Quantum Mechanics I, Correction Sheet 9, Spring 2013

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I. HEISENBERG PICTURE

In Schrödinger picture, the operators are in general time-independent, as for example the position and momentum operators. The time-evolution of the system is completely captured by the quantum state $|\psi(t)\rangle$ which obeys the Schrödinger equation. However all physical predictions of quantum mechanics are given in terms of brackets, which are invariant by performing a unitary transformation on operators and states simultaneously. The idea of Heisenberg picture is to choose this unitary transformation such that the transformation of the state $|\psi(t)\rangle$ becomes time-independent; of course the transformed operators will then become time-dependent. Explicitly a general bracket can be rewritten as

$$\langle\phi(t)|\hat{A}|\psi(t)\rangle = \langle\hat{U}(t)\phi(0)|\hat{A}|\hat{U}(t)\psi(0)\rangle = \langle\phi(0)|\hat{U}(t)^\dagger\hat{A}\hat{U}(t)|\psi(0)\rangle = \langle\phi_H|\hat{A}_H(t)|\psi_H\rangle\,,$$

where $\hat{U}(t)$ is the evolution operator, $|\psi_H\rangle = |\psi(0)\rangle$ and $|\phi_H\rangle = |\phi(0)\rangle$ are the states in Schrödinger picture and $\hat{A}_H$ is the operator A in Heisenberg picture,

$$\hat{A}_H(t) = \hat{U}(t)^\dagger\hat{A}\hat{U}(t)\,.$$

Therefore in Heisenberg picture we obtained that states are time-independent and operators becomes time-dependent.

1. Show that the time-evolution of an operator in Heisenberg picture is given by

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_H(t) = \left[\hat{A}_H(t), \hat{H}_H(t)\right],$$

where $\hat{H}_H(t)$ is the Hamiltonian operator in Heisenberg picture.

By using the equation describing the evolution operator, and its adjoint,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = \hat{H}\hat{U}(t)\,, \qquad \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)^\dagger = -\hat{U}(t)^\dagger\hat{H}\,,$$

we find the time-evolution of an operator in Heisenberg picture,

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_H(t) &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{U}(t)^\dagger\hat{A}\hat{U}(t)\right) = \hat{U}(t)^\dagger\hat{A}\left(\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)\right) - \left(\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)^\dagger\right)\hat{A}\hat{U}(t)\\ &= \hat{U}(t)^\dagger\hat{A}\hat{H}\hat{U}(t) - \hat{U}(t)^\dagger\hat{H}\hat{A}\hat{U}(t)\\ &= \hat{U}(t)^\dagger\hat{A}\hat{U}(t)\hat{U}(t)^\dagger\hat{H}\hat{U}(t) - \hat{U}(t)^\dagger\hat{H}\hat{U}(t)\hat{U}(t)^\dagger\hat{A}\hat{U}(t)\\ &= \hat{A}_H\hat{H}_H - \hat{H}_H\hat{A}_H = \left[\hat{A}_H(t), \hat{H}_H(t)\right],\end{aligned}$$

where $\hat{H}_H(t) = \hat{U}(t)^\dagger\hat{H}\hat{U}(t)$ is the Hamiltonian operator in Heisenberg picture.

2. In one dimension, consider the Hamiltonian of a particle in a potential

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{X})\,.$$

Determine the Hamiltonian in Heisenberg picture $\hat{H}_H$ in terms of the position $\hat{X}_H$ and momentum $\hat{P}_H$ operators in Heisenberg picture. Check that the commutation relations are still valid for the operators in Heisenberg picture. Write the evolution equations for the position $\hat{X}_H$ and momentum $\hat{P}_H$ operators in Heisenberg picture. Compare your result to classical mechanics.

By inserting many times $\hat{U}(t)\hat{U}(t)^\dagger = \hat{I}$, we find

$$\begin{aligned}\hat{H}_H &= \frac{1}{2m}\hat{U}(t)^\dagger\hat{P}^2\hat{U}(t) + \hat{U}(t)^\dagger V(\hat{X})\hat{U}(t)\\ &= \frac{1}{2m}\hat{U}(t)^\dagger\hat{P}\hat{U}(t)\hat{U}(t)^\dagger\hat{P}\hat{U}(t) + \sum_{n=0} f_n\hat{U}(t)^\dagger\hat{X}^n\hat{U}(t)\\ &= \frac{\hat{P}_H^2}{2m} + \sum_{n=0} f_n\left(\hat{U}(t)^\dagger\hat{X}\hat{U}(t)\right)^n = \frac{\hat{P}_H^2}{2m} + \sum_{n=0} f_n\hat{X}_H^n = \frac{\hat{P}_H^2}{2m} + V(\hat{X}_H)\,.\end{aligned}$$

For any operators in Heisenberg picture, we have

$$\begin{aligned}\left[\hat{A}_H, \hat{B}_H\right] &= \hat{A}_H\hat{B}_H - \hat{B}_H\hat{A}_H = \hat{U}(t)^\dagger\hat{A}\hat{U}(t)\hat{U}(t)^\dagger\hat{B}\hat{U}(t) - \hat{U}(t)^\dagger\hat{B}\hat{U}(t)\hat{U}(t)^\dagger\hat{A}\hat{U}(t)\\ &= \hat{U}(t)^\dagger\hat{A}\hat{B}\hat{U}(t) - \hat{U}(t)^\dagger\hat{B}\hat{A}\hat{U}(t) = \hat{U}(t)^\dagger\left[\hat{A}, \hat{B}\right]\hat{U}(t) = \left[\hat{A}, \hat{B}\right]_H\,,\end{aligned}$$

and therefore the commutations relations between Heisenberg picture remains unchanged,

$$\left[\hat{X}_H, \hat{P}_H\right] = \mathrm{i}\hbar\hat{U}(t)^\dagger\hat{U}(t) = \mathrm{i}\hbar\,.$$

By using exercise 1 of sheet 7, the equations of motion are given by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{X}_H &= \left[\hat{X}_H, \hat{H}_H\right] = \frac{1}{2m}\left[\hat{X}_H, \hat{P}_H^2\right] = \frac{\hat{P}_H}{m}\,,\\ \frac{\mathrm{d}}{\mathrm{d}t}\hat{P}_H &= \left[\hat{P}_H, \hat{H}_H\right] = \left[\hat{P}_H, V(\hat{X}_H)\right] = -V'(\hat{X}_H)\,,\end{aligned}$$

which makes an analogy with Hamilton's equations of a particle in a potential.

II. ANGULAR MOMENTUM

Carbon monooxide CO is the second (after hydrogen) most abundant molecule present in the interstellar gas. This molecule is very useful for astrophysics because its rotational spectrum is rather intense and can be observed in the radio-frequency range.
To first approximation, a diatomic molecule of CO can be described as a rigid quantum rotor consisting of two point masses m_O, m_C connected with a massless rod (its length can be taken to be equal $r_b = 1.128 \times 10^{-8}$ cm). The rotation dynamics is given by a Hamiltonian

$$\hat{H}_R = \frac{\hat{J}^2 - \hat{J}_z^2}{2I},$$

where I is the molecule's moment of inertia, and $\hat{J}$ is the angular momentum.

1. Find the energies of transitions from state $|J\rangle$ to state $|J-1\rangle$.

   Since the states $|J\rangle$ are eigenstates of the Hamiltonian the corresponding energies are easily found to be

   $$E_J = \frac{1}{2I}\left[J(J+1) - M_J^2\right],$$

   where M_J is the z-component of the angular momentum.

   At first glance, the transition energies $\Delta E_J \equiv E_J - E_{J-1}$ depend on the value of M_J. However, for a diatomic molecule, such as CO, the energy separation between states with $\Delta M_J = \pm 1$ is proportional to $1/I_z$, which is a huge number and one can thus consider only transitions with $\Delta M_J = 0$ (see also explanation on p. 217 of the text book). For the latter, we have

   $$\Delta E_J \equiv E_J - E_{J-1} = \frac{\hbar^2}{I} J$$

2. Consider two sorts of molecules $^{12}C^{16}O$, $^{13}C^{16}O$ and evaluate the transition frequency $\nu_{1\to 0}$ (between states $J=1$ and $J=0$) for both of them. The following constant values can be used: proton mass $m_p = 1.67 \times 10^{-24}$g, Planck constant $\hbar = 1.055 \times 10^{-27}\,\mathrm{erg}\cdot\mathrm{s}$.

   [*Hint:* Be careful with 2π factors; note that the spectral transition frequency is defined as $\nu = \Delta E/h \equiv \Delta E/(2\pi\hbar)$.]

   Recalling the definition of the moment of inertia for a collection of point masses

   $$I = \sum_i m_i r_i^2,$$

   where r_i is the position relative to the center of mass (r_c), one finds for $I_x = I_y$ of the CO molecule

   $$I_{\mathrm{CO}} \equiv I_x = m_C r_c^2 + m_O (r_b - r_c)^2,$$

   with the position of the center of mass given by the equation

   $$(m_C + m_O) r_c = m_O r_b.$$

   Having found r_c we finally get

   $$I_{\mathrm{CO}} = \frac{m_C m_O}{m_C + m_O} r_b^2$$

   The transition frequency $\nu_{J\to J-1}$ is given by

   $$\nu_{J\to J-1} = \frac{\Delta E_J}{h} = \frac{\hbar}{2\pi I} J.$$

   Finally, the frequencies $\nu_{1\to 0}$ for the two sorts of molecules are obtained as

   $$^{12}C^{16}O : \nu_{1\to 0} \approx 115.238 \text{ GHz},$$
   $$^{13}C^{16}O : \nu_{1\to 0} \approx 110.172 \text{ GHz}.$$

   These values are to be compared to the ones observed by radiotelescopes (source: www.splatalogue.net): $\nu_{1\to 0}(^{12}C^{16}O) = 115.27120$ GHz, $\nu_{1\to 0}(^{12}C^{16}O) = 110.20135$ GHz.

III. ROTATION OF SPIN-1/2 PARTICLES

Neutrons are prepared at $t = 0$ in the state given by the superposition of the eigenvectors of the spin operator $\hat{S}_z$. Then there are injected in the experimental setup described on Figure 1 (Werner et al. Phys. Rev. Lett. 35, 1053 (1975)). We suppose that the lower beam remains a time T between $t = 0$ and $t = T$ in the uniform magnetic field B_z. At point D, we measure the mean value of μ_z. What are the results in function of time T?

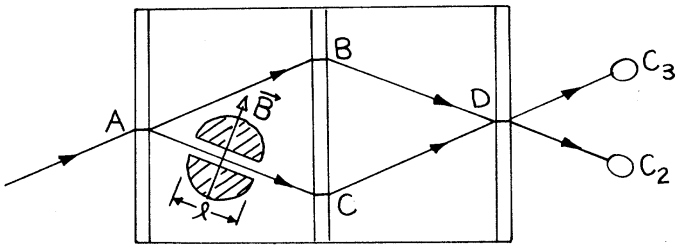

FIG. 1. A schematic diagram of the neutron interferometer. On the path AC the neutrons are in a magnetic field B (0 to 500 G) for a distance l (2 cm).

The initial state of neutrons right after the beam splitter can be defined by a spinor

$$\Psi(t=0) = \begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix},$$

where the z-axis is the quantization axis.
The upper beam propagates freely and its spin state remains intact, while the lower beam interacts with the magnetic field during the period of time T. The interaction term for the field B_z poiting along z-axis is $-g\mu_B(\hat{\sigma}_z/2)B_z \approx -\mu_B\hat{\sigma}_z B_z$, and the evolution of the spin components is described by

$$\begin{aligned} i\hbar\frac{d\alpha(t)}{dt} &= -\mu_B B_z \alpha(t), \\ i\hbar\frac{d\beta(t)}{dt} &= \mu_B B_z \beta(t), \end{aligned}$$

which are solve to give

$$\begin{aligned} \alpha(t) &= \alpha_0 \exp(i\omega_0 t), \\ \beta(t) &= \beta_0 \exp(-i\omega_0 t), \end{aligned}$$

with $\omega_0 = -\mu_B B_z/\hbar$ (this is half the Larmor frequency $\omega_L = egB_z/(2m)$).
Being exposed to the magnetic field for the period of time T, the lower beam will experience the phase shift different for each spin component, $\exp(\pm i\omega_0 T)$. At point D the beams interfere and their combined wave function is then

$$\Psi_D(t) \propto \begin{pmatrix} \alpha_0[1+\exp(i\omega_0 T)] \\ \beta_0[1+\exp(-i\omega_0 T)] \end{pmatrix}.$$

For the mean value of μ_z we then get

$$\begin{aligned} \mu_z &\propto |\alpha_0(1+e^{i\omega_0 T})|^2 - |\beta_0(1+e^{-i\omega_0 T})|^2 \\ &= 2(|\alpha|^2 - |\beta|^2)(1+\cos\omega_0 T). \end{aligned}$$

One concludes that as a function of T the value of μ_z will oscillate proportional to $[1+\cos(\mu_B B_z T/\hbar)]$.

IV. (*) REVISION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

A. δ-function potential

Consider a one-dimensional δ-function potential $V(x) = -g\delta(x)$. There is only one bound state ($E < 0$) in this potential. Find the energy and the wave function corresponding to this bound state.

[*Hint:* Start off with splitting the space into three ranges $(-\infty, a)$, $[-a, a]$, (a, ∞), where a is a small number, which will eventually be put to zero.]

Outside the small region $[-a, a]$ the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi,$$

and has a general solution

$$\Psi(x) = C_1 e^{\kappa x} + C_2 e^{-\kappa x}, \quad \kappa = \sqrt{-\frac{2mE}{\hbar^2}}.$$

The solution must be continuous at zero as $a \to 0$; matching the solutions in the left and right regions, one can write the wave function in the form

$$\Psi(x) = Ce^{-|\kappa|x},$$

where the normalizing constant C is easily found to be $C = \sqrt{\kappa}$.

To find the energy of this bound state, let us integrate the Schrödinger equation over the region $[-a, a]$,

$$\begin{aligned}\int_{-a}^{a} dx \left[-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} - g\delta(x)\right] &= E\int_{-a}^{a}\Psi(x)dx,\\ \int_{-a}^{a} dx \left[-\frac{d^2\Psi}{dx^2} - \frac{2mg}{\hbar^2}\delta(x)\right] &= \frac{2mE}{\hbar^2}\int_{-a}^{a}\Psi(x)dx.\end{aligned}$$

Since $\Psi(x)$ is a bounded function its integral vanishes as $a \to 0$. We, thus, get in this limit

$$\begin{aligned}-\left.\frac{d\Psi}{dx}\right|_{0^-}^{0^+} &= \frac{2mg}{\hbar^2}\Psi(0),\\ 2\kappa\sqrt{\kappa} &= \frac{2mg}{\hbar^2}\sqrt{\kappa},\\ \kappa &= \frac{mg}{\hbar^2},\end{aligned}$$

from which we find

$$E = -\frac{mg^2}{2\hbar^2}.$$

B. Double δ-function potential

A double δ-function potential is defined as $V(x) = -g[\delta(x-d) + \delta(x+d)]$. The one-dimensional Schrödinger equation for a particle in this potential has two distinct solutions.

1. Using symmetry arguments prove that the two eigen wave functions correspond to the same eigenenergy.

2. Construct boundary conditions for the two wave functions and show explicitly that they result in equivalent equations for the eigenenergy.

3. Evaluate the normalization constants for the wave functions.

Unfortunately, the problem statement here is wrong... :(

C. Limit of an extremely narrow square-well potential

Start out with a square-well potential,

$$V(x) = \begin{cases} -V_0, & |x| \le a, \\ 0, & \text{otherwise}, \end{cases}$$

and show that in the limit $a \to 0$, only one bound state is left, and its energy is the same as for the δ-function potential with $g = V_0 a$. Keep in mind that to perform a well-defined limiting procedure, one has to keep the product $V_0 a$ (potential strength) constant.
Errata: the potential strength is $g = 2V_0 a$, i.e. it is a product of the well depth and width.
We start with a Hamiltonian for a square-well potential,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\Psi(x) = E\Psi(x), \quad \text{with}$$

$$V(x) = \begin{cases} -V_0, & |x| < a, \\ 0, & |x| > a. \end{cases}$$

Introducing as usual

$$\kappa = \sqrt{-\frac{2mE}{\hbar^2}}, \qquad k = \sqrt{-\frac{2m(E+V_0)}{\hbar^2}},$$

we obtain the solutions in the three regions $(-\infty, -a)$, $[-a, a]$, (a, ∞), respectively,

$$\begin{aligned} \Psi_1(x) &= A_1 e^{\kappa(x+a)}, \\ \Psi_2(x) &= A_2 e^{ikx} + B_2 e^{-ikx}, \\ \Psi_3(x) &= A_3 e^{-\kappa(x-a)}. \end{aligned}$$

From a general solution of this problem (see pp. 86-87 of the textbook) we expect that as the width of the well is decreased down to a certain point, only the lowest bound state corresponding to an even solution survives. This allows us to write, $\Psi_2(x) = 2A_2 \cos kx$.
Designating $C \equiv A_2$, the continuity conidtion is written as

$$A_1 = A_3 = 2C \cos ka.$$

The continuity of the first derivative gives

$$\begin{aligned} \kappa A_1 &= 2kC \sin ka, \\ -\kappa A_3 &= -2kC \sin ka, \end{aligned}$$

from which we get the equation for the energy of the (even) bound state

$$\tan ka = \frac{\kappa}{k}.$$

Taking into account that $V_0 = g/2a \to \infty$ as $a \to 0$, we see that $\kappa/k \to 0$. We, thus, can expand the tangent around zero to get

$$\begin{aligned}\frac{\kappa}{k} \approx& ka,\\ \kappa \approx& k^2 a.\end{aligned}$$

Neglecting terms linear in a, one can exactly solve this equation:

$$\begin{aligned}\sqrt{-\frac{2mE}{\hbar^2}} =& -\frac{2m}{\hbar^2}(Ea + V_0 a),\\ -\frac{2mE}{\hbar^2} =& \left(\frac{2m}{\hbar^2}\right)^2 \frac{g^2}{4},\\ E =& -\frac{mg^2}{2\hbar^2},\end{aligned}$$

that is the same value as we got in problem IV A.