Master M1 Parcours International 2010-2011

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Travaux Dirigés Quantum Mechanics

Sheet 1 : *Vectors & Operators*

I. Vectors

Let $|u\rangle$, $|v\rangle$ be any two finite-norm vectors in the Hilbert space.

I.A Derive the *Schwarz inequality*

$$|\langle u|v\rangle| \leq \sqrt{\langle u|u\rangle}\sqrt{\langle v|v\rangle} \ .$$

I.B Show that

$$\mathrm{Tr}(|u\rangle\langle v|) = \langle v|u\rangle \ .$$

II. Operators

Consider any two operators A, B.

II.A Show that

$$(AB)^\dagger = B^\dagger A^\dagger \ .$$

II.B Assuming that the inverse A^{-1} of A exists, derive an expression for $(A - \lambda B)^{-1}$ as a power series in λ :

$$(A - \lambda B)^{-1} = A^{-1} + \lambda A^{-1}BA^{-1} + \lambda^2 A^{-1}BA^{-1}BA^{-1} + \dots$$

II.C If $[[A, B], A] = 0$, show that

$$[A^n, B] = nA^{n-1}[A, B]$$

holds for all integers $n \geq 1$.

III. Hermitian operators

Let A be a hermitian (self-adjoint) operator and let λ_a be the eigenvalue corresponding to the eigenket $|a\rangle$.

III.A Show that $\lambda_a \in \mathbb{R}$, i.e. the eigenvalues of a A are real.

III.B Show that $\lambda_a \neq \lambda_{a'}$ implies $\langle a|a'\rangle = 0$, i.e. the eigenkets corresponding to different eigenvalues are orthogonal.

III.C We may assume that the eigenkets $\{|a\rangle\}$ form an orthonormal basis of the Hilbert space. Moreover, let $|\alpha\rangle$ be a normalized vector, and let $|\alpha\rangle = \sum c_a|a\rangle$ be its expansion on the basis of eigenkets of the operator A. Show that

$$\sum |c_a|^2 = 1 \ .$$

IV. Positive-definite operators

A hermitian operator A is called *positive-definite* if, for any vector $|u\rangle$, $\langle u|A|u\rangle \geq 0$.

IV.A Show that the operator $|a\rangle\langle a|$ is hermitian and positive-definite.

IV.B If A is a hermitian positive-definite operator, then

$$|\langle u|A|v\rangle| \leq \sqrt{\langle u|A|u\rangle}\sqrt{\langle v|A|v\rangle} \ .$$

IV.C Show that $\mathrm{Tr}A \geq 0$, and that the inequality is saturated if and only if $A = 0$.

V. Momentum operator

Let $\hat{p}$ be the momentum operator in one dimension, conjugate to the position operator $\hat{x}$, i.e. $[\hat{p}, \hat{x}] = -i\hbar$.

V.A For any integer $n \geq 1$, show that

$$[\hat{p}, \hat{x}^n] = -in\hbar\hat{x}^{n-1} \ .$$

Hint : take into account that $[A, BC] = [A, B]C + B[A, C]$ for any operators A, B, C, and proceed by induction.

V.B Show that

$$[\hat{p}, f(\hat{x})] = -i\hbar\frac{\partial}{\partial\hat{x}}f(\hat{x}) \ ,$$

where $f(x)$ is a differentiable function of x.

V.C Show that

$$\langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x - x') \ .$$

Travaux Dirigés Quantum Mechanics

Sheet 2 : *Measurements & Pictures*

I. Operators and measurement

Consider the linear operators A and B of a three-dimensional Hilbert space :

$$A = \frac{1}{2}\begin{pmatrix} 5 & 0 & 0 \\ 0 & 2-\sqrt{3} & -3 \\ 0 & -3 & 2+\sqrt{3} \end{pmatrix} , \quad B = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} .$$

I.A Are A, B (i) hermitian ? (ii) unitary ? (iii) projectors ?

I.B Compute $[A, B]$.

I.C Compute the eigenvalues of A.

I.D A first measurement of the observalble A gives the highest eigenvalue of A. What is the probability that an immediately subsequent measurement of the observable B will give zero ?

I.E In which states can the observables A and B both be measured exactly at the same time ?

II. Density operator

A system in a *mixed state* is described by the density operator :

$$\rho = \sum_{n=1}^{N} p_n |\psi_n\rangle\langle\psi_n| \ , \quad \sum_{n=1}^{N} p_n = 1 \ ,$$

assuming for simplicity a discrete set of states in the sum above ; the $|\psi_n\rangle$'s can be assumed orthonormal ; the p_n's obey $0 \leq p_n \leq 1$. The density operator can be used to describe a situation where the exact state of the system is not known, and one can only say that the system has a probability p_n to be in the state $|\psi_n\rangle$. (ρ can also be used to describe an ensemble of particles a fraction p_n of which are in the state $|\psi_n\rangle$).

Show that :

II.A $\mathrm{tr}(\rho) = 1$.

II.B The system is in a pure state if and only if ρ is a projector.

II.C The system is in a pure state if and only if :

$$\mathrm{tr}(\rho^2) = 1.$$

II.D The expectation value of the observable A is given by :

$$\langle A \rangle = \mathrm{tr}(\rho A)$$

II.E In the Schrödinger picture the density operator obeys :

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] \ ,$$

while in the Heisenberg picture it is time-independent.

III. Harmonic oscillator

Consider the simple harmonic oscillator with Hamiltonian :

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2} \ ,$$

III.A Show that in terms of the annihilation, creation operators :

$$a := \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right) \ , \qquad a^\dagger := \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right) \ ,$$

which obey the commutation relations

$$[a, a^\dagger] = 1 \ ,$$

the Hamiltonian can also be expressed as :

$$H = \hbar\omega (a^\dagger a + \frac{1}{2}) \ .$$

III.B Compute $a_H(t)$ and $a_H^\dagger(t)$.

III.C Prove the Hadamard lemma :

$$\begin{aligned} e^X Y e^{-X} &= e^{[X,\ ]} Y && (1) \\ &:= Y + [X, Y] + \frac{1}{2}[X, [X, Y]] + \dots \ , && (2) \end{aligned}$$

and use this result to compute $a_H(t)$, $a_H^\dagger(t)$ directly (i.e. without solving the time evolution first-order differential equation).

III.D Compute $[\hat{x}_H(t_1), \hat{x}_H(t_2)]$ and $[\hat{x}_H(t_1), \hat{p}_H(t_2)]$.

Master M1 Parcours International 2010-2011

IPNL, Université Lyon 1

Travaux Dirigés Quantum Mechanics

Sheet 3 : *Angular momentum & rotations*

I. Parity & selection rules

The parity operator P reverses the sign of vectors, according to $P : \mathbf{r} \to -\mathbf{r}$.

I.A Determine the parity of the state $|lm\rangle$.

I.B Using the previous result, show that the matrix elements $\langle l'm'|z|lm\rangle$ vanish when $(l + l')$ is even.

II. Rotations & position operator

II.A Determine the commutator $[L_z, \mathbf{r}]$, where $\mathbf{r} = (x, y, z)$ is the position vector operator.

II.B Compute $e^{-i\varphi L_z/\hbar}\mathbf{r}e^{i\varphi L_z/\hbar}$ using the Hadamard lemma (see exercise sheet no.2)

II.C Rederive the previous result by taking into account that the angular momentum is the generator of rotations.

III. Rotations & angular momentum

III.A Compute $e^{-i\varphi J_x/\hbar}J_z e^{i\varphi J_x/\hbar}$.

III.B Using the previous result and the relation between angular momentum and rotation operators, $R_{\mathbf{n}}(\theta) = e^{-i\theta\mathbf{n}\cdot\mathbf{J}/\hbar}$, prove that

$$R_{\tilde{\mathbf{n}}}(\theta) = \tilde{R} \cdot R_{\mathbf{n}}(\theta) \cdot \tilde{R}^{-1} \ , \tag{1}$$

where $\mathbf{n}$ and $\tilde{\mathbf{n}}$ are two unit vectors related by a rotation $\tilde{R}$ through

$$\tilde{\mathbf{n}} = \tilde{R} \cdot \mathbf{n} \ .$$

(Hint : you may identify $\mathbf{n}$ with $\hat{\mathbf{z}}$ and $\tilde{R}$ with $R_x(\varphi)$.) What is the geometric interpretation of eqn. (1) ?

IV. Pauli matrices & rotation operator

IV.A Consider two vector operators $\mathbf{a}$, $\mathbf{b}$ which commute with the Pauli matrices, but not necessarily with each other. Prove the identity :

$$(\sigma \cdot \mathbf{a})(\sigma \cdot \mathbf{b}) = (\mathbf{a} \cdot \mathbf{b})\mathbb{I} + i(\mathbf{a} \times \mathbf{b})\sigma \ , \tag{2}$$

where $\mathbb{I}$ is the two by two identity matrix and σ is a three-vector whose components are the Pauli matrices,

$$\sigma := (\sigma_x, \sigma_y, \sigma_z) \ .$$

IV.B Use eqn. (2) to show that

$$e^{i\theta \mathbf{n}\cdot\sigma} = \mathbb{I}\cos\theta + i\mathbf{n}\cdot\sigma\sin\theta \ ,$$

where $\mathbf{n}$ is a unit vector and θ is an arbitrary angle.

IV.C Use the previous result to compute the matrix elements of the rotation operator $D^j_{mm'}(\alpha, \beta, \gamma)$, where

$$D^j_{mm'}(\alpha, \beta, \gamma) = \langle jm|D(\alpha, \beta, \gamma)|jm'\rangle \ ,$$

for the special case $j = 1/2$.

Travaux Dirigés Quantum Mechanics

Sheet 4 : *Spin & magnetic field*

The electron (charge $-e$, mass m_e) is a particle of spin $\frac{1}{2}$. Consider an electron in a uniform, time-independent magnetic field $\vec{B} = B\hat{z}$ along the z-axis. Neglecting all other degrees of freedom, the Hamiltonian of the electron is given by

$$H = -\vec{\mu} \cdot \vec{B} \ ,$$

where $\vec{\mu} = \frac{-e}{m_e}\vec{S}$ is the so-called magnetic moment.

I. Time evolution

I.A What is the interpretation of the sign in the expression for H ?

I.B Solve the eigenvalue problem for the Hamiltonian. (Set $\omega = \frac{eB}{m_e}$.)

I.C Determine the explicit expression for the time evolution operator $U(t, t_0 = 0)$. Express your answer as a linear combination of the projectors $|+\rangle\langle+|$ and $|-\rangle\langle-|$.

II. Larmor precession

Suppose that at $t = 0$ the electron is in an eigenstate $|\Psi(0)\rangle$ of the operator S_x corresponding to eigenvalue $+\hbar/2$.

II.A Determine $|\Psi(0)\rangle$ and $|\Psi(t)\rangle$.

II.B What is the probability, as a function of time, for the electron to be in an eigenstate of S_x corresponding to eigenvalue $\hbar/2$?

II.C What are the expectation values, as functions of time, of S_x, S_y, S_z ?

III. Heisenberg picture

III.A Write down and solve the equations of motion satisfied by the time-dependent operators S_x^H, S_y^H, S_z^H in the Heisenberg picture.

III.B Verify your previous answer by a direct computation using the explicit form of the time evolution operator computed in I.C.

III.C Verify that the expectation values of S_x^H, S_y^H, S_z^H agree with those computed in II.C in the Schrödinger picture.

Travaux Dirigés Quantum Mechanics

Sheet 5 : *Addition of angular momenta*

I. Coupling of two spins $\frac{1}{2}$

Consider a system of two particles of spin $\frac{1}{2}$, i.e. $j_1 = \frac{1}{2} = j_2$, and let $\mathbf{J}_1$, $\mathbf{J}_2$ be their respective spin operators. Moreover, let

$$\{\, |j_1 m_1; j_2 m_2\rangle := |j_1 m_1\rangle \otimes |j_2 m_2\rangle \;\; \text{with} \;\; -j_1 \leq m_1 \leq j_1 \;\; \text{and} \;\; -j_2 \leq m_2 \leq j_2 \,\}$$

be the orthonormal basis consisting of common eigenstates of the observables $\mathbf{J}_1^2$, J_{1z}, $\mathbf{J}_2^2$ and J_{2z}. The total angular momentum is defined by

$$\mathbf{J} \;=\; \mathbf{J}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \mathbf{J}_2 \;\equiv\; \mathbf{J}_1 + \mathbf{J}_2 \,.$$

I.A Determine the matrices J_z and $\mathbf{J}^2$ with respect to the basis $|j_1 m_1; j_2 m_2\rangle$ by a direct matrix calculation (i.e. using the matrix representation of the spin operators for a particle of spin $\frac{1}{2}$).

I.B Verify your answer to the previous question by computing the action of the operators J_z and $\mathbf{J}^2$ on the $|j_1 m_1; j_2 m_2\rangle$ basis.

I.C Recover your previous results by computing the action of the operators J_z and $\mathbf{J}^2$ on the $|j_1 j_2, JM\rangle$ basis, and using the table of Clebsch-Gordan coefficients.

II. Symmetric & antisymmetric tensor products

Consider the states $|jm_1; jm_2\rangle_{\mathrm{s}}$, $|jm_1; jm_2\rangle_{\mathrm{a}}$, $j \in \mathbb{N}$, defined by

$$\begin{aligned} |jm_1; jm_2\rangle_{\mathrm{s}} &:= |jm_1; jm_2\rangle + |jm_2; jm_1\rangle \\ |jm_1; jm_2\rangle_{\mathrm{a}} &:= |jm_1; jm_2\rangle - |jm_2; jm_1\rangle \;. \end{aligned}$$

II.A Show that $|jm_1; jm_2\rangle_{\mathrm{s}}$ is a linear combination of states in the $|jj, JM\rangle$ basis with even angular momentum J.

II.B Show that $|jm_1; jm_2\rangle_{\mathrm{a}}$ is a linear combination of states in the $|jj, JM\rangle$ basis with odd angular momentum J.

III. Hyperfine structure of the hydrogen atom

Consider a hydrogen atom in the $1s$ state. Denote the Pauli spin operator for the electron by $\vec{\sigma}_1 = (\sigma_{1x}, \sigma_{1y}, \sigma_{1z})$ (acting on the Hilbert space $\mathcal{H}_1$ of the spin states of the electron) and the Pauli spin operator for the proton by $\vec{\sigma}_2$ (acting on the Hilbert space $\mathcal{H}_2$ of the spin states of the proton). In the presence of a uniform magnetic field in the z-direction, $\vec{B} = (0, 0, B)$, the magnetic interaction terms in the Hamiltonian read

$$H = H_0 + \Delta H\,, \qquad \text{with } \; H_0 = W\vec{\sigma}_1 \cdot \vec{\sigma}_2 \quad \text{and} \quad \Delta H = \mu B\,\sigma_{1z}\,,$$

where W and μ are real constants. The Hamiltonian H_0 represents the magnetic dipole interaction between the electron and proton; the Hamiltonian ΔH describes the coupling of the magnetic dipole moment of the electron with the external magnetic field $\vec{B}$. (The coupling of the magnetic dipole moment of the proton with $\vec{B}$ is negligible as compared to that of the electron.)

III.A In the case of a vanishing magnetic field, i.e. for $H = H_0$, determine the eigenvalues and eigenstates of the Hamiltonian.

III.B Determine the eigenvalues and eigenstates of the Hamiltonian in the presence of a non-vanishing magnetic field.

III.C Draw the eigenvalues of the previous question as functions of B. Label each curve with the angular momentum of the corresponding eigenstate.

Master M1 Parcours International 2010-2011

IPNL, Université Lyon 1

Travaux Dirigés Quantum Mechanics

Sheet 6 : *Many particles*

I. Symmetrization & antisymmetrization

Consider the symmetrization & antisymmetrization operators S, A defined by :

$$S = \frac{1}{N!} \sum P \ , \qquad A = \frac{1}{N!} \sum (-)^P P \ ,$$

where the sums above are over all permutations P of N particles. Show that S, A are orthogonal projector operators, i.e. they satisfy

$$S^2 = S \ , \quad A^2 = A \ , \quad SA = AS = 0 \ .$$

II. Symmetric & antisymmetric tensor products

II.A Use the Clebsch-Gordan coefficients to obtain the $|j_1, j_2, J, M\rangle$ states in terms of the $|j_1 m_1; j_2 m_2\rangle$ states, for a system of two particles of spin $j_1 = j_2 = \frac{1}{2}$. Compute the action of S, A of the previous exercise on the $|j_1, j_2, J, M\rangle$ states and comment on their symmetry properties.

II.B Repeat the preceding computation for a system of two particles of spin $j_{1,2} = 1$. Compare your answer with exercise II of sheet # 5.

III. Identical particles

III.A Show that for a system of two identical particles, each of which can be in one of n quantum states, there are

$$\frac{1}{2} n(n+1) \ \text{ symmetric}$$

and

$$\frac{1}{2} n(n-1) \ \text{ antisymmetric}$$

states of the system.

III.B Show that, if the particles have spin j, the ratio of symmetric to antisymmetric spin states is $(j+1)/j$.

IV. The two-body problem

Consider two particles of mass m_1 and m_2, respectively, whose interaction is given by a potential $V(\vec{r}_1 - \vec{r}_2)$. This system is described by the Hamiltonian

$$H = \frac{1}{2m_1}\,\vec{p}_1^{\,2} + \frac{1}{2m_2}\,\vec{p}_2^{\,2} + V(\vec{r}_1 - \vec{r}_2)\,.$$

In order to reduce this two-body problem to a one-body problem, one introduces the *coordinates of the center of mass* and the *coordinates of relative position*

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}\,, \qquad \vec{r} = \vec{r}_1 - \vec{r}_2\,,$$

as well as the *total mass* M and the *reduced mass* μ defined by

$$M = m_1 + m_2\,, \qquad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}\,.$$

IV.A Recall that in classical mechanics, the momentum $\vec{P}$ of the center of mass particle (of mass M) and the momentum $\vec{p}$ of the relative particle (of mass μ) are respectively given by

$$\vec{P} = \vec{p}_1 + \vec{p}_2\,, \qquad \vec{p} = \frac{m_2}{M}\,\vec{p}_1 - \frac{m_1}{M}\,\vec{p}_2\,.$$

Show that the same relations hold in quantum mechanics between the operators of momentum given by

$$\vec{p}_1 = \frac{\hbar}{\mathrm{i}}\,\vec{\nabla}_{\vec{r}_1}\,, \qquad \vec{p}_2 = \frac{\hbar}{\mathrm{i}}\,\vec{\nabla}_{\vec{r}_2}\,, \qquad \vec{P} = \frac{\hbar}{\mathrm{i}}\,\vec{\nabla}_{\vec{R}}\,, \qquad \vec{p} = \frac{\hbar}{\mathrm{i}}\,\vec{\nabla}_{\vec{r}}\,.$$

Furthermore, show that Heisenberg's commutation relations for the pairs of canonical variables $(\vec{r}_1, \vec{p}_1)$ and $(\vec{r}_2, \vec{p}_2)$, respectively, imply Heisenberg's commutation relations for the pairs of variables $(\vec{r}, \vec{p})$ and $\left(\vec{R}, \vec{P}\right)$, respectively.

IV.B Show that the Hamiltonian takes the following form if written in terms of the center of mass and relative coordinates :

$$H = H_{\mathrm{CM}} + H_{\mathrm{rel}} \qquad \text{with} \qquad \begin{cases} H_{\mathrm{CM}} = \frac{1}{2M}\,\vec{P}^{\,2} \\ H_{\mathrm{rel}} = \frac{1}{2\mu}\,\vec{p}^{\,2} + V(\vec{r})\,, \end{cases}$$

where H_{CM} describes the free motion of the center of mass while H_{rel} describes the dynamics of a "relative particle" of mass μ in the potential $V(\vec{r})$; i.e. H_{rel} is a Hamiltonian for a one-body problem.

IV.C Since the wave function for a free particle is given by a plane wave, we look for a solution to the eigenvalue problem

$$H\Psi_n = E_n\Psi_n$$

of the form

$$\Psi_n(\vec{R}, \vec{r}) = \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}}\,\psi_n(\vec{r})\,.$$

Show that the energy levels of the two-body problem take the form

$$E_n = \frac{\hbar^2\vec{k}^{\,2}}{2M} + \varepsilon_n\,.$$

It follows from the above that the transition energies $\hbar\omega_{n,n'} := E_n - E_{n'}$ do not depend on the center of mass energy.

Master M1 Parcours International 2010-2011

IPNL, Université Lyon 1

Travaux Dirigés Quantum Mechanics

Sheet 7 : *Time-independent perturbation theory*

I. Non-degenerate two-level system

Consider a non-degenerate two-level system which is perturbed by a small time-independent interaction. The perturbation is assumed to be non-diagonal with respect to the Hilbert space basis consisting of eigenkets associated to the non-perturbed system. You may assume that the solution of the eigenvalue problem for the non-perturbed system is known.

I.A Compare the energy corrections determined by an exact calculation with those found by applying perturbation theory to second order.

I.B Compute the perturbed eigenstates to second order in perturbation theory. Compare with the exact result. Discuss the normalization of vectors.

II. Anharmonic oscillator

A particle of mass m moving on the real axis (parametrized by $x \in \mathbb{R}$) is subject to the anharmonic potential

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \lambda\, x^4 \,,$$

where the second term is assumed to be small compared to the first one.

II.A Recall that

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a + a^\dagger)$$

and

$$a^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \,, \qquad a|n\rangle = \sqrt{n}\, |n-1\rangle \,,$$

where $|n\rangle$ is the energy eigenstate of the unperturbed hamiltonian at level n :

$$H_0 |n\rangle = E_n^{(0)} |n\rangle \,, \quad E_n^{(0)} = \hbar\omega(n + \frac{1}{2}) \,.$$

Determine $\langle n|x^4|n\rangle$ and $E_n^{(1)}$.

What would be the effect (at the first order in perturbation theory) of a term x^3 (rather than x^4) in the potential ?

(Hint : take into account the properties of the operators a and $a^\dagger$.)

II.B Use the wave function of the ground state of the harmonic oscillator :

$$\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} ,$$

in order to determine $\langle 0|x^4|0\rangle$ and $E_0^{(1)}$.

What would be the effect (at the first order in perturbation theory) of a term x^3 (rather than x^4) in the potential ?

(Hint : Recall that $\displaystyle\int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}$; use that to determine $\int_{-\infty}^{+\infty} x^{2n} e^{-\alpha x^2} dx$.)

III. Variational method

III.A Use the variational method to estimate the ground-state energy of the anharmonic oscillator of the previous exercise. Use the following test wavefunction :

$$\varphi_\alpha = e^{-\frac{1}{2}\alpha x^2} .$$

Compare your result with that of the first-order perturbation theory. For simplicity you may take $\hbar = m = \omega = 1$.

(Hint : Solve the resultant third-order equation in α perturbatively, to first order in λ.)

III.B Use the variational method to estimate the ground-state energy of the harmonic oscillator. As a normalized test wavefunction take

$$\varphi_\alpha(x) = \sqrt{\frac{2}{\pi}}\, \alpha^{3/2} \frac{1}{x^2 + \alpha^2} , \qquad \alpha \in \mathbb{R}^* .$$

Make a sketch of the φ_α.

Compare your estimate for the ground state energy with the exact result and determine the relative error.

(Hint : The following integrals appear in the calculation (after integrating by parts the expression $\int \varphi_\alpha \varphi_\alpha'' \, dx$) :

$$\int_{-\infty}^{\infty} \frac{x^2\, dx}{(x^2+\alpha^2)^2} = \frac{\pi}{2\alpha} , \qquad \int_{-\infty}^{\infty} \frac{x^2\, dx}{(x^2+\alpha^2)^4} = \frac{\pi}{16\alpha^5} .$$

As in the previous exercise you may take $\hbar = m = \omega = 1$.)

Travaux Dirigés Quantum Mechanics

Sheet 8 : *Time-independent perturbation theory II*

I. Fine structure of the hydrogenic atom

In its simplest version, the quantum mechanical description of a hydrogenic atom is based on the Hamiltonian

$$H_0 = \frac{p^2}{2m} + V_c(r) = \frac{p^2}{2m} - \hbar c \, \frac{Z\alpha}{r} \ ,$$

where Z is the atomic number and $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \simeq \frac{1}{137}$ the fine structure constant. (The energy spectrum is reviewed in the notes). We can use two different orthonormal bases : the basis given by the kets $|n\ell m\frac{1}{2}m_s\rangle$ which can be decomposed into radial, angular momentum and spin momentum parts according to

$$|n\ell m\frac{1}{2}m_s\rangle = |n\ell\rangle \; |\ell m\rangle \; |\frac{1}{2}m_s\rangle \, ,$$

or the so-called *coupled basis* given by the kets $|n\ell\frac{1}{2}jm_j\rangle$ which can be decomposed into radial and angular/spin momentum parts according to

$$|n\ell\frac{1}{2}jm_j\rangle = |n\ell\rangle \; |\ell\frac{1}{2}jm_j\rangle \, .$$

I.A Specify the ranges of the quantum numbers n, ℓ, m, m_s, j, m_j as well the degeneracy level of $E_n^{(0)}$.

I.B The so-called *spin-orbit term* (i.e. the interaction between the magnetic moment associated with the spin of the electron and the field of the nucleus which is in motion relative to the electron) and the so-called *Darwin term* (i.e. the relativistic correction to the Coulomb energy) yield the following perturbations of the Hamiltonian :

$$h_1 = \frac{1}{2m^2c^2} \, \frac{1}{r} \, \frac{dV_c(r)}{dr} \; \vec{L} \cdot \vec{S} \, , \qquad h_2 = \frac{\hbar^2}{8m^2c^2} \, \nabla^2 V_c(r) \, .$$

Show that, for velocities of the electron which are small as compared to c, the theory of relativity contributes the following correction to the kinetic energy of the electron :

$$h_3 = -\frac{1}{2mc^2} \left(\frac{p^2}{2m} \right)^2 \, .$$

I.C For each of these three perturbations, choose an appropriate basis, i.e. a basis with respect which the perturbation operator is diagonal. Show that the corrections provided by first order perturbation theory have the form

$$\begin{aligned}
\Delta E_1 &= -E_n^{(0)} \frac{(Z\alpha)^2}{n} \left[\frac{P_j(\ell)}{2\ell(\ell+\frac{1}{2})(\ell+1)} \right] \qquad (\text{for } \ell \neq 0) \\
\Delta E_2 &= -E_n^{(0)} \frac{(Z\alpha)^2}{n} \delta_{\ell,0} \\
\Delta E_3 &= E_n^{(0)} \frac{(Z\alpha)^2}{n} \left[\frac{1}{\ell+\frac{1}{2}} - \frac{3}{4n} \right],
\end{aligned}$$

where

$$P_j(\ell) = \begin{cases} \ell & \text{if } j = \ell + \frac{1}{2} \\ -(\ell+1) & \text{if } j = \ell - \frac{1}{2} \,. \end{cases}$$

I.D Show that the fine structure of the energy level $E_n^{(0)}$ does not explicitly depend on the quantum number ℓ and that the total correction to $E_n^{(0)}$ as given by first order perturbation theory reads

$$\Delta E = E_n^{(0)} \frac{(Z\alpha)^2}{n} \left[\frac{1}{j+\frac{1}{2}} - \frac{3}{4n} \right] .$$

II. Helium-like atom

Using the variational method, find the ground state energy of an atom with two electrons and a nuclear number Z, using a trial wavefunction of the form

$$\psi(r_1, r_2) = \left(\frac{Z'^3}{\pi a_0^3} \right) e^{-Z' r_1/a_0} e^{-Z' r_2/a_0} \,.$$

where r_1, r_2 are the distances of the two electrons from the nucleus, a_0 is the Bohr radius, α is the fine structure constant, and Z' is an adjustable parameter. The Hamiltonian describing the system is given by :

$$H = \frac{p_1^2}{2m} + \frac{p_1^2}{2m} - \hbar c \frac{Z\alpha}{r_1} - \hbar c \frac{Z\alpha}{r_2} + \hbar c \frac{\alpha}{r_{12}},$$

where $r_{12} := |\mathbf{r}_1 - \mathbf{r}_2|$.

III. WKB approximation

We have seen that in the WKB approximation to first order in $\hbar$, the time-independent part of the wavefunction becomes :

$$\psi(x) = \frac{c_1}{\sqrt{p}} e^{\frac{i}{\hbar} \int dx p(x)} + \frac{c_2}{\sqrt{p}} e^{-\frac{i}{\hbar} \int dx p(x)} \,,$$

where c_1, c_2 are constants and

$$p(x) := \sqrt{2m(E - V(x))} \,.$$

What is the modification to the above expression for $\psi(x)$ at the next order in $\hbar$?

Relevant formulas for the HYDROGENIC ATOM

Let $e = |e|$ be the charge of the proton. For a simple treatment of the hydrogenic atom, one assumes that the nucleus (of charge Ze) is point-like, static, responsible for the Coulomb potential binding the electron (of mass m and charge $-e$) with an interaction energy

$$E_n = -\frac{1}{n^2}\frac{mc^2\alpha^2 Z^2}{2} .$$

Here, n is the principal quantum number (i.e. a positive integer), $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \simeq \frac{1}{137}$ denotes the fine structure constant and $mc^2 \simeq 511$ KeV. The wave functions corresponding to such a degenerate energy level are given by

$$\phi_{n\ell m}(r,\theta,\varphi) = \langle\vec{r}|n\ell m\rangle = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi) \;,$$

where n, l and m are the usual quantum numbers.
The first few of these wave functions read as

$$\begin{aligned}
\phi_{100} &= 2\,(\frac{Z}{a_0})^{\frac{3}{2}}\, e^{-\frac{Zr}{a_0}}\, Y_{00}(\theta,\varphi)\\
\phi_{200} &= 2\,(\frac{Z}{2a_0})^{\frac{3}{2}}\left[1-(\frac{Zr}{2a_0})\right] e^{-\frac{Zr}{2a_0}}\, Y_{00}(\theta,\varphi)\\
\phi_{21m} &= \frac{2}{\sqrt{3}}\,(\frac{Z}{2a_0})^{\frac{3}{2}}\,(\frac{Zr}{2a_0})\, e^{-\frac{Zr}{2a_0}}\, Y_{1m}(\theta,\varphi)\\
\phi_{300} &= 2\,(\frac{Z}{3a_0})^{\frac{3}{2}}\left[1-2(\frac{Zr}{3a_0})+\frac{2}{3}(\frac{Zr}{3a_0})^2\right] e^{-\frac{Zr}{3a_0}}\, Y_{00}(\theta,\varphi)\\
\phi_{31m} &= 4\sqrt{2}\,(\frac{Z}{3a_0})^{\frac{3}{2}}\,(\frac{Zr}{3a_0})\left[1-\frac{1}{2}(\frac{Zr}{3a_0})\right] e^{-\frac{Zr}{3a_0}}\, Y_{1m}(\theta,\varphi)\\
\phi_{32m} &= \frac{2\sqrt{2}}{3\sqrt{5}}\,(\frac{Z}{3a_0})^{\frac{3}{2}}\,(\frac{Zr}{3a_0})^2\, e^{-\frac{Zr}{3a_0}}\, Y_{2m}(\theta,\varphi)\,,
\end{aligned}$$

where $a_0 = \frac{\hbar}{mc\alpha} \simeq 0.529\,\mathring{A}$ denotes the Bohr radius associated to the ground state and where the involved spherical harmonics are given by

$$Y_{00} = \frac{1}{\sqrt{4\pi}}\,, \qquad Y_{10} = \sqrt{\frac{3}{4\pi}}\,\cos\theta, \qquad Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{\pm i\varphi}\,,$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta-1), \qquad Y_{2\pm1} = \mp\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\, e^{\pm i\varphi}, \qquad Y_{2\pm2} = \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\, e^{\pm 2i\varphi} .$$

We also spell out the the value of the probability density at the origin,

$$|\phi_{n\ell m}(r=0)|^2 = \frac{Z^3}{\pi a_0^3}\frac{1}{n^3}\delta_{\ell,0}\,,$$

as well as the expectation values of certain operators in the state $|n\ell\rangle$:

$$\langle r^k\rangle = \int_0^\infty dr\, r^{2+k}\,[R_{n\ell}(r)]^2$$

$$\langle r\rangle = \frac{1}{2}\left(\frac{a_0}{Z}\right)[3n^2-\ell(\ell+1)], \qquad \langle r^2\rangle = \frac{1}{2}\left(\frac{a_0}{Z}\right)^2 n^2\,[5n^2+1-3\ell(\ell+1)]$$

$$\left\langle\frac{1}{r}\right\rangle = \left(\frac{Z}{a_0}\right)\frac{1}{n^2}, \qquad \left\langle\frac{1}{r^2}\right\rangle = (\frac{Z}{a_0})^2\frac{1}{n^3(\ell+\frac{1}{2})}, \qquad \left\langle\frac{1}{r^3}\right\rangle = \left(\frac{Z}{a_0}\right)^3\frac{1}{n^3\ell(\ell+\frac{1}{2})(\ell+1)} .$$

Some useful INTEGRALS

$$\int_0^\infty dx \, \frac{\sin x}{x} = \frac{\pi}{2}$$

$$\int_0^\infty dx \, e^{-x} x^n = n!$$

$$\int_0^\infty dx \, e^{-\alpha x} x \sin \beta x = \frac{2\alpha\beta}{(\alpha^2 + \beta^2)^2} \qquad (\alpha, \beta \text{ positive})$$

$$\int_{-\infty}^\infty dx \, e^{-\alpha^2 x^2} = \frac{\sqrt{\pi}}{\alpha}$$

$$\int_{-\infty}^\infty dx \, e^{-\alpha^2 x^2 + i\beta x} = \frac{\sqrt{\pi}}{\alpha} \, e^{-\frac{\beta^2}{4\alpha}} \qquad (\beta \text{ real})$$

$$\int_{-\infty}^\infty dx \, x^2 \, e^{-\alpha^2 x^2} = \frac{\sqrt{\pi}}{2\alpha^3}$$

$$\int_{\mathbb{R}^3} d^3 r \, \frac{e^{i\vec{k}\cdot\vec{r}}}{|\vec{r'} - \vec{r}|} = \frac{4\pi}{k^2} e^{i\vec{k}\cdot\vec{r'}}$$

$$\int_{\mathbb{R}^3} d^3 r_1 \int_{\mathbb{R}^3} d^3 r_2 \, \frac{1}{|\vec{r}_1 - \vec{r}_2|} \, e^{-2\frac{r_1 + r_2}{a}} = \pi^2 \frac{5}{8} a^5$$

FORMULAS involving the "δ-function"

$$\Delta \frac{1}{r} = -4\pi \, \delta^{(3)}(\vec{r})$$

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \, e^{ikx} = \delta(x)$$

Travaux Dirigés Quantum Mechanics

Sheet 9 : *WKB, Interaction picture*

I. Bohr-Sommerfeld quantization

A particle moves in a potential well $V(x)$ such that for energy $E \geq V(x)$ there are exactly two turning points. Show that in the WKB approximation the discrete energy levels are determined by the condition

$$\int_a^b p(x)dx = \pi\hbar(n+\frac{1}{2}), \qquad n \in \mathbb{N} ,$$

where a, b are the turning points given by $V(a) = V(b) = E$ and $b > a$; the position-dependent momentum is given by $p(x) := \sqrt{2m(E - V(x))}$.

II. Time evolution operator

We have seen that the time evolution operator in the interaction picture takes the form of a *Dyson series* expansion :

$$U_I(t,t_0) = 1 + \sum_{n=1}^{\infty} U^{(n)}(t,t_0) ,$$

where

$$U^{(n)}(t,t_0) = \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H_{pI}(t_1)\cdots H_{pI}(t_n) ,$$

and H_{pI} is the perturbation in the interaction picture.

II.A Using the above expression, verify explicitly that $U_I(t,t_0)$ obeys the differential equation :

$$i\hbar\frac{d}{dt}U_I(t,t_0) = H_{pI}(t)U_I(t,t_0) .$$

II.B Show that

$$U^{(n)}(t,t_0) = \frac{1}{n!}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n T[H_{pI}(t_1)\cdots H_{pI}(t_n)] ,$$

where the *time-ordering operator* T is defined by

$$T[A_1(t_1)\cdots A_n(t_n)] = A_{P(1)}(t_{P(1)})\cdots A_{P(n)}(t_{P(n)}) ,$$

and P is the permutation of n indices for which

$$t_{P(1)} > t_{P(2)} > \cdots > t_{P(n)} .$$

III. Interaction picture

Consider a particle of mass m moving under the influence of a time-dependent one-dimensional potential $V_S(t, x)$ (in the Schrödinger picture).

III.A Treating $V_S(t, x)$ as a perturbation, solve the equations of motion for the position and momentum operators $x_I(t)$, $p_I(t)$ in the interaction picture.

III.B Compute the commutators $[x_I(t_1), x_I(t_2)]$, $[p_I(t_1), p_I(t_2)]$, $[x_I(t_1), p_I(t_2)]$.

III.C Consider two operators $\mathcal{O}_S$, $\mathcal{O}'_S$ (in the Schrödinger picture) such that

$$[\mathcal{O}_S, \mathcal{O}'_S] = 0 \ .$$

Show that

$$[\mathcal{O}_I(t), \mathcal{O}'_I(t)] = 0 \ .$$

Compare with the result of the previous exercise.

Master M1 Parcours International 2010-2011

IPNL, Université Lyon 1

Travaux Dirigés Quantum Mechanics

Sheet 10 : *Time-dependent perturbation*

I. Two-state system

Consider the two-state system described, in the Schrödinger picture, by the Hamiltonian $H = H_0 + H_p$ where :

$$\begin{aligned} H_0 &= E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| \\ H_p &= \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1| \end{aligned} \tag{1}$$

where γ, ω are real and positive, and $E_2 > E_1$.

I.A For a general state $|\psi(t)\rangle_I$ in the interaction picture, we expand

$$|\psi(t)\rangle_I = \sum_n c_n(t)|n\rangle \ ,$$

where $\{|n\rangle\}$ is an orthonormal set of eigenstates of the unperturbed Hamiltonian H_0. Use the explicit form of the time-evolution operator to express the coefficients $c_n(t)$ in a series expansion in the perturbation H_p.

I.B Assuming that at $t = 0$ the system is in its ground state $|1\rangle$, and treating H_p as a perturbation, use the result of the previous exercise to determine $|c_1(t)|^2$, $|c_2(t)|^2$ for the wavefunction of the system (1) to the first non-vanishing order in time-dependent perturbation theory.

I.C Determine $|c_1(t)|^2$, $|c_2(t)|^2$ exactly by solving a coupled system of first-order differential equations for $c_1(t)$, $c_2(t)$; compare with the previous result.

II. Charged harmonic oscillator

A one-dimensional charged harmonic oscillator (charge e, mass m, angular frequency ω) is in its ground state for $t < t_0$. At time t_0 a constant electric field is turned on. Determine, to first order in time-dependent perturbation theory, the probability that at time $t > t_0$ the oscillator is in the n-th excited state.

III. Hydrogen atom

A hydrogen atom in its $1s$ ground state is placed in a uniform time-dependent electric field given by :

$$\vec{E} = \begin{cases} 0 \,, & t < 0 \\ E_0 e^{-t/\tau} \hat{\mathbf{z}} \,, & t > 0 \end{cases} \,,$$

where $\hat{\mathbf{z}}$ is the unit vector in the positive z axis, and E_0, τ are constants.

III.A Derive the electric potential and the corresponding perturbation H_p for $t > 0$.

III.B Compute the probability that at time $t >> \tau$ the hydrogen atom is in the state $2s$.

III.C Repeat the previous exercise for each of the three $2p$ states.

Hint : Take into account that $z = \sqrt{4\pi/3}\, rY_{10}$. The wavefunction of the state with quantum numbers n,l,m is given by : $\Psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta, \varphi)$. You may further assume that the radial integrals

$$I_1 := \int_0^\infty dr r^3 R^*_{20}(r) R_{10} \,, \quad I_2 := \int_0^\infty dr r^3 R^*_{21}(r) R_{10} \,,$$

are known and non-vanishing.

Master M1 Parcours International 2010-2011

IPNL, Université Lyon 1

Travaux Dirigés Quantum Mechanics

Sheet 11 : *Time-dependent perturbation II*

I. Linear response

We would like to study the change of the expectation value of the operator A (in the Schrödinger picture) under the influence of a perturbation :

$$H_p = -B\, b(t) \ ,$$

where B is a time-independent operator, and the time-dependent function $b(t)$ represents the strength of the perturbation. We shall assume that at $t \to -\infty$ the system is in an energy eigenstate $|n\rangle$ of the unperturbed hamiltonian H_0 with eigenvalue E_n^0. The time-dependent change $\langle \delta A(t) \rangle_n$ of the expectation value of the operator A is given by :

$$\langle \delta A(t) \rangle_n = \langle \Psi_n(t)|A|\Psi_n(t)\rangle - \langle n|A|n\rangle \ ,$$

where $|\Psi_n(t)\rangle$ is the state of the system at time t.

I.A The *linear response function* X_{AB}^n is defined by

$$\langle \delta A(t) \rangle_n = \int_{-\infty}^{\infty} dt_1 X_{AB}^n(t-t_1) b(t_1) \ .$$

Show that

$$X_{AB}^n(t) = \frac{i}{\hbar}\Theta(t) \sum_m \left(\langle n|A|m\rangle\langle m|B|n\rangle e^{-i\omega_{mn}t} - \langle n|B|m\rangle\langle m|A|n\rangle e^{i\omega_{mn}t} \right) \ ,$$

where $\omega_{mn} := (E_m^0 - E_n^0)/\hbar$ and Θ is the step function :

$$\Theta(x) = \begin{cases} 1 \ , & x > 0 \\ 0 \ , & x < 0 \end{cases} \ .$$

I.B The Fourier transform $\tilde{f}(\omega)$ of a function $f(t)$ is given by

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{f}(\omega) e^{-i\omega t} \ .$$

Show that the Fourier transform of a *convolution* :

$$C(t) = \int_{-\infty}^{\infty} dt_1 f(t-t_1) g(t_1) \ ,$$

is given by the product of the Fourier transforms : $\tilde{C}(\omega) = \tilde{f}(\omega)\tilde{g}(\omega)$. Use this result to show that the Fourier transform of $\langle \delta A(t)\rangle_n$ reads : $\langle \widetilde{\delta A}(\omega)\rangle_n = \tilde{X}^n_{AB}(\omega)\tilde{b}(\omega)$, where the Fourier transform of the linear response is given by :

$$\tilde{X}^n_{AB}(\omega) = \frac{1}{\hbar}\sum_m \left(\frac{\langle n|A|m\rangle\langle m|B|n\rangle}{\omega_{mn} - \omega - i\varepsilon} - \frac{\langle n|B|m\rangle\langle m|A|n\rangle}{\omega_{nm} - \omega - i\varepsilon} \right) . \tag{1}$$

Hint : You may use the integral representation of the step function :

$$\Theta(t) = -\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\,\frac{e^{-i\omega t}}{\omega + i\varepsilon} .$$

II. Polarizability

We would now like to apply formuma (1) to the case of atoms in a time-dependent electric field. Consider the perturbation :

$$H_p = e\hat{z}E(t) ,$$

where e is the charge of the electron, $\hat{z}$ is the position operator in the direction of the z-axis, and $E(t)$ is a time-dependent electric field; the operator B of the previous exercise now corresponds to the dipole operator $D := e\hat{z}$, while $b(t)$ corresponds to $E(t)$. The above perturbation leads to an induced dipole moment

$$\langle \widetilde{\delta D}(\omega)\rangle_n = \tilde{X}^n_{DD}(\omega)\tilde{E}(\omega) ,$$

i.e. the operator A of the previous exercise also corresponds to D. The linear response function X^n_{DD} is called *polarizability.*

II.A Show that

$$\tilde{X}^n_{DD}(\omega) = \frac{e^2}{m_e}\sum_m \frac{f_{mn}}{\omega^2_{mn} - (\omega + i\varepsilon)^2} , \tag{2}$$

where m_e is the electron mass and f_{mn} is the so-called *oscillator strength* :

$$f_{mn} := \frac{2m_e}{e^2\hbar}\omega_{mn}|\langle m|D|n\rangle|^2 .$$

II.B Consider formula (2) for the ground state $n = 0$. Near the resonance frequency $\omega \sim \omega_{m0}$ it breaks down. In this case higher energy eigenstates $|m\rangle$ are excited, with life expectancy Γ_m^{-1}. One can take this into account by formally complexifying the corresponding energy eigenvalue $E^0_m \to E^0_m - \frac{i}{2}\hbar\Gamma_m$. Compute the polarizability in the case where $\omega \sim \omega_{m0}$.

II.C It is known from electrodynamics that the polarizability is related to the dielectric constant $\mathcal{E}$ via :

$$\mathcal{E} = 1 + C\tilde{X}^0_{DD} ,$$

where C is a real constant proportional to the number of atoms per volume. Determine and draw the real and imaginary parts of $\mathcal{E}$ as a function of ω.

Interpretation : The dielectric constant is related to the *refractive index* n and the *absorption coefficient* κ through $\mathcal{E} = (n + i\kappa)^2$. In the case of an incoming electric field of the form of a plane wave $E_z = E_0 e^{i(kx-\omega t)}$, inside the medium we obtain $E_z = E_0 e^{-\kappa k x} e^{i(nkx-\omega t)}$; i.e. n determines the dispersion and κ the absorption.

Travaux Dirigés Quantum Mechanics

Sheet 12 : *Scattering*

I. Scattering off a hard sphere

Consider the scattering of an incoming wave e^{ikz} off a hard sphere of radius a, i.e. a spherically symmetric potential of the form

$$V(r) = \begin{cases} \infty \ , & r \leq a \\ 0 \ , & r > a \end{cases} \quad .$$

I.A Take into account the symmetries of the system to justify the following ansatz for the wavefunction :

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos\theta) \ .$$

Determine the differential equation obeyed by the radial part $R_l(r)$. Solve for $R_l(r)$ by taking into account the boundary condition at $r = a$ and the asymptotic form of the wavefunction :

$$\psi(\mathbf{r}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(k,\theta)\frac{e^{ikr}}{r} \ .$$

I.B Determine $\sin^2\delta_l$, where δ_l is defined through :

$$f(k,\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) \ .$$

Compute the total cross section σ_{tot}.

I.C Argue that for $ka << 1$ the $l = 0$ term in the partial wave sum dominates the total cross section ; this is the case of the so-called *s-wave scattering*. Compute σ_{tot} in this limit and compare with the classical cross section.

I.D Consider now the opposite limit $ka >> 1$. In this case one may ignore the terms $l > l_0$, where $l_0 \sim ka$. Compute σ_{tot} in this limit and compare with the classical cross section.

II. Scattering off a spherical well

Consider now an attractive spherically symmetric potential well

$$V(r) = \begin{cases} -V_0 \ , & r \leq a \\ 0 \ , & r > a \end{cases} \quad ,$$

where $V_0 > 0$.

II.A We shall consider the case of s-wave scattering, $ka << 1$, so that the partial waves with $l \geq 1$ may be ignored. Making the same ansatz for the wavefunction as in the previous exercise, determine the wavefunction by taking into account the boundary condition at $r = 0$ and the $r \to \infty$ asymptotics, and imposing continuity for the wavefunction and its first derivative at $r = a$. Determine $\tan \delta_0$.

II.B Assume in addition that

$$\frac{k}{q} \tan(qa) << 1 \ ,$$

where $q^2 := 2m(E + V_0)/\hbar^2$. Use the previous result for $\tan \delta_0$ to compute σ_{tot} in this limit. Under what condition do we have $\sigma_{tot} = 0$?

The vanishing of the total cross section for certain values of the energy of the incoming wave (observed in particular in the scattering of low-energy electrons by atoms of a noble gas) goes under the name *Ramsauer-Townsend effect* and has no classical analogue.

III. Born approximation

Determine the differential cross section $d\sigma/d\Omega$ in the Born approximation for the Yukawa potential $V(\mathbf{r}) = V_0 e^{-\alpha r}/r$. In which limit is the Rutherford formula (for scattering off a Coulomb potential) recovered? Compute the total cross section σ_{tot}.

Useful formulæ : The spherical Bessel and Neumann functions $j_l(\rho)$, $n_l(\rho)$ are linearly independent solutions of the differential equation

$$f_l''(\rho) + \frac{2}{\rho} f_l'(\rho) + f_l(\rho) - \frac{l(l+1)}{\rho^2} f_l(\rho) = 0 \ ,$$

where a prime denotes differentiation with respect to ρ. Their asymptotics are given by :

$$j_l(\rho) = \begin{cases} \rho^l/(2l+1)!! & , \quad \rho \to 0 \\ \frac{\sin(\rho - l\pi/2)}{\rho} & , \quad \rho \to \infty \end{cases}$$

$$n_l(\rho) = \begin{cases} -(2l+1)!!/[(2l+1)\rho^{l+1}] & , \quad \rho \to 0 \\ -\frac{\cos(\rho - l\pi/2)}{\rho} & , \quad \rho \to \infty \end{cases} ,$$

where $(2l+1)!! = 1 \cdot 3 \cdots (2l+1)$. For $l = 0$ we have :

$$j_0(\rho) = \frac{\sin \rho}{\rho} \quad , \qquad n_0(\rho) = -\frac{\cos \rho}{\rho} \ .$$

The spherical Hankel functions of the first and second kind are the linear combinations

$$h_l^{(1)}(\rho) := j_l(\rho) + i n_l(\rho) \quad , \qquad h_l^{(2)}(\rho) := j_l(\rho) - i n_l(\rho) \ ,$$

with asymptotics :

$$h_l^{(1)}(\rho) \underset{\rho \to \infty}{\longrightarrow} (-i)^{l+1} \frac{e^{i\rho}}{\rho} \quad , \qquad h_l^{(2)}(\rho) \underset{\rho \to \infty}{\longrightarrow} i^{l+1} \frac{e^{-i\rho}}{\rho} \ .$$

We also have :

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos\theta) j_l(kr) \ .$$