



# Quantum Mechanics

## Homework Assignment 15

### Fall, 2019

1. **[C-T Exercise 13-1]** Consider a one-dimensional harmonic oscillator of mass  $m$ , angular frequency  $\omega_0$  and charge  $q$ . Let  $|\varphi_n\rangle$  and  $E_n = (n + 1/2)\hbar\omega_0$  be the eigenstates and eigenvalues of its Hamiltonian  $\hat{H}_0$ . For  $t < 0$ , the oscillator is in the ground state  $|\varphi_0\rangle$ . At  $t = 0$ , it is subjected to an electric field “pulse” of duration  $\tau$ . The corresponding perturbation can be written  $\hat{W}(t) = \begin{cases} -q\mathcal{E}\hat{x}, & 0 \leq t \leq \tau, \\ 0, & t < 0, t > \tau. \end{cases}$  Here  $\mathcal{E}$  is the field amplitude and  $\hat{x}$  is the position observable. Let  $\mathcal{P}_{0n}$  be the probability of finding the oscillator in the state  $|\varphi_n\rangle$  after the pulse.
  - (a) Calculate  $\mathcal{P}_{01}$  by using first-order time-dependent perturbation theory. How does  $\mathcal{P}_{01}$  vary with  $\tau$ , for fixed  $\omega_0$ ?
  - (b) Show that, to obtain  $\mathcal{P}_{02}$ , the time-dependent perturbation theory calculation must be pursued at least to second order. Calculate  $\mathcal{P}_{02}$  to this perturbation order.
2. **[C-T Exercise 13-2]** Consider two spin  $1/2$ 's,  $\hat{S}_1$  and  $\hat{S}_2$ , coupled by an interaction of the form  $a(t)\hat{S}_1 \cdot \hat{S}_2$ ;  $a(t)$  is a function of time which approaches zero when  $|t|$  approaches infinity, and takes on non-negligible values (on the order of  $a_0$ ) only inside an interval, whose width is of the order of  $\tau$ , about  $t = 0$ .
  - (a) At  $t = -\infty$ , the system is in the state  $|+-\rangle$  (an eigenstate of  $\hat{S}_1$  and  $\hat{S}_2$  with the eigenvalues  $+\hbar/2$  and  $-\hbar/2$ ). Calculate, without approximations, the state of the system at  $t = +\infty$ . Show that the probability  $\mathcal{P}(+- \rightarrow -+)$  of finding, at  $t = +\infty$ , the system in the state  $| - + \rangle$  depends only on the integral  $\int_{-\infty}^{+\infty} dt a(t)$ .
  - (b) Calculate  $\mathcal{P}(+- \rightarrow -+)$  by using first-order time-dependent perturbation theory. Discuss the validity conditions for such an approximation by comparing the results obtained with those of the preceding question.
  - (c) Now assume that the two spins are also interacting with a static magnetic field  $\vec{B}_0$  parallel to  $Oz$ . The corresponding Zeeman Hamiltonian can be written  $\hat{H}_0 = -B_0(\gamma_1\hat{S}_{1z} + \gamma_2\hat{S}_{2z})$ , where  $\gamma_1$  and  $\gamma_2$  are the gyromagnetic ratios of the two spins, assumed to be different. Assume that  $a(t) = a_0 e^{-t^2/\tau^2}$ . Calculate  $\mathcal{P}(+- \rightarrow -+)$  by first-order time-dependent perturbation theory. With fixed  $a_0$  and  $\tau$ , discuss the variation of  $\mathcal{P}(+- \rightarrow -+)$  with respect to  $B_0$ .
3. A particle of mass  $\mu$  is scattered by the central field  $V(r) = \frac{\alpha}{r^2}$  with  $\alpha > 0$ . Find the differential and total scattering cross sections under the first-order Born approximation.
4. **[C-T Complement C<sub>VIII</sub>-3 Exercise b]** Consider a central potential  $V(r)$  such that  $V(r) = \begin{cases} -V_0, & r < r_0, \\ 0, & r > r_0. \end{cases}$  Here  $V_0$  is a positive constant. Set  $k_0 = \sqrt{2\mu V_0/\hbar^2}$  with  $\mu$  the mass of the particle subject to the potential. We shall confine ourselves to the study of the  $s$  wave ( $\ell = 0$ ).
  - (a) **Bound states ( $E < 0$ )**
    - i. Write the radial equation in the two regions  $r > r_0$  and  $r < r_0$ , as well as the condition at the origin. Show that, if one sets  $\rho = \sqrt{-2\mu E/\hbar^2}$  and  $K = \sqrt{k_0^2 - \rho^2}$ , the function  $u_0(r)$  is necessarily of the form  $u_0(r) = \begin{cases} Ae^{-\rho r}, & r > r_0, \\ B \sin(Kr), & r < r_0. \end{cases}$
    - ii. Write the matching conditions at  $r = R_0$ . Deduce from them that the only possible values for  $\rho$  are those which satisfy the equation  $\tan(Kr_0) = -K/\rho$ .
    - iii. Discuss the equation  $\tan(Kr_0) = -K/\rho$ . Indicate the number of  $s$  bound states as a function of the depth of the well (for fixed  $r_0$ ) and show, in particular, that there are no bound states if this depth is too small.
  - (b) **Scattering resonances ( $E > 0$ )**

- i. Again write the radial equation, this time setting  $k = \sqrt{2\mu E/\hbar}$  and  $K' = \sqrt{k_0^2 + k^2}$ . Show that  $u_{k,0}(r)$  is of the form  $u_{k,0}(r) = \begin{cases} A \sin(kr + \delta_0), & r > r_0, \\ B \sin(K'r), & r < r_0. \end{cases}$
- ii. Choosing  $A = 1$ . Show, using the continuity conditions at  $r = r_0$ , that the constant  $B$  and the phase shift  $\delta_0$  are given by  $B^2 = k^2/[k^2 + k_0^2 \cos^2(K'r_0)]$  and  $\delta_0 = -kr_0 + \alpha(k)$  with  $\tan \alpha(k) = (k/K') \tan(K'r_0)$ .
- iii. Trace the curve representing  $B^2$  as a function of  $k$ . This curve clearly shows resonances, for which  $B^2$  is maximum. What are the values of  $k$  associated with these resonances? What is then the value of  $\alpha(k)$ ? Show that, if there exists such a resonance for a small energy ( $kr_0 \ll 1$ ), the corresponding contribution of the  $s$  wave to the total cross section is practically maximal.

(c) **Relation between bound states and scattering resonances**

Assume that  $k_0 r_0$  is very close to  $(2n+1)\pi/2$ , where  $n$  is an integer, and set  $k_0 r_0 = (2n+1)\pi/2 + \varepsilon$  with  $|\varepsilon| \ll 1$ .

- i. Show that, if  $\varepsilon$  is positive, there exists a bound state whose binding energy  $E = -\hbar^2 \rho^2/2\mu$  is given by  $\rho \simeq \varepsilon k_0$ .
- ii. Show that if, on the other hand,  $\varepsilon$  is negative, there exists a scattering resonance at energy  $E = \hbar^2 k^2/2\mu$  such that  $k^2 \simeq -2k_0 \varepsilon/r_0$ .
- iii. Deduce from this that if the depth of the well is gradually decreased (for fixed  $r_0$ ), the bound state which disappears when  $k_0 r_0$  passes through an odd multiple of  $\pi/2$  gives rise to a low energy scattering resonance.

5. [C-T Exercise 14-3] Consider the state space of an electron, spanned by the two vectors  $|\varphi_{p_x}\rangle$  and  $|\varphi_{p_y}\rangle$  which represent two atomic orbitals,  $p_x$  and  $p_y$ , of wave functions  $\varphi_{p_x}(\vec{r})$  and  $\varphi_{p_y}(\vec{r})$ ,  $\varphi_{p_x}(\vec{r}) = xf(r) = rf(r) \sin \theta \cos \phi$ ,  $\varphi_{p_y}(\vec{r}) = yf(r) = rf(r) \sin \theta \sin \phi$ .

- (a) Write, in terms of  $|\varphi_{p_x}\rangle$  and  $|\varphi_{p_y}\rangle$ , the state  $|\varphi_{p_\alpha}\rangle$  which represents the  $p_\alpha$  orbital pointing in the direction of the  $xOy$  plane which makes an angle  $\alpha$  with  $Ox$ .
- (b) Consider two electrons whose spins are both in the  $|+\rangle$  state, the eigenstate of  $\hat{S}_z$  of eigenvalue  $+\hbar/2$ . Write the normalized state vector  $|\psi\rangle$  which represents the system of two electrons, one of which is in the state  $|\varphi_{p_x}\rangle$  and the other in the state  $|\varphi_{p_y}\rangle$ .
- (c) Same question, with one of the electrons in the state  $|\varphi_{p_\alpha}\rangle$  and the other one in the state  $|\varphi_{p_\beta}\rangle$ , where  $\alpha$  and  $\beta$  are two arbitrary angles. Show that the state vector  $|\psi\rangle$  obtained is the same.
- (d) The system is in the state  $|\psi\rangle$  of question (b). Calculate the probability density  $\mathcal{P}(r, \theta, \phi; r', \theta', \phi')$  of finding one electron at  $(r, \theta, \phi)$  and the other one at  $(r', \theta', \phi')$ . Show that the electronic density  $\rho(r, \theta, \phi)$  [the probability density of finding any electron at  $(r, \theta, \phi)$ ] is symmetrical with respect to revolution about the  $Oz$  axis. Determine the probability density of having  $\phi - \phi' = \phi_0$ , where  $\phi_0$  is given. Discuss the variation of this probability density with respect to  $\phi_0$ .