass m is given by*

$$T = \sqrt{(\vec{p})^2c^2 + m^2c^4} - mc^2 \tag{1.45}$$

(c) *Use the fact that for an electron mc^2 is $0.511\,Mev$ to get the following approximation to the kinetic energy of the electron*

$$T \approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \tag{1.46}$$

(d) *Use the above fomrmula to build a new time independent hamiltonan for the Hydrogen atom. Split your result to show that the p^4 can be thought of as a perturbing term of the usual Hamiltonian. Is the perturbation small?*

(e) *Find the new energy eigenvalues for the $\ell \neq 0$ states of the Hydrogen atom*

Problem 1.18. *spin orbit coupling ....*

[5] What is M?
[6] As in non quantum.

Problem 1.19. PROBLEM TAKEN FROM SAKURAI [3]. *A one-electron Hidrogen-like atom is assumed to be non-degenerate and is placed in a uniform electric field in the z-direction.*

(a) Obtain an approximate expression for the induced electrical dipole moment of the groud state by considering the expectation value of $e\mathbf{Z}$ with respect to the perturbed state vector computed to first order.

(b) Show that the same expression can also be obtained from the energy shift $\Delta = -\alpha|\mathbf{E}|^2/2$, where α stands for the polarizability, of the ground state, computed to second order.

Problem 1.20. PROBLEM TAKEN FROM SAKURAI [3]. *Suppose the electron had an intrinsic* electric *dipole moment analogous to the spin magnetic moment (that is, $\vec{\mu}_{el} \propto \vec{\sigma}$). Treating the hypothetical $-\vec{\mu}_{el} \cdot \mathbf{E}$ interaction as a small perturbation, discuss qualitatively how the energy levels of the* Na *atom (Z=11) would be altered in the absence of any external electromagnetic field. Are the level shifts first order or second order? Obtain an expression for the energy shift of the lowest level that is affected by the perturbation. Assume throughout the problem that only the valence electron is subjected to the hypothetical interaction.*

Problem 1.21. A problem on the variation method PROBLEM TAKEN FROM COHEN-TANNOUDJI ET AL., COMPLEMENT H_{XI}, [1]. *You want to calculate the ground state energy of the hydrogen atom by means of the variational method, choosing as trial functions the spherically symmetrical function $\varphi_\alpha(\mathbf{r})$, whose r-dependance is given by*

$$\varphi_\alpha(\mathbf{r}) = \begin{cases} \mathcal{C}\left(1 - \frac{r}{\alpha}\right), & r \leq \alpha \\ 0, & r > \alpha \end{cases} .$$

$\mathcal{C}$ is a normalization constant and α is the variational parameter.

(a) Calculate the mean value of the kinetic and potential energies of the electron in the state $|\varphi_\alpha\rangle$. Express the mean value of the kinetic energy in terms of $\nabla\varphi$, so as to avoid the "delta functions" which appear in $\Delta\varphi$, since $\nabla\varphi$ is discontinuous.

(b) Find the optimal value α_o of α and compare it to the Bohr radius a_o.

(c) Compare the approximation value obtained for the ground state energy with the exact value $-E_I$.

Chapter 2

Time Dependent Perturbation Theory

We have already studied how to approximately find the energy eigenstates and eigenvalues of a system whose Hamiltonian is of the form $\mathbf{H}_0 + \mathbf{W}$, where the original hamiltonian $\mathbf{H}_0$ and the "small" perturbation $\mathbf{W}$ are both time independent. Let us now consider a somewhat different situation. Suppose that we begin with a system evolving under the Hamiltonian $\mathbf{H}_0$, and then we proceed to act on the system with a time-dependent external force, describable by an interaction term $\mathbf{W}(t)$ added to the Hamiltonian.

This physical situation rises the following question, what effect does the force have on the system?. This situation might model shining light on an atom while asking what are the chances that the light ionizes the atom. It might also model applying a voltage to a piece of metal, to ask how much current is produced.

Let us begin by stating the problem of interest. From a physical point of view think of a system which is initially at stationary state $|\psi_i\rangle$ of $\mathbf{H}_0$ with corresponding eigenvalue E_i. The external force begins acting at $t = 0$ setting the system into evolution so $|\psi_i\rangle$ is no longer and eigenstate of $\mathbf{H}$. What we want is to calculate the probability $\mathcal{P}_{if}$ of finding the system in another eigenstate $|\psi_f\rangle$ of $\mathbf{H}_0$ at a later time t.

In principle, the problem reduces to this, we begin, at time $t = 0$, with the system in a state $|\psi(t)\rangle$ that solves

$$\mathbf{H}_0 \, |\psi(t)\rangle = i\hbar \frac{\partial \, |\psi(t)\rangle}{\partial t} \qquad t < 0 \, . \tag{2.1}$$

and then solve

$$[\mathbf{H}_0 + \mathbf{W}(t)] \, |\psi(t)\rangle = i\hbar \frac{\partial \, |\psi(t)\rangle}{\partial t} \qquad t > 0 \, . \tag{2.2}$$

subject to the initial condition $|\psi(t = 0)\rangle = |\psi\rangle_i$. Once the solution is found, the probability we

are looking for is simply

$$\mathcal{P}_{if} = |\langle\psi_f|\psi_i\rangle|^2 . \tag{2.3}$$

The problem just stated is precisely what time dependent perturbation theory is all about. This technique allows approximate solutions of the Schrödinger equation when the hamiltonian contains a bit with an explicit time dependence as

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{W}(t) \tag{2.4}$$

where $\mathbf{H}_0$ is an already diagonalized piece.

In this case, the full Schrödinger equation is

$$[\mathbf{H}_0 + \mathbf{W}(t)]\,|\psi(t)\rangle = i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} . \tag{2.5}$$

2.1 Elementary Solution

Time dependent perturbation theory may be easily tackled down by the method of *variation of parameters*. As we did in the time independent case, we take advantage of the fact that the eigenstates[1] ($|\phi_n\rangle$) of the unperturbed hamiltonian constitute a complete basis of the state space to try a solution of the form[2]

$$|\psi(t)\rangle = \sum_n c_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle \tag{2.6}$$

The time derivative of the proposed solution times $i\hbar$ is

$$\begin{aligned} i\hbar\,\frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t} &= i\hbar\sum_n \dot{c}_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle + \sum_n \hbar\,\omega_n\,c_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle = \\ &= i\hbar\sum_n \dot{c}_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle + \sum_n c_n(t)\mathrm{e}^{-i\omega_n t}E_n\,|\phi_n\rangle = \\ &= i\hbar\sum_n \dot{c}_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle + \sum_n c_n(t)\mathrm{e}^{-i\omega_n t}\mathbf{H}_0\,|\phi_n\rangle \end{aligned} \tag{2.7}$$

[1] For simplicity, we regard the energy spectrum as discrete.

[2] Recall that the general solution for time independent hamiltonians is

$$|\psi(t)\rangle = \sum_n c_n\,\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle .$$

substituting in Schrödinger's equation we get

$$\begin{aligned}&\sum_n \left[\mathbf{H}_0 + \mathbf{W}(t)\right]\, c_n(t)\mathrm{e}^{-i\omega_n\, t}\,|\phi_n\rangle = \\ &= i\hbar \sum_n \dot{c}_n(t)\mathrm{e}^{-i\omega_n t}\,|\phi_n\rangle + \sum_n c_n(t)\mathrm{e}^{-i\omega_n\, t}\mathbf{H}_0\;|\phi_n\rangle\end{aligned} \tag{2.8}$$

which reduces to

$$\sum_n \dot{c}_n(t)\mathrm{e}^{-i\omega_n\, t}\,|\phi_n\rangle = -\frac{i}{\hbar}\sum_n \mathbf{W}(t)\, c_n(t)\mathrm{e}^{-i\omega_n\, t}\,|\phi_n\rangle \tag{2.9}$$

The obvious step to take here is to apply $\langle\phi_k|\,\mathrm{e}^{i\omega_k\, t}$ to the left of the equation, to get

$$\sum_n \dot{c}_n(t)\mathrm{e}^{i\omega_{nk}\, t}\,\langle\phi_k|\phi_n\rangle = -\frac{i}{\hbar}\,\langle\phi_k|\,\left[\sum_n \mathbf{W}(t)\, c_n(t)\mathrm{e}^{i\omega_{nk}\, t}\,|\phi_n\rangle\right]\,, \tag{2.10}$$

where $\omega_n = E_n/\hbar$, and since $\langle\phi_k|\phi_n\rangle = \delta_{nk}$,

$$\dot{c}_k(t) = -\frac{i}{\hbar}\sum_n \mathrm{e}^{i\omega_{nk}}\,\langle\phi_k|\mathbf{W}(t)|\phi_n\rangle\; c_n(t)\;, \tag{2.11}$$

where

$$\omega_{nk} = \omega_k - \omega_n\,,$$

this in turn can be cast as the integral equation

$$c_k(t) = c_{0k} - \frac{i}{\hbar}\sum_n \lambda \int_{t_0}^{t} \mathrm{e}^{i\omega_{nk}\,\xi}\,\langle\phi_k|\mathbf{W}(\xi)|\phi_n\rangle\; c_n(\xi)\, d\xi\,, \tag{2.12}$$

which is clearly non linear. This kind of equation[3] can be solved iteratively, i.e. we let $c_\ell(t)$ be

$$c_\ell(t) = c_\ell^{(0)}(t) + \lambda\, c_\ell^{(1)}(t) + \lambda^2 c_\ell^{(2)}(t) + \dots\,, \tag{2.13}$$

[3] where we have reinserted the parameter λ to make things easier to visualize

and substitute in the integral equation to obtain:

$$\begin{aligned}
&c_n^{(0)}(t) + \lambda\, c_n^{(1)}(t) + \lambda^2 c_n^{(2)}(t) + \cdots = \\
&c_{0n} - \frac{i}{\hbar}\sum_n \lambda \int_{t_0}^{t} \langle\phi_k|\mathbf{W}(\xi)|\phi_n\rangle \left[c_n^{(0)}(\xi) + \lambda\, c_n^{(1)}(\xi) + \lambda^2 c^{(2)}(\xi) + \dots\right] \mathrm{e}^{i\frac{(E_k-E_n)\xi}{\hbar}} d\xi = \\
&c_{0n} - \frac{i}{\hbar}\sum_n \lambda \int_{t_0}^{\xi} \langle\phi_k|\mathbf{W}(\xi)|\phi_n\rangle\; c_n^{(0)}(\xi)\mathrm{e}^{i\frac{(E_k-E_n)t}{\hbar}} d\xi + \\
&-\frac{i}{\hbar}\sum_n \lambda^2 \int_{t_0}^{t} \langle\phi_k|\mathbf{W}(\xi)|\phi_n\rangle\; c_n^{(1)}(\xi)\mathrm{e}^{i\frac{(E_k-E_n)\xi}{\hbar}} d\xi + \dots
\end{aligned} \tag{2.14}$$

Inspection shows that

$$\begin{aligned}
c_n^{(0)}(t) &= c_{0n} \\
c_n^{(1)}(t) &= -\frac{i}{\hbar}\sum_n \int_{t_0}^{t} \langle\phi_k|\mathbf{W}(\xi)|\phi_n\rangle\; c_{0n}\, \mathrm{e}^{i\frac{(E_k-E_n)\xi}{\hbar}} d\xi \\
&\dots
\end{aligned} \tag{2.15}$$

Freeman Dyson did the magic of unifying Schwinger's and Feynman quantum electrodynamics, in doing so we all learned a technique called the Dyson series approach to time dependent perturbation theory that gives us a unified view of the calculation we had just made and which is the natural way to introduce Feynman diagrams.

2.2 The transition Probability

Since the system is initially at state $|\phi_i\rangle$, $c_{0n} = \delta_{ni}$ and so, its state at time t to first order will be:

$$|\psi(t)\rangle = \mathrm{e}^{iE_i/\hbar}\,|\phi_i\rangle - \frac{i}{\hbar}\left[\sum_k \int_{t_0}^{t} \langle\phi_k|\mathbf{W}(\xi)|\phi_i\rangle\; \mathrm{e}^{i\frac{(E_k-E_i)\xi}{\hbar}} d\xi\; |\phi_k\rangle\right] \tag{2.16}$$

$$\begin{aligned}
S_{fi} = \langle f|i\rangle &= -\frac{i}{\hbar}\,\langle f|\left[\sum_k \int_{t_0}^{t} \langle\phi_k|\mathbf{W}(\xi)|\phi_i\rangle\; \mathrm{e}^{i\frac{(E_k-E_i)\xi}{\hbar}} d\xi\; |\phi_k\rangle\right] \\
&= -\frac{i}{\hbar}\int_{t_0}^{t} \langle\phi_f|\mathbf{W}(\xi)|\phi_i\rangle\; \mathrm{e}^{i\frac{(E_k-E_i)\xi}{\hbar}} d\xi
\end{aligned} \tag{2.17}$$

$$\mathcal{P}_{fi} = \frac{1}{\hbar^2} \left| \int_{t_0}^{t} \langle \phi_f | \mathbf{W}(\xi) | \phi_i \rangle \, \mathrm{e}^{i \frac{(E_k - E_i)\xi}{\hbar}} d\xi \right|^2 \tag{2.18}$$

2.2.1 A couple of examples

2.2.1.1 Sinusoidal Perturbation

Under the influence of a time dependent interaction of the form

$$\mathbf{W} = \mathbf{W}_0 \, sin(\omega \, t) = -i \frac{\mathbf{W}_0}{2} \left[e^{i\omega \, t} - e^{-i\omega \, t} \right] , \tag{2.19}$$

Problem 2.1. *Think of a physical example*

With this particular form of the perturbation, and setting $t_0 = 0$ for simplicity, the transition probability is ($W_{fi} = \langle \phi_f | \mathbf{W}_0 | \phi_i \rangle$)

$$\begin{aligned} \mathcal{P}_{fi} &= \frac{|W_{fi}|^2}{4\hbar^2} \left| \int_0^t \left[e^{i\omega \, t} - e^{-i\omega \, t} \right] \mathrm{e}^{i \frac{(E_k - E_i)\xi}{\hbar}} d\xi \right|^2 = \\ &= \frac{|W_{fi}|^2}{4\hbar^2} \left| \int_0^t \left[e^{i(\omega_{fi} + \omega) \, t} - e^{i(\omega_{fi} - \omega) \, t} \right] \, d\xi \right|^2 = \\ &= \frac{|W_{fi}|^2}{4\hbar^2} \left| \frac{1 - e^{i(\omega_{fi} + \omega) \, t}}{\omega_{fi} + \omega} - \frac{1 - e^{i(\omega_{fi} - \omega) \, t}}{\omega_{fi} - \omega} \right|^2 . \end{aligned} \tag{2.20}$$

As an exercise, show that had the time dependence been $cos(\omega t)$ the transition probability would have resulted in

$$\mathcal{P}_{fi}(t, \omega) = \frac{|W_{fi}|^2}{4\hbar^2} \left| \frac{1 - e^{i(\omega_{fi} + \omega) \, t}}{\omega_{fi} + \omega} + \frac{1 - e^{i(\omega_{fi} - \omega) \, t}}{\omega_{fi} - \omega} \right|^2 , \tag{2.21}$$

where we have written $\mathcal{P}_{fi}(t, \omega)$ in in order to highlight the physical importance of the dependence of the frequency of the perturbation. In this latter case and specializing on a constant perturbation

$(\omega = 0)$ the result is

$$\begin{aligned} \mathcal{P}_{fi}(t, \omega = 9) &= \frac{|W_{fi}|^2}{4\hbar^2} \left| 2\frac{1 - e^{i(\omega_{fi}\, t}}{\omega_{fi}} \right|^2 = \\ &= \frac{|W_{fi}|^2}{\hbar^2} \left[\frac{sen(\omega_{fi}\, t/2)}{\omega_{fi}/2} \right]^2 , \end{aligned} \tag{2.22}$$

2.2.1.2 Resonance

We shall now inquire in to what happens when the frequency of the perturbation is close or equal to the Bohr frequency $\omega_{fi} = (E_f - E_i)/\hbar$ associated to two eigenstates $|\phi_i\rangle$ $|\phi_f\rangle$ of the unperturbed hamiltonian.

We begin by rewriting $\mathcal{P}_{fi}$ as

$$\mathcal{P}_{fi} = \frac{|W_{fi}|^2}{4\hbar^2} |A_+ \pm A_-|^2 , \tag{2.23}$$

where

$$\begin{aligned} A_+ &= \frac{1 - e^{i(\omega_{fi}+\omega)\, t}}{\omega_{fi} + \omega} = -ie^{i(\omega_{fi}+\omega)\, t/2} \frac{sen(\omega_{fi} + \omega)\, t/2)}{(\omega_{fi} + \omega)/2} \\ A_- &= \frac{1 - e^{i(\omega_{fi}-\omega)\, t}}{\omega_{fi} - \omega} = -ie^{i(\omega_{fi}-\omega)\, t/2} \frac{sen(\omega_{fi} - \omega)\, t/2)}{(\omega_{fi} - \omega)/2} . \end{aligned} \tag{2.24}$$

A_- largely dominates formula 2.23 when $\omega \approx \omega_{fi}$ while A_+ does when $\omega \approx -\omega_{fi}$, for these reasons, the second term in fromula 2.23 is called *resonant* and the first one *anti-resonant*

2.3 Coupling with a continuum. Second Fermi's Golden Rule

2.4 Interaction Representation Approach

$$[\mathbf{H}_0 + \mathbf{W}(t)] \, |\psi(t)\rangle = i\hbar \frac{\partial \, |\psi(t)\rangle}{\partial t} . \tag{2.25}$$

Introduce a new time dependent ket $|\Psi\rangle(t)$ as

$$|\psi(t)\rangle \equiv \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle \tag{2.26}$$

so

$$\frac{\partial |\psi(t)\rangle}{\partial t} = -i\frac{\mathbf{H}_0}{\hbar}\, \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle + \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} \frac{\partial |\Psi(t)\rangle}{\partial t}\,, \tag{2.27}$$

after substitution in Schrödinger's equation

$$\begin{aligned} &[\mathbf{H}_0 + \mathbf{W}(t)]\ \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle = \\ &= i\hbar \left[-i\frac{\mathbf{H}_0}{\hbar}\, \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle + \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} \frac{\partial |\Psi(t)\rangle}{\partial t}\right] = \\ &= \mathbf{H}_0\, \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle + i\hbar\, \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} \frac{\partial |\Psi(t)\rangle}{\partial t}\,, \end{aligned} \tag{2.28}$$

we are left with

$$\mathbf{W}(t)\mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} |\Psi(t)\rangle = i\hbar\, \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}} \frac{\partial |\Psi(t)\rangle}{\partial t}\,. \tag{2.29}$$

Which we write as

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \hat{\mathbf{W}}(t) |\Psi(t)\rangle\ . \tag{2.30}$$

where:

$$\hat{\mathbf{W}}(t) \equiv \mathrm{e}^{i\frac{\mathbf{H}_0 t}{\hbar}} \mathbf{W}(t) \mathrm{e}^{-i\frac{\mathbf{H}_0 t}{\hbar}}\,. \tag{2.31}$$

ket $|\Psi\rangle(t)$ and $\hat{\mathbf{W}}(t)$ are said to be in the *interaction representation*

To solve equation 2.30 we recur to an iterative scheme that begins by integrating in time to transform the differential equation into the following integral equation

$$|\Psi(t)\rangle = |\Psi(t_0)\rangle - \frac{i\lambda}{\hbar} \int_{t_0}^{t} \hat{\mathbf{W}}(s) |\Psi(s)\rangle\, ds\,. \tag{2.32}$$

and propose a solution of the form

$$|\Psi(t)\rangle = |\Psi(t_0)\rangle + \lambda \left|\Psi^{(1)}(t)\right\rangle + \lambda^2 \left|\Psi^{(2)}(t)\right\rangle + \lambda^3 \left|\Psi^{(3)}(t)\right\rangle + ... \tag{2.33}$$

From here, one finds that to first order in λ,

$$|\Psi(t)\rangle = |\Psi(t_0)\rangle - \frac{i\lambda}{\hbar} \int_{t_0}^{t} \hat{\mathbf{W}}(s) |\Psi(t_0)\rangle\, ds\,. \tag{2.34}$$

The second order correction is

$$\left|\Psi^{(2)}(t)\right\rangle = -\frac{i\lambda}{\hbar}\int_{t_0}^{t}\hat{\mathbf{W}}(s)\left|\Psi^{(1)}(s)\right\rangle ds = \left(\frac{\lambda}{i\hbar}\right)^2\int_{t_0}^{t}\int_{t_0}^{s}\hat{\mathbf{W}}(s)\hat{\mathbf{W}}(w)\left|\Psi(t_0)\right\rangle dw\, ds\,. \tag{2.35}$$

2.5 Problems

Problem 2.2. Problem taken from Sakurai [3]. *The unperturbed Hamiltonian of a two-state system is represented by*

$$\mathbf{H} = \begin{pmatrix} E_1^o & 0 \\ 0 & E_2^o \end{pmatrix}.$$

There is, in addition, a time-dependent perturbation

$$V(t) = \lambda\cos\omega t\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\quad (\lambda\in\mathbb{R}).$$

(a) At $t=0$ the system is known to be in the first state, represented by

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

*Using time-dependet perturbation theory and assuming that $E_2^o - E_1^o$ is **not** close to $\hbar\omega$, derive an expression for the probability that the system be found in the second state represented by*

$$|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as a function of t $(t>0)$.

Problem 2.3. Problem taken from Gasiorowicz [7]. *Consider a particle in an infinite well, with*

$$V(x) = \begin{cases} 0 & \text{for}\quad 0\le x\le a\,, \\ \infty & \text{everywhere else.} \end{cases}$$

The potential in the region $0\le x\le a$ changes by an additional term

$$V'(x) = \lambda\Big(x-\frac{a}{2}\Big)\sin\omega t\,.$$

(a) Calculate the probability that a particle in the ground state ($n = 1$) makes a transition to the first excited state.

(b) What is the probability that it makes a transition to the second excited state ($n = 3$)?

(c) What happens to this results as $\omega \to 0$?

Problem 2.4. PROBLEM TAKEN FROM GASIOROWICZ [7]. *Repeat the above calculation with*

$$V'(x) = \lambda\Big(x - \frac{a}{2}\Big)\, e^{-\frac{t^2}{\tau^2}}\,.$$

In part (c), consider the limit $\tau \to \infty$. Note that in both cases (c) shows that for a very slowly varying perturbation, transitions become strongly suppressed.

Problem 2.5. PROBLEM TAKEN FROM SAKURAI [3]. *Consider a one-dimensional simple harmonic oscillator whose classical angular frequency is ω_o. For $t < 0$ it is known to be in the ground state. For $t > 0$ there is also a time-dependent potential*

$$V(t) = F_0\, x \cos\omega t\,,$$

where F_0 is a constant in both space and time. Obtain an expression for the expectation value $\langle x\rangle$ as a function of time using time-dependet perturbation theory to the lowest non-vanishing order. Is this procedure valid for $\omega = \omega_0$?

Problem 2.6. PROBLEM TAKEN FROM GASIOROWICZ [7]. *This problem is intended to illustrate the **adiabatic theorem**, originally stated by Max Born and Vladimir A. Fock in 1928: "A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum" [8]. To be specific, consider the ground state, so that $\mathbf{H}_o\phi_o = E_o\phi_o$. Let $V(t) = f(t)V$, where $f(t)$ is a slowly varying function, as shown in figure 2.1. If the ground state of $\mathbf{H} = \mathbf{H}_o + V$ is $|w_o\rangle$, the theorem states that $|\langle w_o|\psi(t)\rangle| \to 1$. The steps to be carried out are the following*

(a) Show that

$$\frac{1}{i\hbar}\int_0^t dt'\, e^{\frac{i}{\hbar}\left(E_m^0 - E_o^0\right)t'} f(t') \;\longrightarrow\; \frac{e^{\frac{i}{\hbar}\left(E_m^0 - E_o^0\right)t'}}{E_m^0 - E_o^0}$$

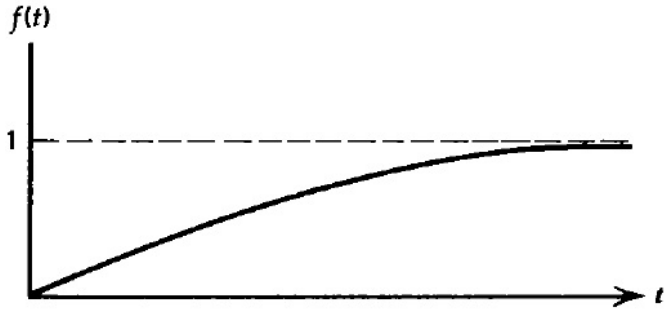

Figure 2.1: Taken from [7].

for times t such that $f(t) = 1$. Use the fact that

$$\frac{\mathrm{d}f(t')}{\mathrm{d}t'} \ll \frac{E_m^0 - E_o^0}{\hbar} f(t').$$

Either construct an example of a function f(t) or use integration by parts; that is, write

$$e^{i\omega t'} = \frac{1}{i\omega} \frac{\mathrm{d}}{\mathrm{d}t'} e^{i\omega t'}$$

in the preceding.

(b) Calculate $\psi(t)$ using (2.6) and (2.15). Compare with (1.26), which here reads

$$|w_o\rangle = |\phi_o\rangle + \sum_{m \neq o} \frac{\langle \phi_m | V | \phi_o \rangle}{E_o^{(0)} - E_m^{(0)}} |\phi_m\rangle$$

and thus show that $|\langle w_o | \psi(t) \rangle| \to 1$.

Problem 2.7. Problem taken from Sakurai [3]. *A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform **force** in the x-direction,*

$$F(t) = F_o e^{-\frac{t}{\tau}}.$$

(a) Using time-dependet perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states?

Problem 2.8. PROBLEM TAKEN FROM SAKURAI [3]. *Consider a particle bound in a simple harmonic oscillator potential. Initially ($t < 0$), it is in the ground state. At $t = 0$ a perturbation of the form*

$$H'(x,t) = Ax^2 e^{-\frac{t}{\tau}}$$

is swithced on. Using time-dependet perturbation theory, calculate the probability that, after a sufficiently long time ($t \gg \tau$), the system will have made a transition to a given excited state. Consider all final states.

Problem 2.9. PROBLEM TAKEN FROM SAKURAI [3]. *A one-dimensional simple harmonic oscillator of angular frequency ω is acted upon by a spatially uniform but time dependent force (**not** potential)*

$$F(t) = F_o \frac{\tau}{\omega\left(\tau^2 + t^2\right)}\,, \quad -\infty < t < \infty\,.$$

(a) At $t = -\infty$, the oscillator is known to be in the ground state. Using the time-dependet perturbation theory to first order, calcluate the probability that the oscillator is found in the first excited state at $t = +\infty$.

*(b) **Challenge:** $F(t)$ is so normalized that the impulse*

$$\int F(t)dt$$

imparted to the oscillator is allways the same, that is, independent of τ; yet for $\tau \gg \frac{1}{\omega}$, the probability for excitation is essentially negligible. Is this reasonable?

Problem 2.10. PROBLEM TAKEN FROM SAKURAI [3]. *Consider a composite system made up of two spin $\frac{1}{2}$ objects. For $t < 0$, the Hamiltonian does not depend on spin and can be taken to be zero by suitably adjusting the energy scale. For $t > 0$, the Hamiltonian is given by*

$$\mathbf{H} = \left(\frac{4\mathbf{\Delta}}{\hbar^2}\right)\mathbf{S}_1 \cdot \mathbf{S}_2\,.$$

Suppose the system is in $|+-\rangle$ for $t \leq 0$. Find, as a function of time, the probability of being found in each of the $\{|\pm\pm\rangle\}$ states:

(a) By solving the problem exactly.

(b) By solving the problem assuming the validity of first-order time-dependent perturbation theory with $\mathbf{H}$ *as a perturbation switched on at* $t = 0$*. Under what condition does this method give the correct results?*

Problem 2.11. *A system with spin and a magnetic moment will absorb energy from a rotating magnetic field, e.g.*

$$\vec{\mathbf{H}} = H_0 \left\{ \cos \omega t \, \hat{\mathbf{e}}_x + \sin \omega t \, \hat{\mathbf{e}}_y \right\},$$

which results which results in a change in the orientation of the spin of the system relative to a constant homogeneous magnetic field, e.g.

$$\vec{\mathbf{H}}' = H_z \, \hat{\mathbf{e}}_z \, .$$

*This leads to the phenomena of "**Magnetic Resonance**". Consider a spin s system subject to a magnetic field*

$$\vec{\mathbf{H}} = H_0 \left\{ \cos \omega t \, \hat{\mathbf{e}}_x + \sin \omega t \, \hat{\mathbf{e}}_y \right\} + H_z \, \hat{\mathbf{e}}_z \, .$$

Let χ *be the spin wave function of the system, so that it satisfies the following equation:*

$$i\hbar \frac{\partial \chi}{\partial t} = -\gamma \, \hbar \left[H_0 (\cos \omega t \, \mathbf{S}_x + \sin \omega t \, \mathbf{S}_y) + H_z \, \mathbf{S}_z \right] \chi \, ,$$

where γ *is the systems gyromagnetic ratio. Suppose that, at* $t = 0$*, the spin is in the state* m_s *and determine the probability of finding it in a state* m_s' *at a latter timer* t *(*$m_s, m_s' \in \{-s, -s+1, ..., s-1, s\}$*). Study in detail the case of a spin* $\frac{1}{2}$ *system.*

Problem 2.12. Problem taken from Sakurai [3]. *Consider a particle in one dimension moving under the influence of some time-independent potential. The energy levels and the corresponding eigenfunctions for this problem are assumed to be known. We now subject the particle to a traveling pulse represented by a time-dependent potential,*

$$V(t) = A \, \delta(x - ct) \, .$$

(a) Suppose at $t = -\infty$ *the particle is known to be in the ground state, whose energy eigenfunction is* $\langle x|i\rangle = u_i(x)$*. Obtain the probability for finding the system in some excited state with energy eigenfuncion* $\langle x|f\rangle = u_f(x)$ *at* $t = +\infty$*.*

(b) Interpret your previous result physically by regarding the δ-function pulse as a superposition of harmonic perturbations; recall

$$\delta(x-ct)=\frac{1}{2\pi c}\int_{-\infty}^{\infty}d\omega\, e^{i\omega\left(\frac{x}{c}-t\right)}.$$

Emphasize the role played by energy conservation, which holds even quantum mechanically as long as the perturbation has been for a very long time.

Problem 2.13. PROBLEM TAKEN FROM SAKURAI [3]. *A hydrogen atom in its ground state* $|n,l,m\rangle=|1,0,0\rangle$ *is placed between the plates of a capacitor. A time-dependent but spatial uniform electric field (**not** potential) is applied as follows:*

$$\vec{\mathbf{E}}=\begin{cases}0 & \text{for}\quad t<0\,,\\ E_0\,e^{-\frac{t}{\tau}}\,\hat{\mathbf{k}} & \text{for}\quad t>0\,.\end{cases}$$

(a) Using first-order time-depended perturbation theory, compute the probability for the atom to be found at $t\gg\tau$ *in each of the three* $2p$ *states:* $\{|2,1,\pm1\rangle\,,|2,1,0\rangle\}$.

(b) Repeat for the $2s$ *state:* $|2,0,0\rangle$.

You need not attempt to evaluate radial integral, but perform all other integrations (with respect to angles and time).

Problem 2.14. PROBLEM TAKEN FROM SAKURAI [3]. *Consider a two-level system with* $E_1<E_2$ *and eigenstates* $\{|1\rangle\,,|2\rangle\}$. *There is a time-dependent potential that connects the two levels as follows:*

$$V_{11}=V_{22}=0,\;\; V_{12}=\gamma e^{i\omega t},\;\; V_{21}=\gamma e^{-i\omega t}\;\; \gamma\in\mathbb{R}.$$

The state of the system at any given time is given by $|\psi(t)\rangle=c_1(t)\,|1\rangle+c_2(t)\,|2\rangle$. *At* $t=0$, *it is known that only the lower level is populated, that is,* $|\psi(t=0)\rangle=|1\rangle$.

(a) Find $|c_1(t)|^2$ *and* $|c_2(t)|^2$ *for* $t>0$ *by **exactly** solving the coupled differential equation*

$$i\hbar\,\dot{c}_k(t)=\sum_{n=1}^{2}V_{kn}(t)\;e^{i\omega_{kn}t}\,c_n(t)\,,\;\;(k=1,2)\,.$$

(b) Repeat using time-dependent perturbation theory to lowest non-vanishing order. Compare the two approaches for small values of γ. Treat the following two cases separately: (i) ω very different from ω_{21} and (ii) ω close to ω_{21}.

Problem 2.15. Problem taken from Sakurai [3]. *The ground state of a hydrogen atom $(n-1,\, l=0)$ is subjected to a time-dependent potential as follows:*

$$V(\mathbf{x},t) = V_o \cos(kz - \omega t)\,.$$

Using time-dependent perturbation theory, obtain an expression for the transition rate at which the electron is emitted with momentum $\mathbf{p}$. Show, in particular, how may you compute the angular distribution of the ejected electron (in terms of θ and ϕ defined with respect to the z-axis). Discuss briefly *the similarities between this problem and the (more realistic) photoelectric effect.*

Help: *The wave function for the ground state of hydrogen is given by*

$$\Psi_{n=1,\,l=0}(\mathbf{x}) = \frac{1}{a_o^{\frac{3}{2}}\sqrt{\pi}}\, e^{-\frac{r}{a_o}}\,.$$

In case you have a normalization problem, the final wave function may be taken to be

$$\psi_f(\mathbf{x}) = \left(\frac{1}{L^{\frac{3}{2}}}\right) e^{\,\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}$$

with L very large, but should be able to show that the observable effects are independent of L.

Problem 2.16. ***Optional:*** *A* ***Josephson Junction*** *consists of two identical superconductors, separated by a thin insulating layer, as shown in figure 2.2.The superconducting electron pairs in each superconductor are in the same state with a single phase. If n_1 denotes the time-independent density of these pairs in SC1, their wave function ψ_1 may be expressed in the form*

$$\psi_1 = \sqrt{n_1}\, e^{i\theta_1}\,,$$

where θ_1 is the common time-independent phase angle. Similarly,

$$\psi_2 = \sqrt{n_2}\, e^{i\theta_2}\,.$$

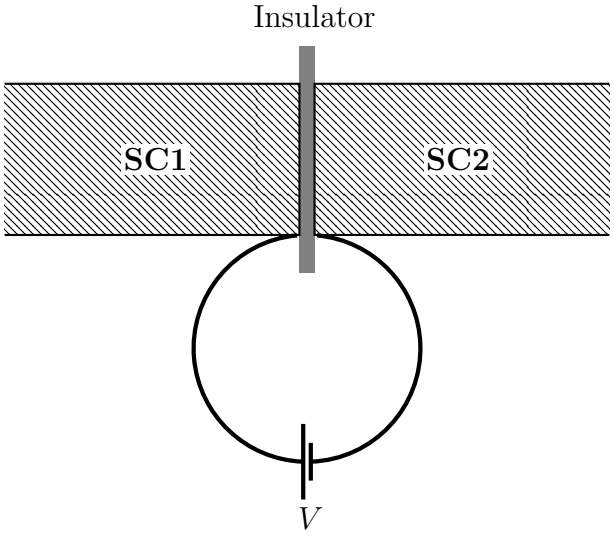

Figure 2.2: A Josephson tunneling Junction. SC1 and SC2 are superconductors.

Since tunneling is taken into account, both ψ_i obey the following equation:

$$\frac{\partial \psi_i}{\partial t} = -\frac{i}{\hbar}(E_i \psi_i - F\psi_j)\,, \quad j \neq i\,.$$

(a) Search for applications of Josephson Junctions in active research fields. Based on this, estimate a number of annually published papers dealing with Josephson Junctions and verify your estimate in **arXiv** *for 2019.*

(b) Show that

$$\frac{\partial n_1}{\partial t} = 2\,\Omega\, n\, \sin\left(\theta_2 - \theta_1\right),$$

where $\Omega = \frac{F}{\hbar}$ and $n \sim n_1 \sim n_2$.

(c) Show that if a steady voltage V is applied across the junction, the current of superconducting electrons oscillates with frequency $\nu = 2\frac{e\,V}{\hbar}$.

Chapter 3

Scattering

This chapter is really fundamental, most of our knowledge of the world at very small scales is thanks to scattering experiments. Indeed, perhaps the most famous example of this is Rutherford's discovery of the atomic nucleus in 1911.

Being this important, we strongly recommend you to review how scattering experiments are usually performed. The Physics Girl has an amusing video on this topic

Scattering theory requires a particular set of tools to be introduced in this chapter. Complex variables, residue's theorem, regularization procedures and generalized functions are some of them.

3.1 Scattering and Cross Sections

The basic HEP experiment is a scattering experiment. In the simplest case it is a **fixed target experiment** see figure 3.1. To completely understand the discussion we must ask a couple of questions: *what is a fixed target scattering experiment?, how is such an experiment performed?*. The answers are fairly simple. A collimated quasi monochromatic beam of particles is thrown into a target, the beam then impinges on the target interacting with it, the interaction in turn modifies the beam. Detectors are placed far from the target in order to capture the modified beam. Some measurements are made of several parameters such as angular and energy distribution, etc. The observations are then reduced and interpreted and from the interpretation the researchers get information regarding the target.

In order to become quantitative, we need to understand the terms, for the sake of simplicity let us

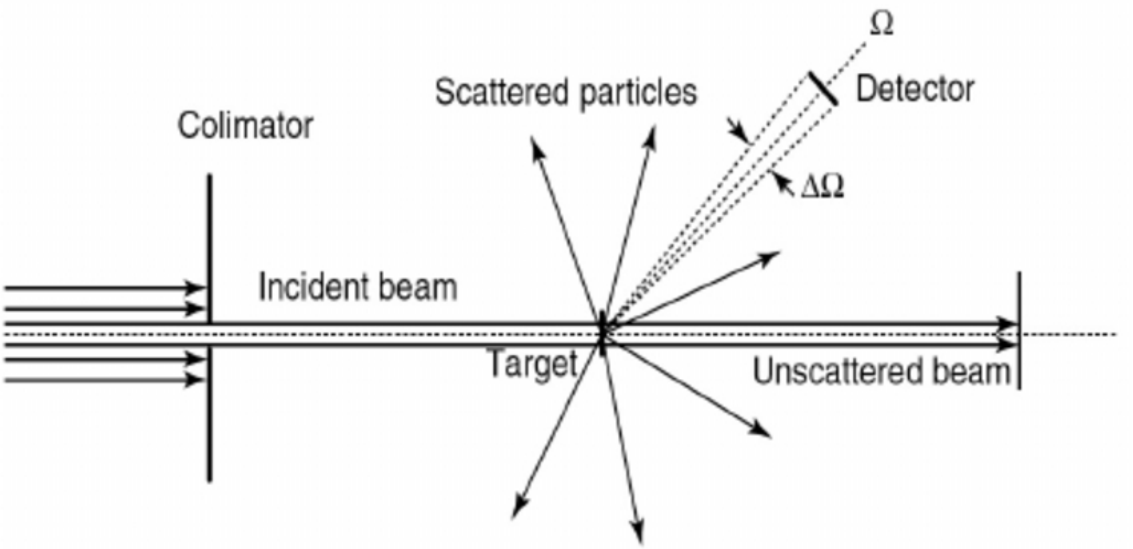

Figure 3.1: Typical fixed target scattering experiment.

imagine we perform a classical[1] scattering experiment. Then a *collimated beam* would be a current of particles having almost parallel momenta[2], *Quasi monochromatic* means that the energies or the particles in the beam are all close to a well defined mean value. The particles hit the target which of course exerts forces into them causing something to happen with the particle momenta[3], the rest of the experiment is clear, there is a setup of detectors that allow the measurements to be performed.

Scattering data are presented in terms of two **observables** (i.e. measurable quantities), namely *the differential cross section* and *the cross section itself*.

Let us use figure 3.1 to clearly define some terms. The collimated (incident) **beam** comes from the left of the figure, it impinges on the target and the particles get scattered all over the place. The **detector**, which you may think as a Geiger counter, is at a large distance R from the target and has a transverse area ΔA to be thought of in terms of a solid angle, $\Delta A = R^2\,\Delta\Omega$, we also need the following two observable quantities,

$$\begin{aligned} n &\equiv \textit{number of scattered particles per unit solid angle} \\ N &\equiv \textit{number of incoming particles per unit area} \end{aligned} \tag{3.1}$$

[1] non quantum

[2] I apologize for the military implications, but you may be safe imagining the beam as being bullets shot form a machine gun

[3] Deflection with no reduction of kinetic energy would be the simplest case

given such observables, a new quantity is introduced

Definition 3.1.1. *The differential cross section is given by*

$$\frac{d\sigma}{d\Omega} \equiv \frac{n}{N} \tag{3.2}$$

The first thing to notice at this point is that the differential cross section is indeed an observable in the sense that it is calculated form things that can -and are- actually measured. A second remark is the differential cross section is a measure of probability. We may finally note that N and n might also be quantities per unit time.

Definition 3.1.2. *The cross section is the sum of the differential cross section over the whole solid angle, i.e.*

$$\sigma \equiv \int_{\Omega} \left(\frac{d\sigma}{d\Omega}\right) d\Omega \tag{3.3}$$

The theoretical physicist Rudolf Peierls once explained the measurement of cross sections with this analogy: *...For example, if I throw a ball at a glass window one square foot in area, there may be one chance in ten that the window will break, and nine chances in ten that the ball will just bounce. In the physicists' language, this particular window, for a ball thrown in this particular way, has a "disintegration cross-section" of* 1/10 *square foot and an "elastic cross-section" of* 9/10 *square foot* (see P282 of reference [9]).

Scattering is used both to discover new physics and to confirm theoretical findings. One of the best examples of this is the famous Rutherford's experiment in which he scattered alpha particles off the atoms in a thin gold foil, Rutherford's results brought the atomic nucleus to existence in 1911. The story began with the Geiger Marsden experiment and ended with Rutherford's brilliant calculation of the differential cross section for the scattering of an electrical charged particle impinging on a Coulomb potential, i.e. a point like fixed charged target. According to the atomic model of Thomson, the beam should have passed through the foil with almost non deviation, the results were completely different, there were particles scattered even to big angles and this could not be explained, Rutherford thought of a centred charged point like nucleus and did the calculation for the expected differential cross section (formula 3.4, the comparison of data and experiment was unmistakable, the nucleus did, in fact, exist.

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_i\, Z_N \alpha\, \hbar\, c}{4\, E\, sin^2(\theta/2)}\right)^2 \tag{3.4}$$

In this formula $e_i = Z_i\, e$ is the electric charge of the scattered particles, $e_N = Z_N\, e$ the nuclear

charge, E the energy of the projectiles, θ the scattering angle and $\alpha \approx 1/137$ the fine structure constant and we have the numerical value $\hbar c = 197\, Mev\, fm$

Surprisingly, scattering of classical particles are remarkably hard to model, while quantum mechanical calculations, at least to first order are relatively simple.

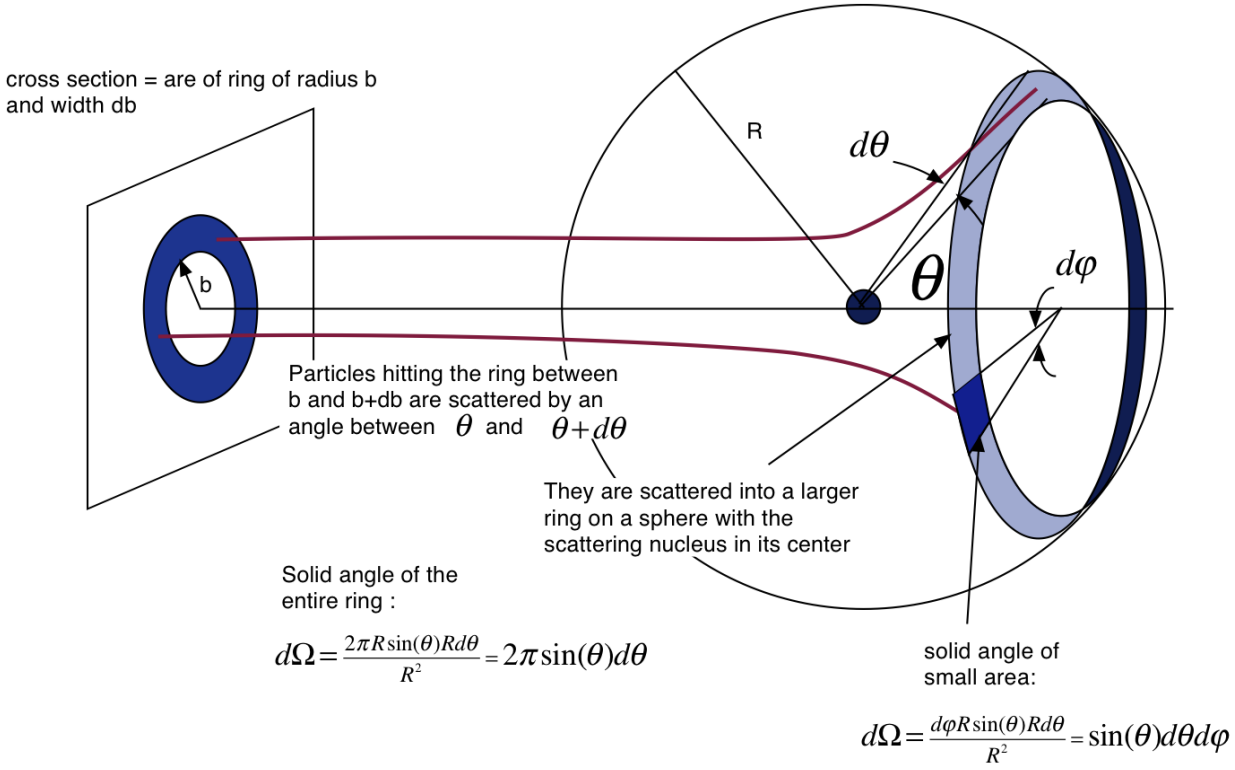

Figure 3.2: Notation for the calculation of Rutherford Scattering formula.

3.2 The Scattering Problem

At this point we should understand that a scattering experiment is perfomed as follows:

- A collimated beam of free cuasi monoenergetic particles is directed to a region of typical linear dimensions a.
- The particles impinge the target, which is represented by a potential with range of the order of a length a
- In the case of elastic scattering, the wave function of the particles after the collision is ψ, finding ψ after the collision is practically the solution to the scattering problem.

It should also be clear that the incoming particles might be loosely modeled by a plane wave[4]

$$\psi_{in} \propto e^{i(\vec{k}.\vec{r}-E\,t/\hbar)}\,, \quad E = \frac{\hbar^2\,k^2}{2m} > 0 \tag{3.5}$$

After the scattering has taken place, and far from the scattering region, intuition tells us that the time independent wave function should somehow look -up to normalization- as

$$\psi(\vec{r}) \sim e^{i\vec{k}.\vec{r}} + f(\theta,\phi)\frac{e^{i\,k\,r}}{r}\,, \tag{3.6}$$

the second part being the scattered wave. If f were constant the second term would clearly resemble a spherically symmetric outgoing wave which is exactly what we would expect if we imagined the scattering center as a source of secondary waves which is exactly what it is. The angular dependence of f represents the effect of the non trivial interaction of the wave function with the scattering potential

For the full solution of the scattering problem we need to solve the time independent Schrödinger equation for free energy states, i.e. $E > 0$ benging to the continuum part of the spectrum, i.e. we need the solution of

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\,\psi(\vec{r}) = E\,\psi(\vec{r})\,, \qquad E > 0 \tag{3.7}$$

we may change the way of writing the equation to

$$\left(\nabla^2 + k^2\right)\,\psi(\vec{r}) = U(r)\,\psi(\vec{r}) \tag{3.8}$$

with

$$k^2 = \frac{2\,m\,E}{\hbar^2} \qquad U = \frac{2\,m\,V}{\hbar^2} \tag{3.9}$$

Now, if we wanted to solve

$$\left(\nabla^2 + k^2\right)\,\psi(\vec{r}) = F(\vec{r})\,, \tag{3.10}$$

for F independent of ψ the solution would obviously be

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int\,d^3x'\,G(\vec{r},\vec{r}')\,F(\vec{r}') \tag{3.11}$$

[4]To be rigorous we should model the incident particles as a wave packet with a very sharp distribution of momenta around a value $\vec{k}_0$ and very little to none spreading

with $\psi_0(\vec{r})$ the general solution of the homogeneous equation, and

$$\left(\nabla^2 + k^2\right)\, G(\vec{r},\vec{r}') = -4\pi\, \delta^3(\vec{r},\vec{r}') \tag{3.12}$$

a Green's function, indeed, given a linear operator $\mathbf{L}$, the most general solution to the nonhomogeneous problem

$$\mathbf{L}u = f \tag{3.13}$$

is

$$u = u_0 + F \tag{3.14}$$

where u_0 is the most general solution to the homogeneous problem and F a particular solution to the nonhomogenous problem.

Green's functions differ on a solution to the homogeneous problem and that is why, we may choose almost any Green's funtion in order to write 3.11 as a solution.

Our problem is not so simple since the r.h.s. of equation 3.8 contains the wave function itself. Nevertheless we may use the Green's function method to transform Schrödinger's equation 3.8 into the following integral equation

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi(\vec{r}')\,. \tag{3.15}$$

Fortunately, and even the formidable appearance of this integral equation, it is known that under certain very general circumstances it can be solved iteratively, we will go back to that later.

3.3 A comment on the Green's Functions

Loosely speaking, Green's functions are distributions associated with point (Dirac's delta) sources, they always differ in solutions to a homogeneous problems, and are not unique in exactly such sense.

There are two very interesting and useful Greens functions for our problem, namely:

$$G_{\pm}(\vec{r},\vec{r}') = \frac{e^{\pm ik\,|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\,, \tag{3.16}$$

they have the look of the space part of spherically symmetric that outgo/income from/to the scattering center which should not be surprising since the time independent problem we are addressing

in equation 3.12 is exactly that of our old friend the Green's function problem for the Helmholtz equation.

An important part of the scattering problem is then, showing that indeed the Green's functions for the scattering problem are given by formula 3.16. We leave the proof for section 3.9, and for that the first section of the chapter will be of importance.

3.4 Solving the Scattering Integral Equation

Let us for the moment think that we have found the the Green's function $G(\vec{r},\vec{r}')$, then our starting point is the integral equation

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi(\vec{r}')\,, \tag{3.17}$$

to solve it we follow an iteration procedure (we are now experts in perturbative solutions), the first approximation ψ_1 is found using the general homogeneous solution (ψ_0) as

$$\psi_1(\vec{r}) = \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi_0(\vec{r}') \tag{3.18}$$

ψ_2 is built from ψ_1 and so on,

$$\psi_2(\vec{r}) = \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi_1(\vec{r}')\,, \tag{3.19}$$

substitution yields

$$\begin{aligned}\psi_2(\vec{r}) &= \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}') \left[\psi_0(\vec{r}') + \int d^3x''\, G(\vec{r'},\vec{r}'')\, U(\vec{r}'')\psi_0(\vec{r}'')\right] = \\ &= \psi_0(\vec{r}) + \int d^3x'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi_0(\vec{r}') + \\ &+ \int d^3x'\, d^3x''\, G(\vec{r},\vec{r}')\, U(\vec{r}')G(\vec{r}',\vec{r}'')\, U(\vec{r}'')\psi_0(\vec{r}'')\,.\end{aligned} \tag{3.20}$$

This last identity shows that higher order corrections get messy as one might expect.

In the next section we study the first order approximation for the far field regime.

3.5 Born Approximation

Substitution of the Green's functions, into the first order approximation to the integral scattering equation yields

$$\begin{aligned}\psi_1(\vec{r}) &= \psi_0(\vec{r}) + \int d^3\, r'\, G(\vec{r},\vec{r}')\, U(\vec{r}')\psi_0(\vec{r}') = \\ &= \psi_0(\vec{r}) + \int d^3\, r'\, \frac{e^{\pm ik\,|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\, U(\vec{r}')\psi_0(\vec{r}')\,.\end{aligned} \tag{3.21}$$

We now consider some geometrical aspects of the above formula[5], we begin by noticing that

$$\begin{aligned}|\vec{r}-\vec{r}'| &= \left(r^2 + r'^2 - 2\,\vec{r}.\vec{r}'\right)^{1/2} = r\left(1 + \left(\frac{r'}{r}\right)^2 - 2\,\frac{\vec{r}.\vec{r}'}{r^2}\right)^{1/2} = \\ &= r\left[1 + \frac{1}{2}\left(\left(\frac{r'}{r}\right)^2 - 2\,\frac{\vec{r}.\vec{r}'}{r^2}\right) - \frac{1}{8}\left(\left(\frac{r'}{r}\right)^2 - 2\,\frac{\vec{r}.\vec{r}'}{r^2}\right)^2 + \dots\right] = \\ &= r\left[1 - \frac{\vec{r}.\vec{r}'}{r^2} + \frac{1}{2}\left(\left(\frac{r'}{r}\right)^2 - \left(\frac{\vec{r}.\vec{r}'}{r^2}\right)^2\right) + \dots\right] = \\ &= r\left[1 - \frac{\vec{r}.\vec{r}'}{r^2} + \frac{1}{2}\left(\frac{r'^2 - (\hat{r}.\vec{r}')^2}{r^2}\right) + \dots\right] = \\ &= r - \hat{r}.\vec{r}' + \frac{(\hat{r}\times r')^2}{2r} + \dots\end{aligned} \tag{3.22}$$

which for $r' << r$, allows the approximation

$$|\vec{r}-\vec{r}'| = r - \hat{r}.\vec{r}' + \frac{(\hat{r}\times r')^2}{2r} + \dots \tag{3.23}$$

When working with scattering problems, one usually thinks that the potential has a typical range a meaning that $U \neq 0$ for distances shorter than a around the interaction region.

Such assumption has interesting consequences for the integration in formula 3.21. Indeed, if we are in the far field region

$$a << r\,, \tag{3.24}$$

[5]
$$(1+x)^{1/2} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \dots$$

the values of r' can be disregarded in favor of those of r, and $k\,|\vec{r}-\vec{r}'|$ can be approximated as

$$k\,r \approx kr - k\hat{r}.\vec{r}'\,, \tag{3.25}$$

As for $|\vec{r}-\vec{r}'|^{-1}$

$$\frac{1}{|\vec{r}-\vec{r}'|} \approx \frac{1}{r}\,, \tag{3.26}$$

which, in turn implies

$$\psi_1(\vec{r}) \approx \psi_0(\vec{r}) + \frac{e^{ikr}}{4\pi\,r}\int d^3\,r'\,e^{ik\hat{r}.\vec{r}'}\,U(\vec{r}')\psi_0(\vec{r}') \tag{3.27}$$

but in the far field, $k\hat{r}$ is essentially the wave vector, so

$$\psi_1(\vec{r}) \approx \psi_0(\vec{r}) + \frac{e^{ikr}}{4\pi\,r}\int d^3\,r'\,e^{i\vec{k}.\vec{r}'}\,U(\vec{r}')\psi_0(\vec{r}') \tag{3.28}$$

We set the coordinates to make the incident wave be

$$\psi_0(\vec{r}) = e^{ikz} \tag{3.29}$$

so the incident wave vector is $\vec{k}_{in} = k\hat{e}_z$ after substitution in eq. 3.28 we get

$$\psi_1(\vec{r}) = \psi_0(\vec{r}) + \frac{e^{ikr}}{4\pi\,r}\int d^3\,r'\,e^{i\vec{K}.\vec{r}'}\,U(\vec{r}')\,, \tag{3.30}$$

where $\vec{K} = \vec{k} - \vec{k}_{in}$ is the transferred momentum

The final result is that the scattering amplitude equals the F. Transform of the potential muajajajajajaja

3.6 Physics: back to the fun

Let us now put together all that we have learned up to this point.

We begin by recalling the probability current

$$\mathbf{J} = \frac{\hbar}{i}\frac{1}{m}\psi^*\nabla(\psi) \tag{3.31}$$

We now think of the incident beam of a fixed target experiment and notice that the number (N)

of particles that cross a unit surface perpendicular to the incident beam is proportional to the flux of the current through such surface,

$$N = C\,|\vec{J}| = C\frac{\hbar\,k}{m} \tag{3.32}$$

Let us turn opur attention to the scattered particles *scattered current*, to that end we set spherical coordinates centered at the target and calculate the components of the current as follows,

$$\begin{aligned}
\mathbf{J}_r &= \frac{\hbar\,k}{m}\psi^*\frac{1}{i}\nabla_r(\psi) \\
\mathbf{J}_\theta &= \frac{\hbar}{m}\psi^*\frac{1}{i}\nabla_\theta(\psi) \\
\mathbf{J}_\phi &= \frac{\hbar}{m}\psi^*\frac{1}{i}\nabla_\phi(\psi)\,.
\end{aligned} \tag{3.33}$$

Recalling the formulas for the components of the gradient we easily obtain general expressions for the components of the scattered current we can easily find the following explicit formulas

$$\begin{aligned}
\mathbf{J}_r &= \frac{\hbar\,k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 \\
\mathbf{J}_\theta &= \frac{\hbar}{m}\frac{1}{r^3}\,Re\left[\frac{1}{i}f^*(\theta,\phi)\partial_\theta f^*(\theta,\phi)\right] \\
\mathbf{J}_\phi &= \frac{\hbar}{m}\frac{1}{r^3\,sen\theta}\,Re\left[\frac{1}{i}f^*(\theta,\phi)\partial_\theta f^*(\theta,\phi)\right]
\end{aligned} \tag{3.34}$$

due to the powers of r it is clear that for large distances, the scattered current is radial.

With this at hand, we calculate the number of particles that cross an element of area of the detector per unit time is

$$dn = C\,\vec{J}.\hat{n}dS = C\frac{\hbar\,k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,r^2 d\Omega = C\frac{\hbar\,k}{m}\,|f(\theta,\phi)|\,d\Omega \tag{3.35}$$

recalling the definition of the differential cross section

$$dn = N\,\frac{d\sigma(\theta,\phi)}{d\Omega}\,d\Omega \tag{3.36}$$

we finally obtain

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = |f(\theta,\phi)|^2 \tag{3.37}$$

3.7 A section on examples is badly needed...I am laaazyyy

3.8 A reminder and a tool

For reasons which will become apparent later on, we begin this chapter with the following calculation,

$$I = \int_{\mathrm{Re}} d\omega \, \frac{e^{-i\omega t}}{\omega} \, . \tag{3.38}$$

There's clearly a pole at $\omega = 0$ which must be carefully dealt with. A regularization procedure must be imposed on I and we should take advantage of this opportunity to learn at once and forever that, regularization procedures are intrinsically non unique in the following sense: different regularizations usually lead to different results.

An amusing example is

$$\sum_{n=1}^{\infty} n = 1 + 2 + 3 + 4 + ... = -\frac{1}{12} \, , \tag{3.39}$$

a result widely used in string theory and which can be obtained either by a zeta function regularization scheme or through what is known as *Ramanujan summation* 3.3.

Example 3.8.1. *As a motivational example let us examine the sum*

$$\mathcal{S} = \sum_{n=1}^{\infty} n \, , \tag{3.40}$$

we replace this sum by another having a convergence factor

$$\lim_{\epsilon \to 0} \mathcal{S}(\epsilon) = \sum_{n=1}^{\infty} n \, e^{-\epsilon \, n} \, , \tag{3.41}$$

clearly

$$\mathcal{S}(\epsilon) = - \left[\frac{d}{d\alpha} \sum_{n=1}^{\infty} e^{-n\alpha} \right] |_{\alpha = \epsilon} \, , \tag{3.42}$$

the sum is convergent for all $0 < \alpha$*, after summing and taking the derivative one gets*

$$\mathcal{S}(\epsilon) = \frac{e^{-\alpha}}{(e^{-\alpha} - 1)^2} \, , \tag{3.43}$$

this has the Laurent series POLCHINSKI; Vol 1.

$$\mathcal{S}(\epsilon) = \frac{1}{\epsilon^2} - \frac{1}{12} + \frac{\epsilon^2}{240} + \frac{\epsilon^4}{6048} + \textit{higher powers of } \epsilon\,, \tag{3.44}$$

this sum has three very distinctive terms, a singular divergent par (ϵ^{-2}), a finite (regular) part (-1/12) and a part that goes to zero when ϵ goes to nill. The Dirichlet regularization comes in by defining the finite part as the value of the sum.

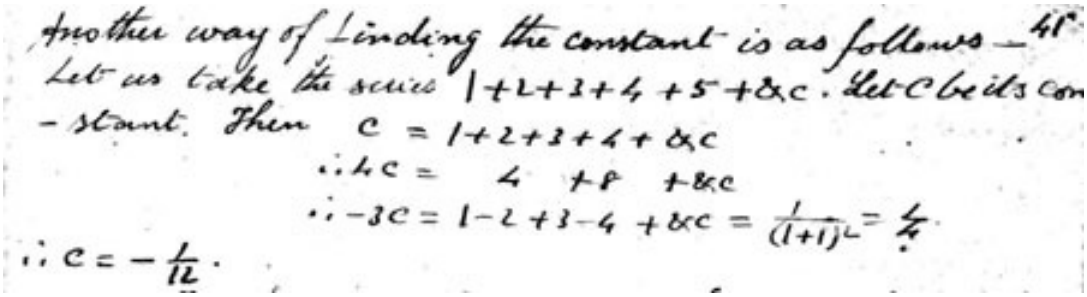

Figure 3.3: Ramanujan Notebook 1 Chapter 8 on 1234 series

The fact that different regularization procedures lead to different results should not be a total surprise since we should already be familiar with what happens with Cauchy's principal value.

Having the above been said, and going back to formula 3.38 we consider the integral

$$\mathcal{I} = \int_{\mathcal{C}} dz\, \frac{e^{-i\,z\,t}}{z}\,, \tag{3.45}$$

where $\mathcal{C}$ is a trajectory we are going to look for. Choosing the trajectory is equivalent to choosing a regularization procedure.

We note that for $z = \omega + i\zeta$, iz is $iz\,t = i\omega\,t - \zeta\,t$, so for $t > 0$, a semicircle in the half space $\zeta > 0$ does not contribute to the integral, this suggests choosing an infinite radius semicircle on the upper half plane to integrate for $t > 0$. To handle the pole on the real axis, we circumventing it with a tiny half circle of radius $\epsilon \to 0$ around $\omega = 0$ which goes into the $\zeta < 0$ region.

According to our choosing of $\mathcal{C}$, and the residue theorem,

$$\mathcal{I} = \int_{\mathcal{C}} d\,z\, \frac{e^{-i\,z\,t}}{z} = 2\pi\,i\,Res\left(\frac{e^{-i\,z\,t}}{z}\right) = 2\pi\,i \times 1\,, \quad t > 0\,, \tag{3.46}$$

for $t < 0$ we use the same trajectory over the real numbers but close $\mathcal{C}$ with a circle in the lower complex half plane so

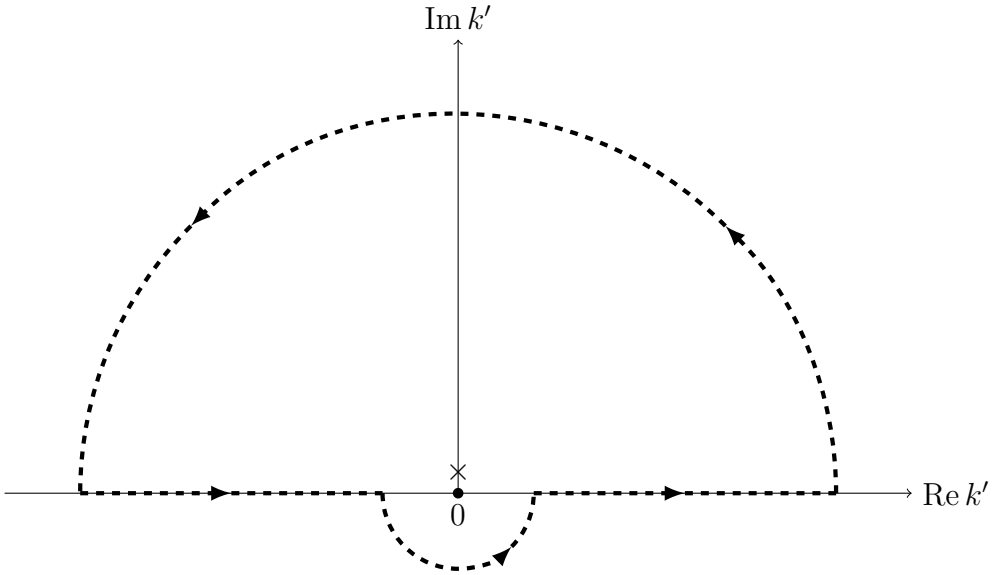

Figure 3.4: Path of integration for $t > 0$, it encloses the first order pole at $z = 0$

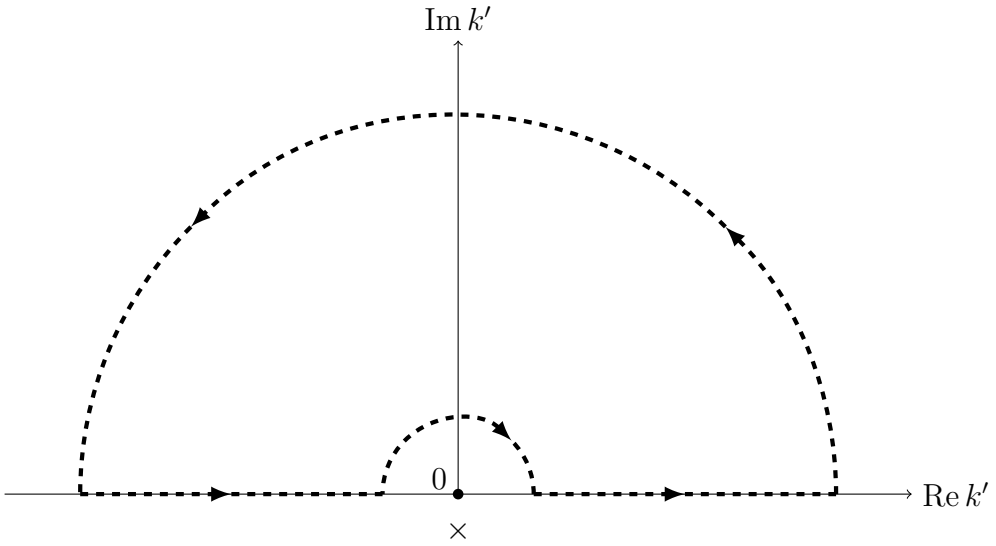

Figure 3.5: $\mathcal{C}$ for $t < 0$, no poles enclosed inside the pqath

$$\mathcal{I} = \int_{\mathcal{C}} dz \, \frac{e^{-i\,z\,t}}{z} = 2\pi\, i\, Res\left(\frac{e^{-i\,z\,t}}{z}\right) = 2\pi\, i \times 0\,, \quad t < 0\,, \tag{3.47}$$

since there are no poles inside the path.

We conclude:

$$FT^{-1}\left(\frac{1}{\omega}\right) \propto i\Theta(t) \tag{3.48}$$

We may reach the same conclusion by a far simpler approach as follows,

$$1 = FT\left(\delta(t)\right) = FT\left(\frac{d\Theta(t)}{dt}\right) = i\omega\, FT\left(\Theta(t)\right) \tag{3.49}$$

3.9 Finding the Green's Function

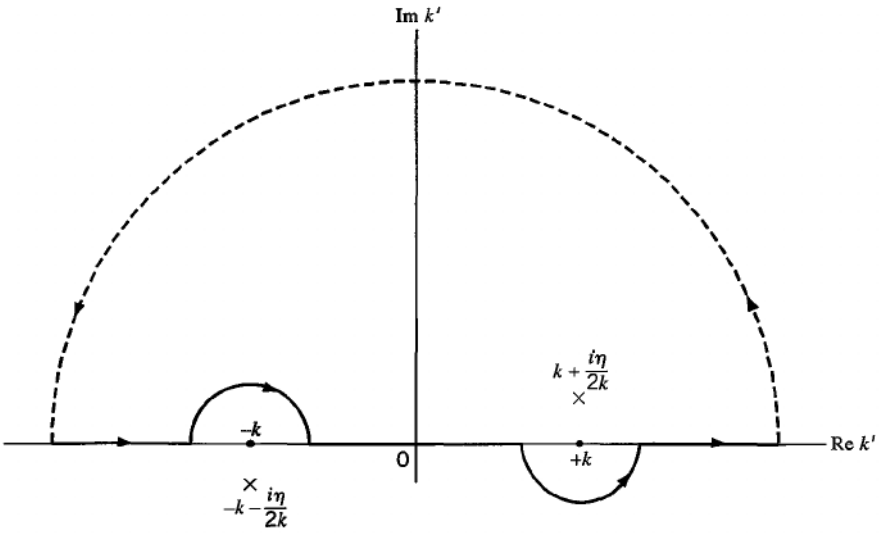

Figure 3.6: The path to build the Green's function. Taken from Merzbacher [4].

In this section we carry out the details of the calculation leading to formula 3.16 for the Green's funtion.

The starting point is of course the non-homogeneous equation

$$\left(\nabla^2 + k^2\right)\, G(\vec{r}, \vec{r}') = -4\pi\delta^3(\vec{r}, \vec{r}')\,, \tag{3.50}$$

the first step in the calculation is taking the $3D$ Fourier transform form the position (coordinate) space to the momentum space. We perfectly know that space derivatives transform on $\sqrt{-1}$ times the components of the wave vector implying that after transforming we get

$$\left(-k'^2 + k^2\right)\, \hat{G}(\vec{k}') = -4\pi \tag{3.51}$$

where $\vec{k}'$ is the momentum in the transformed domain.

We then have a simple algebraic equation (the magic of the Fourier transform) and get

$$\hat{G}(\vec{k}') = -4\pi \frac{1}{k^2 - k'^2}\,, \tag{3.52}$$

from here

$$\hat{G}(\vec{r}) = -4\pi\,\mathcal{N} \int d^3k' \frac{e^{i\vec{k}'.\vec{r}}}{k^2 - k'^2}\,, \tag{3.53}$$

where $\mathcal{N}$ is the normalization for the Fourier transform.

To perform the integration we fix the momentum space axis parallel to the z, so

$$\begin{aligned}
\hat{G}(\vec{r}) &= -4\pi\,\mathcal{N} \int_0^{2\pi} d\phi \int_0^{\infty} ds s^2 \int_0^{\pi} sen\theta d\theta\, \frac{e^{isr\,cos\theta}}{k^2 - s^2} = \\
&= -8\pi^2\,\mathcal{N} \int_0^{\infty} ds\, s^2 \int_1^{-1} (-d\mu)\, d\phi \frac{e^{ikr\,\mu}}{k^2 - s^2} = \\
&= -8\pi^2\,\mathcal{N} \left[\int_0^{\infty} ds\, s^2\, \frac{e^{isr}}{irs(k^2 - s^2)} - \int_0^{\infty} ds\, s^2\, \frac{e^{-isr}}{irs(k^2 - s^2)} \right] = \\
&= 8i\pi^2\,\mathcal{N} \left[\int_0^{\infty} ds\, s^2\, \frac{e^{isr}}{rs(k^2 - s^2)} + \int_0^{-\infty} (-ds)\, s^2\, \frac{e^{isr}}{rs(k^2 - s^2)} \right] = \\
&= 8i\pi^2\,\mathcal{N} \left[\int_0^{\infty} ds\, s^2\, \frac{e^{isr}}{rs(k^2 - s^2)} + \int_{-\infty}^{0} (ds)\, s^2\, \frac{e^{isr}}{rs(k^2 - s^2)} \right] = \\
&= 8i\pi^2\,\mathcal{N} \int_{-\infty}^{\infty} ds\, s\, \frac{e^{isr}}{r(k^2 - s^2)}
\end{aligned} \tag{3.54}$$

The calculation of the Green's function has cleanly come down to

$$G(\vec{r}) = 8i\pi^2\,\mathcal{N} \int_{-\infty}^{\infty} dq\, q\, \frac{e^{iqr}}{r(k^2 - q^2)} \tag{3.55}$$

To go back to the space domain we must perform the q integration. Rewriting the integrand

$$G(\vec{r}) = 8i\pi^2\,\mathcal{N} \int_{-\infty}^{\infty} dq\, q\, \frac{e^{iqr}}{r(k+q)(k-q)}\,, \tag{3.56}$$

it is clear that there are two simple poles along the real q axis and therefore we must use a regularization procedure for the calculation. Here is when the situation we had in section 3.8 becomes handy, indeed, the treatment of the poles goes along the same lines. If we use the

integration path shown in figure 3.6 the result is (notice the slight change in notation)

$$G_+(\vec{r}) = 2\pi\, i\, 8i\pi^2\, \mathcal{N}(k)\, \frac{e^{ikr}}{r(2k)}\,, \tag{3.57}$$

i.e.

$$G_+(\vec{r}) = -8\pi^3\, \mathcal{N}\, \frac{e^{ikr}}{r}\,. \tag{3.58}$$

Now, we must recall what we learned, regularizations are not unique, we might have used a different integration path and would have gotten a different (but valid) result.

Problem 3.1. *Use the path shown in figure xxx to show that*

$$G_-(\vec{r}) = -8\pi^3\, \mathcal{N}\, \frac{e^{-ikr}}{r}\,, \tag{3.59}$$

is also a Green's function.

Problem 3.2. *Use Cauchy principal value (what is the corresponding path?) to show that*

$$G_s(\vec{r}) = 8\pi^3\, \mathcal{N}\, \frac{cos(kr)}{r}\,, \tag{3.60}$$

is also a Green's function. Write G_s as

$$G_s(\vec{r}) = \frac{1}{2}\left[G_+(\vec{r}) + G_-(\vec{r})\right]\,. \tag{3.61}$$

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Appendices

Appendix A

Time independent Perturbation Theory: Solutions

Solution to problem 1.2 We begin by noting that $\mathbf{W}$ can be split as the sum of two matrices, namely,

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \tag{A.1}$$

and

$$\mathbf{B} = \begin{bmatrix} -0.05 & -0.05 & 0 \\ -0.05 & 0 & 0 \\ 0 & 0 & -0.05 \end{bmatrix} = \lambda \begin{bmatrix} -1 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{A.2}$$

With $\lambda = 5 \times 10^{-2}$.

And regard $\mathbf{A}$ as an unperturbed operator and $\mathbf{B}$ as a perturbation.

We will solve this exercise we do some things

1. Solve the eigen problem for $\mathbf{W}$ by computer means, i.e. by coding in both R and Python 3
2. Find the first order corrections **by hand**, i.e. using the formula $\Delta\lambda_k^{(1)} = \langle k|B|k\rangle$
3. Find by hand the first order corrected eigenvectors
4. Find the second order corrections -if needed-

R solves the eigen problem for $\mathbf{W}$ with a simple function.

```
W<-as.matrix(data.frame ( c (1.95 ,-0.05 ,0) , c (-0.05 ,1 ,0) , c (0 ,0 ,2.95) ) )
eigen<-eigen(W)
eigen$values

[1] 2.9500000 1.9526243 0.9973757

eigen$vectors
      [,1]        [,2]       [,3]
[1,]    0  0.99862542 0.05241444
[2,]    0 -0.05241444 0.99862542
[3,]    1  0.00000000 0.00000000
```

In this result we must notice that R sorts the eigenvalues in decreasing order and gives the list of eigenvectors as columns accordingly. We note that (using an obvious notation),

$$|1.9526243\rangle = \begin{pmatrix} 0 \\ 0.99862542 \\ 0.05241444 \end{pmatrix}, |0.9973757\rangle = \begin{pmatrix} 0.05241444 \\ 0.99862542 \\ 0.0 \end{pmatrix}, |2.95\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{A.3}$$

These clearly show that the eigenproblem for $\mathbf{W}$ comes from the perturbation of the eigen problem for $\mathbf{A}$ which, being diagonal has the following spectrum $\lambda_1 = 2$, $\lambda_2 = 1$ and $\lambda_3 = 3$ with associated eigenvectors

$$|\lambda_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\lambda_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\lambda_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{A.4}$$

we further note that the eigenvalues of both problems are very close, moreover,

$$|0.9973757\rangle \approx |\lambda_1\rangle, |1.9526243\rangle \approx |\lambda_2\rangle, |2.95\rangle \approx |\lambda_3\rangle, \tag{A.5}$$

which seems to justify perturbation theory. Let us now check whether this is true.

We know that the first order perturbed eigenvalues and eigenvectors, of a perturbed hamiltonian ($\mathbf{H} = \mathbf{H}_0 + \mathbf{W}$) are given by the formulas:

$$E_n = E_n^{(0)} + E_n^{(1)} = E_n^{(0)} + \langle\psi_n|\mathbf{W}|\psi_n\rangle \tag{A.6}$$

$$|\Psi_n(\lambda)\rangle = |\psi_n\rangle + \sum_{p\neq n} \frac{\langle\psi_p|\mathbf{W}|\psi_n\rangle}{E_n^0 - E_p^0}|\psi_p\rangle \tag{A.7}$$

For the problem at hand, the first order corrected eigenvalues of $\mathbf{A}$ are,

$$\lambda_1^{(corr)} = \lambda_1 + \langle 1|\mathbf{B}|1\rangle = 2 + \langle 1|\mathbf{B}|1\rangle \tag{A.8}$$

$$\lambda_1^{(corr)} = 2 - \lambda \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{A.9}$$

$$\boxed{\lambda_1^{(corr)} = 2 - 0.05 = 1.95} \tag{A.10}$$

Similarly

$$\lambda_2^{(corr)} = \lambda_2 + \langle 2|\mathbf{B}|2\rangle = 1 + \langle 2|\mathbf{B}|2\rangle \tag{A.11}$$

$$\lambda_2^{(corr)} = 1 - \lambda \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{A.12}$$

$$\boxed{\lambda_2^{(corr)} = 1 - 0 = 1} \tag{A.13}$$

and

$$\boxed{\lambda_3^{(corr)} = 3 - 0.05 = 2.95} \tag{A.14}$$

We note that λ_2 does not pick any first order correction.

We can make a code for calculating these values

```
#firt define the vector E of the perturbed energies
E <- vector(length = 3 )
#then using the formula for the perturbation at first order we perform the
    calculation
for (i in 1:3){
  E[i] <- eigen$values[i]+eigen$vectors[,i]%*%B%*%eigen$vectors[,i]
}
#The result is
> E
[1] 2.95 1.95 1.00
#these are the perturbed eigenvalues to the respective unperturbed eigenvalues
> eigen$values
[1] 3 2 1
```

To find the perturbed eigenvectors we use

$$|\lambda_\ell^{(corr)}\rangle = |\lambda_\ell\rangle + \sum_{p\neq\ell} \frac{\langle\lambda_p|\mathbf{B}|\lambda_\ell\rangle}{\lambda_\ell^{(0)} - \lambda_p^{(0)}}|\lambda_p\rangle \tag{A.15}$$

We find:

$$|\lambda_1^{(corr)}\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix} - \lambda\frac{\begin{bmatrix}0 & 1 & 0\end{bmatrix}\begin{bmatrix}1 & 1 & 0\\1 & 0 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}}{2-1}\begin{bmatrix}0\\1\\0\end{bmatrix} - \lambda\frac{\begin{bmatrix}0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 1 & 0\\1 & 0 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}}{2-3}\begin{bmatrix}0\\0\\1\end{bmatrix} \tag{A.16}$$

$$\boxed{|\lambda_1^{(corr)}\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix} - 0.05\begin{bmatrix}0\\1\\0\end{bmatrix} = \begin{bmatrix}1\\-0.05\\0\end{bmatrix}} \tag{A.17}$$

$$|\lambda_2^{(corr)}\rangle = |\lambda_2\rangle + \sum_{p\neq1} \frac{\langle\lambda_p|\mathbf{B}|\lambda_2\rangle}{\lambda_2^{(0)} - \lambda_p^{(0)}}|\lambda_2\rangle \tag{A.18}$$

$$|\lambda_2^{(corr)}\rangle = \begin{bmatrix}0\\1\\0\end{bmatrix} - \lambda\frac{\begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{bmatrix}1 & 1 & 0\\1 & 0 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix}}{1-2}\begin{bmatrix}1\\0\\0\end{bmatrix} - \lambda\frac{\begin{bmatrix}0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 1 & 0\\1 & 0 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix}}{1-3}\begin{bmatrix}0\\0\\1\end{bmatrix} \tag{A.19}$$

$$\boxed{|\lambda_2^{(corr)}\rangle = \begin{bmatrix}0\\1\\0\end{bmatrix} + 0.05\begin{bmatrix}1\\0\\0\end{bmatrix} = \begin{bmatrix}0.05\\1\\0\end{bmatrix}} \tag{A.20}$$

And

$$|\lambda_3^{(corr)}\rangle = |\lambda_3\rangle + \sum_{p\neq1} \frac{\langle\lambda_p|\mathbf{B}|\lambda_3\rangle}{\lambda_3^{(0)} - \lambda_p^{(0)}}|\lambda_3\rangle \tag{A.21}$$

$$|\lambda_3^{(corr)}\rangle =\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix} - \lambda\frac{\begin{bmatrix}1&0&0\end{bmatrix}\begin{bmatrix}1&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}}{3-2}\begin{bmatrix}1\\0\\0\end{bmatrix} - \lambda\frac{\begin{bmatrix}0&1&0\end{bmatrix}\begin{bmatrix}1&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}}{3-1}\begin{bmatrix}0\\1\\0\end{bmatrix} \quad \text{(A.22)}$$

$$\boxed{|\lambda_3^{(corr)}\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix} + 0\begin{bmatrix}1\\0\\0\end{bmatrix} + 0\begin{bmatrix}0\\1\\0\end{bmatrix} = \begin{bmatrix}0\\0\\1\end{bmatrix}} \quad \text{(A.23)}$$

And making a R code:

```
psi <- list() #define a list of perturbed vectors
#now we perform an algorithm over each i'th  unperturbed vector
for (i in 1:3){
  pert <- 0 #we beging defining perturbation 0 for each vector
  #then we perform the calculus of the perturbation
  for (j in 1:3){
    if (j!=i){
      pert <- pert + (eigen$vectors[,j]%*%B%*%eigen$vectors[,i])*eigen$vectors[,j]/
   (eigen$values[i]-eigen$values[j])
    }
  }
  then we add the perturbation to the unperturbed vector
  psi[[i]]<-eigen$vectors[,i] + pert
}

#the result is

> psi
[[1]]
[1] 0 0 1

[[2]]
[1]  1.00 -0.05  0.00

[[3]]
```

```
[1] 0.05 1.00 0.00

#over each vector
> list(eigen$vectors[,1], eigen$vectors[,2], eigen$vectors[,3])
[[1]]
[1] 0 0 1

[[2]]
[1] 1 0 0

[[3]]
[1] 0 1 0
```

We see that the perturbation does not affect the third dimension of the orthonormal basis of A, we notice, seeing at Matrix B of the perturbation that the linear transformation over a generalized vector $v = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ performs a rotation of the x and y axes around the z axis, then the direction on the z axis of v is not affected by B

The second order corrections are still missing

Solution to problem 1.3

As with problem 1.2, we might split , $\mathbf{W}$ as the sum of two matrices:

An unperturbed one

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \tag{A.24}$$

and a perturbation

$$\mathbf{B} = \begin{bmatrix} 0 & -0.05 & 0 \\ -0.05 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \lambda \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{A.25}$$

and follow the same steps we did in problem 1.2.

Nevertheless it is much better to realize that $\mathbf{W}$ has block form, i. e.

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_1 & 0 \\ 0 & w_{33} \end{pmatrix} \tag{A.26}$$

with

$$\mathbf{W}_1 = \begin{pmatrix} 2 & -0.05 \\ -0.05 & 1 \end{pmatrix} \quad \text{and} \quad w_{33} = 3\,, \tag{A.27}$$

this makes a simple fact manifest, perturbation theory can be applied in the two dimensional subspace on which $\mathbf{W}_1$ acts, i.e. we just need to perform perturbation theory on $\mathbf{W}_1$ which splits as

$$\mathbf{W}_1 = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} + 0.05 \times \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{A.28}$$

Since the perturbation is on the off diagonal elements only, there is no first order correction, indeed:

$$\lambda_1^{(corr)} = 2 - 0.05 \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{A.29}$$

$$\boxed{\lambda_1^{(corr)} = 2 - 0 = 2} \tag{A.30}$$

Similarly

$$\lambda_1^{(corr)} = 1 - 0.05 \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{A.31}$$

$$\boxed{\lambda_2^{(corr)} = 1 - 0 = 1} \tag{A.32}$$

The eigenvectors pick first order corrections, indeed

$$|\lambda_1^{(corr)}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - 0.05 \frac{\begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}}{2 - 1} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{A.33}$$

$$\boxed{|\lambda_1^{(corr)}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - 0.05 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -0.05 \end{pmatrix}} \tag{A.34}$$

$$|\lambda_2^{(corr)}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} - 0.05 \frac{\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}}{1 - 2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{A.35}$$

$$\boxed{|\lambda_2^{(corr)}\rangle = \begin{bmatrix}0\\1\end{bmatrix} + 0.05\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}0.05\\1\end{bmatrix}} \tag{A.36}$$

And clearly, $|\lambda_3\rangle$ remains invariant.

Solution to problem 1.4

$$A = \begin{bmatrix}2&0&0&0\\0&1&0&0\\0&0&2&0\\0&0&0&3\end{bmatrix} \tag{A.37}$$

$$W = \begin{bmatrix}0&0.1&0&0\\0.1&0&0&0\\0&0&-0.05&-0.05\\0&0&-0.05&-0.05\end{bmatrix} \tag{A.38}$$

With the R script we did, we have the new eigenenergies

$$2, 1, 1.95, 2.95$$

. Indeed the perturbed eigenenergies are related to the diagonal of the perturbation in the folowing form

$$E_n = E_n^0 + H_{nn} \tag{A.39}$$

$$E_1 = 2 + 0 = 2$$

$$E_2 = 1 + 0 = 1$$

$$E_3 = 2 - 0.05 = 1.95$$

$$E_4 = 3 - 0.05 = 2.95$$

And the eigenstates are :

$$|\psi_1\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \frac{0.1}{1-2}\begin{bmatrix}0\\1\\0\\0\end{bmatrix} + \frac{-0.05}{} \tag{A.40}$$