QUANTUM MECHANICS I (Dr. T. Brandes): COURSEWORKS 2001

The lecture homepage is **http://bursill.phy.umist.ac.uk/QM/**

Project 1: Production of an Internet web–page 'QUANTUM MECHANICS FROM 1900 UNTIL 1925'

Form a project team of up to four people. The aim of this project is the production of an Internet web–page that illustrates the main concepts, experiments and theories of the so–called 'old quantum theory'. Your task is to produce a web–page (alternatively: a report produced with some text–processing system) which a second–year physics student can understand. In case of a successful completion of this project, your work (including your names as authors) will be published on UMIST physics Internet sites so that it can be used by other students and people interested in that topic.

Project 2: Production of an Internet web–page 'THE PROPAGATOR'

Form a project team of up to four people. The aim of this project is the production of an Internet web–page that illustrates the concept of the 'propagator', sometimes also called Green's function. Your task is to produce a web–page (alternatively: a report produced with some text–processing system) which a second–year physics student can understand after the first half of the quantum mechanics 1 lecture. In case of a successful completion of this project, your work (including your names as authors) will be published on UMIST physics Internet sites so that it can be used by students attending this course in the future (and other people interested in Quantum Mechanics).

The propagator is an important concept in theoretical physics that appears when time–dependent problems have to be solved. An example is the Feynman propagator in relativistic quantum mechanics, that basically describes the time evolution of wave functions for elementary particles.

In this project, we discuss only the case of the (non–relativistic) Schrödinger equation to describe, for example, non–relativistic electrons in 'mesoscopic systems', solid crystals etc. In the first two parts, we concentrate on the case of the motion of a particle in free space (zero potential).

Part 1: Show that for a free particle of mass m in three dimensions, the solution of the Schrödinger equation at time $t > 0$ can be written as

$$\Psi(\mathbf{x}, t) = \int d^3x G_0(\mathbf{x}, \mathbf{x}'; t)\Psi(\mathbf{x}', t = 0). \quad (1.1)$$

You should explain and illustrate how to calculate the propagator $G_0(\mathbf{x}, \mathbf{x}'; t)$ by Fourier transformation explicitly.

Part 2: Integrate the example (1.4.6) of the time evolution of a wave packet from the example sheet 1 into your presentation. Work out the detailed solution of this

problem using the 'propagator' concept. Of course, you may use text books to check that your results are correct.
Part 3: This last part is voluntary work, but you are strongly encouraged to work on it, too.

Consider the motion of a particle of mass m in the infinite potential well $[0, L]$. Show that the time–evolution of the wave function can be written using the propagator $G(x, x'; t)$ as

$$\begin{aligned}\Psi(x, t > 0) &= \int_0^L dx' G(x, x'; t)\Psi(x', t = 0)\\ G(x, x'; t > 0) &= \frac{2}{L}\sum_{n=1}^{\infty} \sin(n\pi x/L)\sin(n\pi x'/L)e^{-i(\pi n/L)^2 t}. \end{aligned} \tag{1.2}$$

Here, we set $\hbar = 2m = 1$ for convenience.

These three parts form a sort of frame–work, but you are free to add things: you should work as a 'scientific author'. It is only important that the final form of your web–page (or your report) is coherent and consistent; it should reflect your own work and your own way of presenting things. You are allowed to use any additional material you like.

Project 3: Production of an Internet web–page or a report on a free topic related to the course QUANTUM MECHANICS 1

As in project 1 and 2 (maximum team of four people), but with a topic of your own choice.

Project 4: Oral presentation (15 Minutes) of a free topic related to the course QUANTUM MECHANICS 1

Please discuss with me in advance if your choice is this project. Each presentation is by one person; a maximum of four slots for these projects is available.

1.1 Problem No. 1

1.1.1 Wien and Stefan–Boltzmann

Show that from Wien's law (scaling law), the Stefan–Boltzmann law follows, that is

$$u(\nu, T) = \nu^3 f(\nu/T) \rightsquigarrow U(T) := \int_0^{\infty} d\nu u(\nu, T) = \sigma T^4, \quad \sigma = const. \tag{1.3}$$

1.1.2 Microscopic Object

Calculate the de Broglie wave length of a thermal neutron with energy $E \approx k_B T$ at $T = 300$K. Compare it to typical atom distances in crystals.

1.1.3 Commutator

Prove the commutator relation for a differentiable function $F(x)$ in one dimension, $[p, F(x)] = \frac{\hbar}{i}\frac{d}{dx}F(x)$.

1.2 Problem No. 2

1.2.1 Transfer matrix of a Delta barrier

We consider the stationary Schrödinger equation for a particle of mass m in a one–dimensional delta–function potential

$$V(x) = V_0\delta(x - x_1), V_0 > 0.$$

Here, we set $x_1 = 0$ and $\hbar = 2m = 1$.

1. Write down the stationary Schrödinger equation for energy $E > 0$

2. Integrate the Schrödinger equation over x from $x_1 - \epsilon$ until $x_1 + \epsilon$ and derive a condition for the discontinuity (the jump) of the wave function derivative $\psi'(x)$ from the right to the left of the barrier.

3. From 2. and the continuity of the wave function itself at $x = x_1$ you obtain two equations for the coefficients a_i and b_i in

$$\Psi(x) = \begin{cases} a_1 e^{ik_1 x} + b_1 e^{-ik_1 x}, & -\infty < x \le x_1 \\ a_2 e^{ik_2 x} + b_2 e^{-ik_2 x}, & x_1 < x < \infty \end{cases} \tag{1.4}$$

In our case, $k_1 = k_2 = k = \sqrt{E}$ (why?). Express a_1 and b_1 as a function of a_2 und b_2. Write this in matrix form, that is

$$\mathbf{u}_1 = T^1\mathbf{u}_2, \quad \mathbf{u}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}, \quad i = 1, 2. \tag{1.5}$$

4. Calculate (as a function of energy E) the transmission and relection coefficient of a particle that comes from the left.

1.2.2 Fabry–Perot Formula

We investigate resonant tunneling of electrons through a 'Fabry-Perot resonator'. This is motivated by an experiment of T. Heinzel et al., *Europhysics Letters* **26**, 689 (1994).

1. Calculate the generalization of T^1 from above for arbitrary x_1: show that

$$T^1 = \frac{1}{2k}\begin{pmatrix} 2k + iV_0 & iV_0 e^{-2ikx_1} \\ -iV_0 e^{2ikx_1} & 2k - iV_0 \end{pmatrix}. \tag{1.6}$$

2. Express T^1 by the transmission amplitude $t_1 := 2k/(2k + iV_0)$ and the terms $e^{\pm 2ikx_1}$.

3. Now consider two Delta–function barriers

$$V(x) = V_0\delta(x - x_1) + V_1\delta(x - x_2).$$

Calculate (by matrix multiplication) the transfer matrix $M = T^1T^2$ of the whole system, where T^1 and T^2 are expressed (as in 2.) by the transmission amplitudes t_1, t_2, and the exponentials. Show that

$$\frac{1}{M_{11}} = \frac{t_1t_2}{1 - (1 - t_1)(1 - t_2)e^{2ik(x_2 - x_1)}}.$$

4. Discuss the total transmission coefficient $T_{tot} = |1/M_{11}|^2$.

1.3 Problem No. 3

1.3.1 Orthonormality

Consider the Hilbert space $\mathcal{H}$ of wave functions $\psi(x)$ of the infinite potential well on the interval $[0, L]$ with $\psi(0) = \psi(L) = 0$. Show that the basis vectors

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

form an orthonormal system.

1.3.2 Expansion into eigenmodes

Consider the vector $f \in \mathcal{H}$, $f(x) = cx(L - x)$.
a) Calculate the constant c such that f is normalized, i.e. $\|f\| = 1$. Show that $c = \sqrt{30/L}/L^2$.
b) Show that f can be expanded in the basis ψ_n as

$$f = \sum_{n=1}^{\infty} c_n\psi_n, \quad c_n = 2\sqrt{60}\frac{1 - (-1)^n}{n^3\pi^3} \tag{1.7}$$

c) Use b) to prove the formula

$$\frac{\pi^3}{32} = \sum_{k=0}^{\infty}\frac{(-1)^k}{(2k + 1)^3}.$$

1.3.3 Scalar Product

a) Use the bra and ket notation to show that for an orthonormal basis $\{|\psi_n\rangle\}$ and two Hilbert space vectors $|\psi\rangle$ and $|\chi\rangle$, one has

$$\langle\psi|\chi\rangle = \sum_{n=0}^{\infty}\langle\psi|\psi_n\rangle\langle\psi_n|\chi\rangle. \tag{1.8}$$

b) Show that in the case of vectors $\mathbf{x}$, $\mathbf{y} \in R^d$, this reduces to the standard formula for the scalar product in R^d,

$$\langle \mathbf{x}|\mathbf{y}\rangle = \sum_{i=1}^{d} x_i^* y_i.$$

c) (Extra, voluntary problem) Use Eq.(1.8) and Eq.(1.7) to prove

$$\frac{\pi^6}{960} = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^6}$$

1.4 Problem No. 4

1.4.1 Model

We consider the Hamiltonian of the two–level system,

$$\hat{H} = \left(\begin{array}{cc} \varepsilon_L & T \\ T* & \varepsilon_R \end{array} \right), \tag{1.9}$$

see Fig. 1.1.

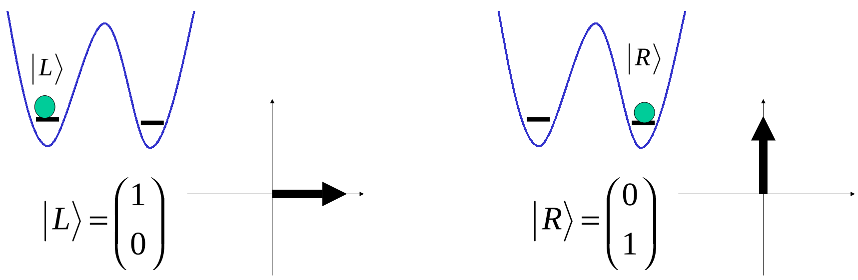

Fig. 1.1: Vector representation of left and right lowest states of double well potential.

a) and b) Calculate the two eigenvectors $|i\rangle$ and eigenvalues ε_i of $\hat{H}$, eq. (1.9), that is the solutions of

$$\hat{H}|i\rangle = \varepsilon_i|i\rangle, \quad i = 1, 2. \tag{1.10}$$

Show that

$$\begin{aligned}
|1\rangle &= \frac{1}{N_1}\left[-2T|L\rangle + (\Delta+\varepsilon)|R\rangle\right], \quad \varepsilon_1 = \frac{1}{2}(\varepsilon_L + \varepsilon_R - \Delta) \\
|2\rangle &= \frac{1}{N_2}\left[\ \ 2T|L\rangle + (\Delta-\varepsilon)|R\rangle\right], \quad \varepsilon_2 = \frac{1}{2}(\varepsilon_L + \varepsilon_R + \Delta) \\
\varepsilon &:= \varepsilon_L - \varepsilon_R, \quad \Delta := \varepsilon_2 - \varepsilon_1 = \sqrt{\varepsilon^2 + 4|T|^2} \\
N_{1,2} &:= \sqrt{4|T|^2 + (\Delta \pm \varepsilon)^2}.
\end{aligned} \tag{1.11}$$

1.4.2 Absorption Experiment

In an experiment, microwaves are irradiated upon a double quantum well. An absorption peak is observed when electrons absorb a photon $h\nu$ that matches the energy difference between the lowest state 1 and the first excited state 2 of the system. Plot the absorption peak photon energy as a function of the tunnel coupling T between both wells, when the energies in both wells are kept fixed.