# Introduction to Quantum Mechanics I

## Exam 2023-2024

#### 3 hours

Please write as neatly as possible. Any unreadable text will be ignored.

This exam is composed of two independent problems. Use separate sets of paper to deal with the two problems.

It is probably not possible to complete both problems in the 3 hours.

The grading will be adjusted accordingly.

Each problem comes with some more general questions and more specific calculations.

The answer to a given question is not always necessary to deal with the following questions, so don't spend too much time with questions you don't know how to answer

- you can probably still do (part) of the following questions

You can write in English or French.

# Problem 1: A one-dimensional circular "wire"

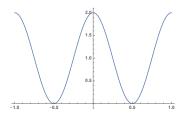
One considers a one-dimensional circular "wire" of circumference  $2\ell$  to which a particle of mass m, called an electron, is confined. We introduce a coordinate  $x \in [-\ell, \ell]$  along this "wire" and the circular geometry imposes periodic boundary conditions, i.e.  $x = -\ell$  and  $x = \ell$  are identical points.

- 1) Briefly describe what should be the appropriate Hilbert space of wave functions  $\psi(x)$  in this setting. What is the appropriate hermitian inner product  $(\psi, \chi)$ ? How the norm of  $\psi$  is defined in terms of this inner product?
- 2) What should be the appropriate domains of definitions of the linear operators X, acting as  $(X\psi)(x) = x\psi(x)$ , and P, acting as  $(P\psi)(x) = -i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}x}(x)$ ? Are they self-adjoint or only symmetric? Motivate your answer by a one-line computation. What about  $X^n$  and  $P^n$  for  $n \geq 2$ ?

The electron carries an electric charge q and we add a static electric field such that the potential energy of the electron due to the electrostatic potential is

$$V(x) = V_0 \left(\cos \frac{2\pi x}{\ell} + 1\right) , {(1.1)}$$

see the figure (where the horizontal axis is  $x/\ell$  and the vertical axis  $V/V_0$ ). We insist that the right edge of the figure is to be identified with the left edge.



We assume that the Hamiltonian operator in this setting is

$$H = \frac{1}{2m}P^2 + V(X) \ . \tag{1.2}$$

- 3) Of which simple situations discussed in the lecture does this remind you? Discuss qualitatively what should be the expectations for the spectrum of the Hamiltonian. There will be a finite number of discrete eigenvalues (which we could call bound states). How do you expect this number to depend on the quantities m,  $V_0$  and  $\ell$ ? More precisely, what should be the dimensionless quantity made from m,  $\ell$ ,  $V_0$  (and  $\hbar$ ) that can control the number of bound states?
- **4)** We begin by restricting our attention to the vicinity of the minimum of the potential at  $x = x_R$  with  $x_R = \frac{\ell}{2}$ . Taylor expand the potential to second order around  $x_R$ . You should get  $V(x) \simeq V_{\text{harm},R}(x)$  with

$$V_{\text{harm,R}}(x) = \frac{m\omega^2}{2}(x - x_R)^2$$
, (1.3)

with some angular frequency  $\omega$  to be determined. What are the corresponding energy levels  $\epsilon_{R,n}$ ,  $n=0,1,2,\ldots$  (i.e eigenvalues of  $P^2/(2m)+V_{\rm harm,R}(x)$ ) in this approximation? (The subscript R refers to the fact that we are only treating the right part of the potential.) Discuss, depending on  $m,\ell$  and  $V_0$  for which values of n this harmonic approximation should be a good approximation. Compare with your result from question 3. The corresponding eigenfunctions in this approximation will be called  $\varphi_{R,n}(x)$ . (In particular, we do not try to make them periodic.)

5) We now assume that  $V_0 = 10 \,\hbar\omega$  and assume the electron is in the "ground state"  $|\varphi_{R,0}\rangle$ , i.e. that its wave function is  $\varphi_{R,0}(x)$ . Using the result from the lecture notes, explicitly give this function  $\varphi_{R,0}(x)$ . Give the formula for computing the probability P to find the electron in the interval  $[-\ell,0]$  ("on the other side" of the potential barrier). Do not attempt to evaluate the integral explicitly but give an order of magnitude estimate for this probability P. How does this compare to the general formula (7.41) for a tunnel probability given in the lecture? Give the formula for computing the expectation value  $\langle X \rangle_{R,0}$  of the position operator in this state  $|\varphi_{R,0}\rangle$  and argue that approximately

$$\langle X \rangle_{R,0} \simeq x_R = \frac{\ell}{2} \ . \tag{1.4}$$

6) We can of course similarly approximate the left part of the potential around its minimum at  $x_L = -\frac{\ell}{2}$  and obtain  $V_{\text{harm},L}(x) = \frac{m\omega^2}{2}(x - x_L)^2$ , with the same  $\omega$  as before and corresponding energy levels  $\epsilon_{L,n'}$ ,  $n' = 0, 1, 2, \ldots$  (i.e. eigenvalues of  $P^2/(2m) + V_{\text{harm},L}$ ) and eigenfunctions  $\varphi_{L,n'}(x)$ . Explain why the probability to find the electron in  $[0,\ell]$ , if it is in the state  $\varphi_{L,0}$ , is given by the same P as above, and why also approximately

$$\langle X \rangle_{L,0} \simeq x_L = -\frac{\ell}{2} \ .$$
 (1.5)

Show that one also has (exactly)

$$\langle \varphi_{L,0} | X | \varphi_{R,0} \rangle = 0 . \tag{1.6}$$

7) We now restrict our attention to the 2-state system formed by  $|\varphi_{R,0}\rangle$  and  $|\varphi_{L,0}\rangle$ . The probability P determined above should somehow reflect the tunnel probability that an electron "initially" localised around the right potential minimum can be found "later-on" around the left potential minimum, and vice versa. To make this precise, one needs to obtain a transition probability per unit time. We will start with a Hamiltonian for this 2-state system which in the  $\{\varphi_{R,0}, \varphi_{L,0}\}$  basis takes the form

$$H_0 = \frac{\hbar\omega}{2} \begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix} , \quad a > 0 , \qquad (1.7)$$

where  $a \sim \sqrt{P}$ . Explain why this is a reasonable Hamiltonian, in particular why a should be related to the *square root* of P. (If this takes you more than 3 minutes, continue to questions 8, 9 and 10, and then come back to the present question.)

8) Determine the eigenvalues  $E_{\pm}$  and eigenvectors  $|\varphi_{\pm}\rangle$  / eigenfunctions  $\varphi_{\pm}(x)$  of this Hamiltonian. In particular express  $|\varphi_{\pm}\rangle$  in terms of  $|\varphi_{R,0}\rangle$  and  $|\varphi_{L,0}\rangle$ , and vice versa.

- 9) Assume at t = 0 the electron is in the state  $|\psi(0)\rangle = c_+ |\varphi_+\rangle + c_- |\varphi_-\rangle$ . What condition the coefficients  $c_{\pm}$  should satisfy? Give the state at any later time t.
- 10) Assuming the electron is initially "on the right", i.e. in the state  $|\varphi_{R,0}\rangle$ , compute the probability  $\mathcal{P}_{R\to L}(t)$  that, at a later time t, it is found "on the left", i.e. in the state  $|\varphi_{L,0}\rangle$ . Give the state  $|\psi(t)\rangle$  in the basis of the  $\{|\varphi_{L,0}\rangle, |\varphi_{R,0}\rangle\}$ .
- 11) Compute the expectation value of the position operator  $\langle X \rangle$  as a function of time and comment whether your result is consistent with  $\mathcal{P}_{R\to L}(t)$ . (Use the results (1.18) and (1.19).)
- 12) Actually, the electron also has a spin (corresponding to the observable  $\vec{S} = (S_x, S_y, S_z)$ ) and corresponding magnetic moment  $\vec{\mu} = \frac{e}{m}\vec{S}$ . In the presence of a magnetic field  $\vec{B}$  this leads to an interaction with corresponding Hamiltonian

$$H_{\rm spin} = -\vec{\mu} \cdot \vec{B} \tag{1.8}$$

We assume that the magnetic field is constant and uniform in the z-direction,  $\vec{B} = B_0 \vec{e}_z$ . As usual we call  $|\pm\rangle$  the eigenstates of  $S_z$  with eigenvalues  $\pm \frac{\hbar}{2}$ . Recall how the eigenstates  $|x:\pm\rangle$  of  $S_x$  are related to the  $|\pm\rangle$ . Considering for the time being only the spin, and assuming that at t=0 the spin of the electron is measured along the x-axis and found to be  $+\frac{\hbar}{2}$ , what is the probability to find  $-\frac{\hbar}{2}$  in a measurement of  $S_x$  at a later time t?

13) Now we consider the problem of the electron in the spatial potential as above, approximated by the two-state system with basis  $\{|\varphi_{L,0}\rangle, |\varphi_{R,0}\rangle\}$ , and interacting via its spin with the magnetic field. The corresponding Hilbert space then is the tensor product with basis

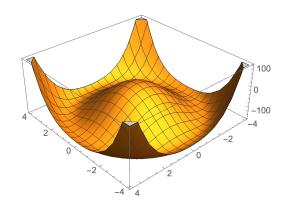
$$\{|\varphi_{R,0}\rangle\otimes|+\rangle, \{|\varphi_{R,0}\rangle\otimes|-\rangle, |\varphi_{L,0}\rangle\otimes|+\rangle, \{|\varphi_{L,0}\rangle\otimes|-\rangle\}.$$
 (1.9)

The full Hamiltonian then is "the sum" of  $H_0$  and  $H_{\rm spin}$ . Give a more precise writing of the sum in terms of an operator acting on the tensor product space. Give the eigenstates and eigenvalues of this full Hamiltonian. What is the lowest possible energy value?

- 14) Assuming that at t=0 the electron is measured "on the right" with it's spin component in the x-direction being  $+\frac{\hbar}{2}$ , what is its state  $|\psi(0)\rangle$  just after this initial measurement and what is it at later times t? Suppose at some time  $t=t_1>0$  a measurement of the spin in the x-direction is done and one finds  $-\frac{\hbar}{2}$ . What is the state  $|\widetilde{\psi}\rangle$  immediately after this measurement? What is the expectation value of X for this state? Compare with the result found in 11). Comment?
- 15) Now still assume that at t=0 the electron is measured "on the right" with it's spin component in the x-direction being  $+\frac{\hbar}{2}$  (i.e. same  $|\psi(0)\rangle$ ), but at the later time  $t=t_1$  one measures the total energy and finds the lowest possible value. What was the probability to find this result? Give the state right after this measurement. What are the probabilities that a later measurement, at  $t_2 > t_1$ , of the x-component of the spin finds  $+\frac{\hbar}{2}$  or  $-\frac{\hbar}{2}$ ? Same question for the y-component of the spin.

## Problem 2: A particle in a Mexican hat potential

Consider a particle of mass m in a two-dimensional potential  $V(x,y) = \frac{V_0}{r_0^4} (x^2 + y^2 - r_0^2)^2$ . This potential usually is referred to as a Mexican hat potential and a picture is shown in the figure.



The potential obviously is invariant under rotations in the xy-plane. If one introduces polar coordinates r and  $\phi$  (such that  $x = r \cos \phi$  and  $y = r \sin \phi$ ) then  $x^2 + y^2 = r^2$  and the invariance under rotations manifests itself in that V only depends on r, namely  $V = V(r) = V_0 \left(\frac{r^2}{r_0^2} - 1\right)^2$ . As a function of r, this has a minimum at  $r = r_0$ , and  $V''(r_0) = \frac{8V_0}{r_0^2}$ . Around its minimum, V(r) can be approximated by the harmonic potential

$$V(r) \simeq \widetilde{V}(r) = \frac{m}{2}\omega^2(r - r_0)^2$$
 ,  $\omega^2 = \frac{8V_0}{mr_0^2}$  . (1.10)

There is actually one such minimum for every value of the polar angle  $\phi \in [0, 2\pi]$ . This harmonic approximation will be a good approximation for the few lowest oscillator levels if  $V_0 \gg \hbar \omega$  i.e.  $V_0 \gg \frac{\hbar^2}{mr_0^2}$ . We will assume that this condition is satisfied. One can then also simplify the "kinetic part" of the Hamiltonian  $\widehat{H}$  (acting on wave functions of r and  $\phi$ ). The result is

$$\widehat{H} = \widehat{H}_r + \widehat{H}_{\phi} \quad , \quad \widehat{H}_r = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + \frac{m}{2} \omega^2 (r - r_0)^2 \quad , \quad \widehat{H}_{\phi} = -\frac{\hbar^2}{2m} \frac{1}{r_0^2} \frac{\partial^2}{\partial \phi^2} . \tag{1.11}$$

It is consistent with this harmonic approximation to consider  $r \in (-\infty, \infty)$ , as well as  $\phi \in [0, 2\pi]$ . The corresponding Hilbert space then is  $L^2(\mathbf{R} \times S^1) \simeq L^2(\mathbf{R}) \otimes L^2(S^1)$  where  $S^1$  is the unit circle with coordinate  $\phi$ . The inner product is defined as  $(\psi, \chi) = \int_{-\infty}^{\infty} \mathrm{d}r \, \int_{0}^{2\pi} \mathrm{d}\phi \, \psi^*(r, \phi) \chi(r, \phi)$ .

- 1) First consider the angular part. Show that  $\frac{\hbar}{i} \frac{\partial}{\partial \phi}$  is a symmetric operator which is moreover self-adjoint. Give an orhonormal basis in  $L^2(S^1)$  of eigenfunctions  $f_k(\phi)$  of this operator (where  $k \in \mathbf{Z}$ ). We will call the corresponding kets  $|k\rangle_{\text{angular}}$ . Show that these eigenfunctions also are eigenfunctions of  $\widehat{H}_{\phi}$  and give the corresponding eigenvalues.
- 2) Now consider the radial part. Relate  $\frac{\partial}{\partial r}$  to an operator  $P_r$  and define a corresponding operator R such that  $H_r = \frac{P_r^2}{2m} + \frac{m}{2}\omega^2 R^2$ . Give the commutator of R and  $P_r$ . Define appropriate operators a

and  $a^{\dagger}$  such that  $[a, a^{\dagger}] = \mathbf{1}$  and express  $H_r$  in terms of a and  $a^{\dagger}$ . Using the results from the lecture, give the orthonormal basis of eigenvectors  $|n\rangle_{\text{radial}}$  of  $H_r$  by applying the  $a^{\dagger}$  to an appropriate state  $|0\rangle_{\text{radial}}$ . Write down the wave function  $\langle r | 0 \rangle_{\text{radial}}$ .

- **3)** A basis of the full Hilbert space then is given by the  $|n\rangle_{\text{radial}} \otimes |k\rangle_{\text{angular}} \equiv |n,k\rangle$  with  $n=0,1,2,\ldots$  and  $k \in \mathbf{Z}$ . Is this an eigenbasis of H and if so what are the eigenvalues?
- 4) A somewhat more careful treatment would replace  $\hat{H}_{\phi}$  by  $-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}$ . The difference is

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} - \frac{1}{r_0^2}\right) \frac{\partial^2}{\partial \phi^2} \simeq -\frac{\hbar^2}{2m} \frac{r_0^2 - r^2}{r_0^4} \frac{\partial^2}{\partial \phi^2} \simeq \frac{\hbar^2}{m} \frac{r - r_0}{r_0^3} \frac{\partial^2}{\partial \phi^2} = \widehat{H}_2$$
 (1.12)

Compute the matrix elements

$$\langle n, k | H_2 | n', k' \rangle . \tag{1.13}$$

Determine the corresponding corrections to the energies to first and second order in perturbation theory.

5) We now disregard the corrections due to  $H_2$ , but instead suppose the particle carries an electric charge q and we add an electric field  $\mathcal{E}$  in the x-direction. This amounts to adding an extra term  $-q\mathcal{E}x = -q\mathcal{E}r\cos\phi = -q\mathcal{E}r(e^{i\phi} + e^{-i\phi})/2$  to the potential. Determine the corresponding additional Hamiltonian  $H_1$  and give its matrix elements

$$\langle n, k | H_1 | n', k' \rangle . \tag{1.14}$$

(You should find that they vanish if n and n' or k and k' differ by more than  $\pm 1$ ).

6) Treat this additional  $H_1$  in perturbation theory. Show that to first order in perturbation theory the eigenvalues of H remain unchanged, and compute their change to second order in perturbation theory.

# Introduction à la mécanique quantique I

## Examen 2023-2024

#### durée 3 heures

Veuillez écrire aussi lisiblement que possible. Tout texte illisible sera ignoré.

Cet examen est composé de deux problèmes indépendants. Utilisez des feuilles séparées pour traiter les deux problèmes.

Il n'est probablement pas possible de traiter les deux problèmes complètement en 3 heures. La notation sera ajustée en conséquence.

Chaque problème contient des questions plus générales et des calculs plus spécifiques.

La réponse à une question donnée n'est pas toujours nécessaire pour traiter les questions suivantes.

Ne perdez donc pas trop de temps avec des questions auxquelles vous ne savez pas répondre - vous pouvez probablement encore faire (une partie) des questions suivantes.

Vous pouvez écrire en anglais ou en français.

## Problème 1: Un "fil" circulaire unidimensionnel

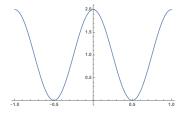
On considère un "fil" circulaire unidimensionnel de circonférence  $2\ell$  dans lequel une particule de masse m, appelée électron, est confinée. Nous introduisons une coordonnée  $x \in [-\ell, \ell]$  le long de ce "fil" et la géométrie circulaire impose des conditions aux limites périodiques, c'est-à-dire que  $x = -\ell$  et  $x = \ell$  sont des points identiques.

- 1) Décrire brièvement l'espace de Hilbert approprié des fonctions d'onde  $\psi(x)$  dans ce contexte. Quel est le produit intérieur hermitien approprié  $(\psi, \chi)$ ? Comment la norme de  $\psi$  est définie en termes de ce produit intérieur?
- 2) Quels sont les domaines appropriés de définition des opérateurs linéaires X, agissant comme  $(X\psi)(x) = x\psi(x)$ , et P, agissant comme  $(P\psi)(x) = -i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}x}(x)$ ? Sont-ils auto-adjointes ou seulement symétriques? Motivez votre réponse par un calcul en une ligne. Qu'en est-il de  $X^n$  et  $P^n$  pour  $n \geq 2$ ?

L'électron porte une charge électrique q et nous ajoutons un champ électrique statique tel que l'énergie potentielle de l'électron due au potentiel électrostatique est

$$V(x) = V_0 \left(\cos \frac{2\pi x}{\ell} + 1\right) , \qquad (1.15)$$

voir la figure (où l'axe horizontal est  $x/\ell$  et l'axe vertical  $V/V_0$ ). Nous insistons sur le fait que le bord droit de la figure doit être identifié au bord gauche.



Nous supposons que l'opérateur hamiltonien dans ce cadre est

$$H = \frac{1}{2m}P^2 + V(X) \ . \tag{1.16}$$

- 3) A quelles situations simples discutées dans le cours cela vous fait-il penser ? Discutez qualitativement à quel spectre de l'hamiltonien on s'attend. Il y aura un nombre fini de valeurs propres discrètes (que nous pourrions appeler états liés). Comment pensez-vous que ce nombre dépend des quantités m,  $V_0$  et  $\ell$ ? Plus précisément, quelle devrait être la quantité sans dimension composée de m,  $\ell$ ,  $V_0$  (et  $\hbar$ ) qui contrôle le nombre d'états liés ?
- 4) Nous commençons par porter notre attention au voisinage du minimum du potentiel à  $x = x_R$  avec  $x_R = \frac{\ell}{2}$ . Ecrire le développement de Taylor du potentiel au second ordre autour de  $x_R$ . Vous devriez obtenir  $V(x) \simeq V_{\text{harm},R}(x)$  avec

$$V_{\text{harm,R}}(x) = \frac{m\omega^2}{2}(x - x_R)^2$$
, (1.17)

avec une fréquence angulaire  $\omega$  à déterminer. Quels sont les niveaux d'énergie correspondants  $\epsilon_{R,n}, n=0,1,2,\ldots$  (c'est-à-dire les valeurs propres de  $P^2/(2m)+V_{\rm harm,R}(x)$ ) dans cette approximation? (L'indice R indique que nous ne traitons que la partie droite du potentiel). Discuter, en fonction de  $m,\ell$  et  $V_0$  pour quelles valeurs de n cette approximation harmonique devrait être une bonne approximation. Comparez avec votre résultat de la question 3. Les fonctions propres correspondantes dans cette approximation seront appelées  $\varphi_{R,n}(x)$ . (En particulier, nous n'essayons pas de les rendre périodiques).

5) Nous supposons maintenant que  $V_0 = 10 \,\hbar\omega$  et supposons que l'électron est dans l'"état fondamental"  $|\varphi_{R,0}\rangle$ , c'est-à-dire que sa fonction d'onde est  $\varphi_{R,0}(x)$ . En utilisant les résultats du cours, donner explicitement cette fonction  $\varphi_{R,0}(x)$ . Donner la formule pour calculer la probabilité P de trouver l'électron dans l'intervalle  $[-\ell,0]$  ("de l'autre côté" de la barrière de potentiel). N'essayez pas d'évaluer l'intégrale explicitement mais donnez un ordre de grandeur de cette probabilité P. Comment cela se compare-t-il à la formule générale (7.41) donnée dans le cours pour une probabilité de tunnel ? Donner la formule pour calculer la valeur moyenne  $\langle X\rangle_{R,0}$  de l'opérateur de position dans l'état  $|\varphi_{R,0}\rangle$  et argumenter qu'approximativement on a

$$\langle X \rangle_{R,0} \simeq x_R = \frac{\ell}{2} \ .$$
 (1.18)

6) Nous pouvons bien sûr approximer de la même manière la partie gauche du potentiel autour de son minimum en  $x_L = -\frac{\ell}{2}$  et obtenir  $V_{\text{harm},L}(x) = \frac{m\omega^2}{2}(x-x_L)^2$ , avec le même  $\omega$  que précédemment et les mêmes niveaux d'énergie  $\epsilon_{L,n'}$ ,  $n' = 0, 1, 2, \dots$  (c'est-à-dire les valeurs propres de  $P^2/(2m) + V_{\text{harm},L}$ ) et fonctions propres  $\varphi_{L,n'}(x)$ . Expliquer pourquoi la probabilité de trouver l'électron dans  $[0,\ell]$ , s'il est dans l'état  $\varphi_{L,0}$ , est donnée par le même P que ci-dessus, et pourquoi aussi approximativement

$$\langle X \rangle_{L,0} \simeq x_L = -\frac{\ell}{2} \ . \tag{1.19}$$

Montrer que l'on a aussi (exactement)

$$\langle \varphi_{L,0} | X | \varphi_{R,0} \rangle = 0 . \tag{1.20}$$

7) Nous limitons maintenant notre attention au système à deux états formé par  $|\varphi_{R,0}\rangle$  et  $|\varphi_{L,0}\rangle$ . La probabilité P déterminée ci-dessus devrait en quelque sorte refléter la probabilité tunnel qu'un électron "initialement" localisé autour du minimum de potentiel de droite puisse être retrouvé "plus tard" autour du minimum de potentiel de gauche, et vice versa. Afin de rendre ceci plus précis, il faut obtenir une probabilité de transition par unité de temps. Nous commençons par considérer un hamiltonien pour ce système à deux états qui, dans la base  $\{\varphi_{R,0}, \varphi_{L,0}\}$ , prend la forme suivante

$$H_0 = \frac{\hbar\omega}{2} \begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix} \tag{1.21}$$

où  $a \sim \sqrt{P}$ . Expliquez pourquoi il s'agit d'un hamiltonien raisonnable, en particulier pourquoi a devrait être lié à la racine carrée de P (si cela vous prend plus de 3 minutes, passez aux questions 8, 9 et 10, puis revenez à la présente question).

- 8) Déterminer les valeurs propres  $E_{\pm}$  et les vecteurs propres  $|\varphi_{\pm}\rangle$  / fonctions propres  $\varphi_{\pm}(x)$  de cet hamiltonien. En particulier, exprimer  $|\varphi_{\pm}\rangle$  en termes de  $|\varphi_{R,0}\rangle$  et  $|\varphi_{L,0}\rangle$ , et vice versa.
- 9) Supposons qu'à t=0 l'électron soit dans l'état  $|\psi(0)\rangle=c_+|\varphi_+\rangle+c_-|\varphi_-\rangle$ . Quelle condition les coefficients  $c_{\pm}$  doivent-ils satisfaire? Donner l'état à un instant ultérieur t.
- 10) En supposant que l'électron soit initialement "à droite", c'est-à-dire dans l'état  $|\varphi_{R,0}\rangle$ , calculer la probabilité  $\mathcal{P}_{R\to L}(t)$  que, à un instant ultérieur t, il se trouve "à gauche", c'est-à-dire dans l'état  $|\varphi_{L,0}\rangle$ . Donner l'état  $|\psi(t)\rangle$  dans la base des  $\{|\varphi_{L,0}\rangle, |\varphi_{R,0}\rangle\}$ .
- 11) Calculez la valeur moyenne de l'opérateur de position  $\langle X \rangle$  en fonction du temps. Est-ce que votre résultat est cohérent avec le  $\mathcal{P}_{R\to L}(t)$  obtenu précédemment ? (Utilisez les résultats (1.18) et (1.19).)
- 12) En réalité, l'électron a également un spin (correspondant à l'observable  $\vec{S} = (S_x, S_y, S_z)$ ) et un moment magnétique correspondant  $\vec{\mu} = \frac{e}{m}\vec{S}$ . En présence d'un champ magnétique  $\vec{B}$ , cela conduit à une interaction donnée par

$$H_{\rm spin} = -\vec{\mu} \cdot \vec{B} \tag{1.22}$$

Nous supposons que le champ magnétique est constant et uniforme dans la direction z, soit  $\vec{B} = B_0 \vec{e}_z$ . Comme d'habitude, nous appelons  $|\pm\rangle$  les états propres de  $S_z$  avec des valeurs propres  $\pm \frac{\hbar}{2}$ . Rappelez comment les états propres  $|x:\pm\rangle$  de  $S_x$  sont liés aux  $|\pm\rangle$ . En ne considérant pour l'instant que le spin, et en supposant qu'à t=0 le spin de l'électron est mesuré le long de l'axe x et vaut  $+\frac{\hbar}{2}$ , quelle est la probabilité de trouver  $-\frac{\hbar}{2}$  lors d'une mesure de  $S_x$  à un instant ultérieur t?

13) Considérons maintenant le problème de l'électron dans le potentiel spatial comme ci-dessus, approximé par le système à deux états avec la base  $\{|\varphi_{L,0}\rangle, |\varphi_{R,0}\rangle\}$ , et interagissant par son spin avec le champ magnétique. L'espace de Hilbert correspondant est alors le produit tensoriel avec comme base

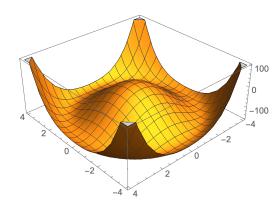
$$\{|\varphi_{R,0}\rangle\otimes|+\rangle, \{|\varphi_{R,0}\rangle\otimes|-\rangle, |\varphi_{L,0}\rangle\otimes|+\rangle, \{|\varphi_{L,0}\rangle\otimes|-\rangle\}.$$
 (1.23)

Le hamiltonien complet est "la somme" de  $H_0$  et  $H_{\rm spin}$ . Donner une écriture plus précise de la somme en termes d'un opérateur agissant sur l'espace du produit tensoriel. Donnez les états propres et les valeurs propres de ce hamiltonien complet. Quelle est la plus petite valeur d'énergie possible ?

- 14) En supposant qu'à t=0 l'électron est mesuré "à droite" avec sa composante de spin dans la direction x étant  $+\frac{\hbar}{2}$ , donnez son état  $|\psi(0)\rangle$  juste après cette mesure initiale et aux temps t ultérieurs. Supposons qu'à un moment donné  $t=t_1>0$  une mesure du spin dans la direction x soit effectuée et que l'on trouve  $-\frac{\hbar}{2}$ . Quel est l'état  $|\widetilde{\psi}\rangle$  immédiatement après cette mesure ? Quelle est la valeur moyenne de X pour cet état ? Comparer avec le résultat trouvé en 11).
- 15) Supposons encore qu'à t=0 l'électron soit mesuré "à droite" avec sa composante de spin dans la direction x étant  $+\frac{\hbar}{2}$  (c'est-à-dire le même  $|\psi(0)\rangle$ ), mais qu'au moment ultérieur  $t=t_1$  on mesure l'énergie totale et trouve la valeur la plus basse possible. Quelle était la probabilité de trouver ce résultat? Donnez l'état juste après cette mesure. Quelles sont les probabilités qu'une mesure ultérieure, à  $t_2 > t_1$ , de la composante x du spin trouve  $+\frac{\hbar}{2}$  ou  $-\frac{\hbar}{2}$ ? Même question pour la composante y du spin.

# Problème 2 : Une particule dans un potentiel ayant la forme d'un chapeau mexicain

Considérons une particule de masse m dans un potentiel bidimensionnel  $V(x,y) = \frac{V_0}{r_0^4} (x^2 + y^2 - r_0^2)^2$ . Ce potentiel est généralement appelé potentiel du chapeau mexicain et une image est présentée dans la figure.



Le potentiel est évidemment invariant sous l'effet des rotations dans le plan xy. Si l'on introduit les coordonnées polaires r et  $\phi$  (telles que  $x = r\cos\phi$  et  $y = r\sin\phi$ ) alors  $x^2 + y^2 = r^2$  et l'invariance sous les rotations se manifeste par le fait que V ne dépend que de r, à savoir  $V = V(r) = V(r) = V(r)^2 - 1$ . Cette fonction a un minimum à  $r = r_0$ , et  $V''(r_0) = \frac{8V_0}{r_0^2}$ . Autour de son minimum, V(r) peut être approximé par le potentiel harmonique

$$V(r) \simeq \widetilde{V}(r) = \frac{m}{2}\omega^2(r - r_0)^2$$
 ,  $\omega^2 = \frac{8V_0}{mr_0^2}$ . (1.24)

Il existe en fait un tel minimum pour chaque valeur de l'angle polaire  $\phi \in [0, 2\pi]$ . Cette approximation harmonique sera une bonne approximation pour les quelques niveaux les plus bas de l'oscillateur si  $V_0 \gg \hbar \omega$  c'est-à-dire  $V_0 \gg \frac{\hbar^2}{mr_0^2}$ . Nous supposerons que cette condition est satisfaite. On peut alors également simplifier la "partie cinétique" de l'hamiltonien  $\hat{H}$  (agissant sur les fonctions d'onde de r et  $\phi$ ). Le résultat est

$$\widehat{H} = \widehat{H}_r + \widehat{H}_{\phi} \quad , \quad \widehat{H}_r = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + \frac{m}{2} \omega^2 (r - r_0)^2 \quad , \quad \widehat{H}_{\phi} = -\frac{\hbar^2}{2m} \frac{1}{r_0^2} \frac{\partial^2}{\partial \phi^2}$$
 (1.25)

Il est cohérent dans cette approximation harmonique de considérer  $r \in (-\infty, \infty)$ , ainsi que  $\phi \in [0, 2\pi]$ . L'espace de Hilbert correspondant est alors  $L^2(\mathbf{R} \times S^1) \simeq L^2(\mathbf{R}) \otimes L^2(S^1)$  où  $S^1$  est le cercle unitaire avec la coordonnée  $\phi$ . Le produit intérieur est défini comme  $(\psi, \chi) = \int_{-\infty}^{\infty} \mathrm{d}r \int_{0}^{2\pi} \mathrm{d}\phi \, \psi^*(r, \phi) \chi(r, \phi)$ .

1) Considérons d'abord la partie angulaire. Montrer que  $\frac{\hbar}{i} \frac{\partial}{\partial \phi}$  est un opérateur symétrique qui est de plus auto-adjoint. Donner une base orhonormée dans  $L^2(S^1)$  de fonctions propres  $f_k(\phi)$  de cet opérateur (où  $k \in \mathbf{Z}$ ). Nous appellerons les kets correspondants  $|k\rangle_{\text{angulaire}}$ . Montrer

que ces fonctions propres sont aussi des fonctions propres de  $\widehat{H}_{\phi}$  et donner les valeurs propres correspondantes.

- 2) Considérons maintenant la partie radiale. Relier  $\frac{\partial}{\partial r}$  à un opérateur  $P_r$  et définir un opérateur correspondant R tel que  $H_r = \frac{P_r^2}{2m} + \frac{m}{2}\omega^2R^2$ . Donner le commutateur de R et  $P_r$ . Définir les opérateurs appropriés a et  $a^{\dagger}$  tels que  $[a, a^{\dagger}] = 1$  et exprimer  $H_r$  en termes de a et  $a^{\dagger}$ . En utilisant les résultats du cours, donner la base orthonormée des vecteurs propres  $|n\rangle_{\text{radial}}$  de  $H_r$  en appliquant le  $a^{\dagger}$  à un état approprié  $|0\rangle_{\text{radial}}$ . Ecrire la fonction d'onde  $\langle r | 0\rangle_{\text{radial}}$ .
- **3** Une base de l'espace de Hilbert complet est alors donnée par les  $|n\rangle_{\text{radial}} \otimes |k\rangle_{\text{angulaire}} \equiv |n,k\rangle$  avec  $n=0,1,2,\ldots$  et  $k\in\mathbf{Z}$ . S'agit-il d'une base propre de H et si oui, quelles sont ses valeurs propres ?
- 4) Un traitement un peu plus rigoureux conduit à remplacer  $\widehat{H}_{\phi}$  par  $-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}$ . La différence est

$$-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} - \frac{1}{r_0^2}\right) \frac{\partial^2}{\partial \phi^2} \simeq -\frac{\hbar^2}{2m} \frac{r_0^2 - r^2}{r_0^4} \frac{\partial^2}{\partial \phi^2} \simeq \frac{\hbar^2}{m} \frac{r - r_0}{r_0^3} \frac{\partial^2}{\partial \phi^2} = \widehat{H}_2$$
 (1.26)

Calculer les éléments de la matrice

$$\langle n, k | H_2 | n', k' \rangle . \tag{1.27}$$

Déterminer les corrections correspondantes aux énergies au premier et au second ordre dans la théorie des perturbations.

5) Maintenant nous n'allons plus tenir compte des corrections dues à  $H_2$ , mais nous supposons que la particule porte une charge électrique q et nous ajoutons un champ électrique  $\mathcal{E}$  dans la direction x. Cela revient à ajouter un terme supplémentaire  $-q\mathcal{E}x = -q\mathcal{E}r\cos\phi = -q\mathcal{E}r(e^{i\phi} + e^{-i\phi})/2$  au potentiel. Déterminer l'hamiltonien  $H_1$  qui correspond à cette interaction et donner ses éléments de matrice

$$\langle n, k | H_1 | n, k \rangle$$
 (1.28)

(Vous devriez trouver qu'ils s'annulent si n et n' ou k et k' diffèrent de plus de  $\pm 1$ .)

6) Traiter ce  $H_1$  en théorie des perturbations. Montrer qu'au premier ordre de la théorie des perturbations, les valeurs propres de H restent inchangées, et calculer leur changement au second ordre de la théorie des perturbations.

# Introduction to Quantum Mechanics I

# Exam 2023-2024 : Solutions

## Problem 1: A one-dimensional circular "wire"

1) The Hilbert space should consist of the periodic, square-integrable functions on  $[-\ell,\ell]$ . Since  $-\ell$  and  $+\ell$  are identified, this is actually a circle  $S^1$  so that the Hilbert space is  $\mathcal{H}=L^2(S^1)$ . Now,  $S^1$  has no boundary and there is actually no boundary condition. Also, continuity is not a requirement for being square-integrable. What then means the periodicity condition  $\psi(-\ell)=\psi(\ell)$ ? If we want to think of  $\psi$  as a function of the real variable x then we define it on  $[-\ell,\ell)$  together with  $2\ell$  periodicity. This means indeed that  $\psi(\ell)=\psi(-\ell)$  by definition, but we do not require that  $\lim_{\epsilon\to 0}\psi(\ell-\epsilon)=\psi(\ell)=\psi(-\ell)$ . Square-integrability then is simply written as

$$\psi \in \mathcal{H} \quad \Leftrightarrow \quad \int_{-\ell}^{\ell} \mathrm{d}x \, |\psi(x)|^2 < \infty \ .$$
 (1.29)

The inner product and norm are

$$(\psi, \chi) = \int_{-\ell}^{\ell} dx \, \psi^*(x) \chi(x) \quad , \quad ||\psi|| = \sqrt{(\psi, \psi)} .$$
 (1.30)

2)  $\mathcal{D}(X)$  consist of all functions  $\psi \in \mathcal{H}$  such that  $x\psi(x)$  is again square-integrable. But since x is bounded on  $[-\ell,\ell]$  we have that  $x\psi(x)$  is square-integrable if  $\psi(x)$  is. Obviously  $x\psi(x)$  will not take identical values at  $x=\ell$  and at  $x=-\ell$  unless  $\psi(\pm\ell)=0$ . This seems to impose an extra restriction on the domain of definition of X, but actually it does not. As explained above, we define the action of X only on  $x \in [-\ell,\ell)$  and at any other real x by periodicity. In particular then we have automatically  $(X\psi)(\ell)=(X\psi)(-\ell)$ . Of course, if  $\psi(-\ell)\neq 0$  this implies that  $(X\psi)(x)$  is not continuous at  $x=\ell\equiv -\ell$  but jumps by  $2\ell\psi(-\ell)$ . Finally we conclude that  $\mathcal{D}(X)=\mathcal{H}=L^2(S^1)$ 

 $\mathcal{D}(P)$  consist of the differentiable functions on  $S^1$ . A differentiable function is necessarily continuous and hence square-integrable over the finite interval  $[-\ell,\ell]$ . Being continuous, for these functions periodicity imposes  $\psi(\ell) = \psi(-\ell)$ . Hence,  $\mathcal{D}(P) = C^1(S^1)$ .

To see that X is symmetric one writes  $(X\chi,\psi) = \int_{-\ell}^{\ell} \mathrm{d}x \, (x\chi(x))^* \psi(x) = \int_{-\ell}^{\ell} \mathrm{d}x \, \chi(x)^* \, x \, \psi(x) = (\chi, X\psi)$  which uses the fact that x is real. To see that P is symmetric one uses that  $i^* = -i$  generates a minus sign and an integration by parts generates another minus sign:

$$(P\chi,\psi) = \int_{-\ell}^{\ell} dx \left(\frac{\hbar}{i} \frac{d}{dx} \chi(x)\right)^* \psi(x) = \int_{-\ell}^{\ell} dx \, \chi(x)^* \frac{\hbar}{i} \frac{d}{dx} \, \psi(x) = (\chi, P\psi) . \tag{1.31}$$

Of course, this requires that also  $\chi \in C^1(S^1)$ . No boundary terms are generated because all functions are periodic, or actually because the circle  $S^1$  has no boundary. For this same reason there is no distinction between the domains of definition of P and  $P^{\dagger}$  or between those of X and  $X^{\dagger}$  and these operators are self-adjoint. The discussion for  $X^n$  and  $P^n$  goes exactly in the same way.

3) The potential presents two minima, which ressemble two potential wells of finite depth  $2V_0$ . They are separated by a sort of potential barrier. For a finite potential well one expects a finite number of discrete eigenvalues of the Hamiltonian at  $E < 2V_0$ , as well as a continuous spectrum for  $E \ge 0$ . Very roughly (cf the infinite potential well) the eigenvalues in a well of width  $\ell$  are  $\frac{\hbar^2}{2m} \left(\frac{2\pi n}{\ell}\right)^2$ . Then we expect  $\frac{\hbar^2}{2m} \left(\frac{2\pi}{\ell}\right)^2 n_{\text{max}}^2 \simeq V_0$ , so that

$$n_{\text{max}} \simeq \frac{\ell}{2\pi\hbar} \sqrt{2mV_0} \ . \tag{1.32}$$

4) First of all,  $V'(x) = -\frac{2\pi}{\ell}V_0\sin\frac{2\pi x}{\ell}$  which vanishes at the two minima  $x_R = \frac{\ell}{2}$  and  $x_L = -\frac{\ell}{2}$  (as well as at the maximum x = 0). The value of the potential at these minima is  $V(\pm \frac{\ell}{2}) = 0$ . Taylor expanding around the minimum  $X_R$  means to approximate

$$V(x) \simeq \frac{1}{2} V''(\frac{\ell}{2}) \left(x - \frac{\ell}{2}\right)^2 = \frac{V_0}{2} \left(\frac{2\pi}{\ell}\right)^2 \left(x - \frac{\ell}{2}\right)^2 = \frac{m}{2} \omega^2 \left(x - \frac{\ell}{2}\right)^2, \tag{1.33}$$

with

$$\omega = \frac{2\pi}{\ell} \sqrt{\frac{V_0}{m}} \ . \tag{1.34}$$

The corresponding energy levels are of course  $E_n = \hbar \omega (n + \frac{1}{2})$ . However, we do not expect the approximation to make sense if  $E_n$  becomes similar or greater than  $\alpha V_0$  where  $\alpha$  is some number between 1 and 2. Choosing  $\alpha = \sqrt{2}$  we get

$$\hbar\omega n_{\text{max}} \simeq \sqrt{2}V_0 \quad \Rightarrow \quad n_{\text{max}} \simeq \frac{\sqrt{2}V_0}{\hbar\omega} = \frac{\ell}{2\pi\hbar}\sqrt{2mV_0} ,$$
(1.35)

which agrees with the previous estimate. The eigenfunctions we will use in this approximations should be the corresponding harmonic oscillator wave-functions centered at  $x = x_R = \frac{\ell}{2}$ .

5) If  $V_0 = 10\hbar\omega$  one has  $n_{\text{max}} \simeq 14$  and one expects the harmonic approximation to be very good for n = 0, i.e. for the ground state wave functions. In particular

$$\varphi_{R,0}(x) = \varphi_0\left(x - \frac{\ell}{2}\right) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}(x - \frac{\ell}{2})^2} . \tag{1.36}$$

Note that this is not periodic and that it is only correctly normalised if one integrates from  $-\infty$  to  $+\infty$ , but the error one commits is exponentially small. Similarly, the probability to find the

electron in the interval  $[-\ell, 0]$  is

$$P = \int_{-\ell}^{0} dx \, |\varphi_{R,0}(x)|^{2} = \int_{-\ell}^{0} dx \, |\varphi_{0}(x - \frac{\ell}{2})|^{2} = \int_{-3\ell/2}^{-\ell/2} dx \, |\varphi_{0}(x)|^{2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-3\ell/2}^{-\ell/2} dx \, e^{-\frac{m\omega}{\hbar}x^{2}}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-3\sqrt{\frac{m\omega}{\hbar}}\ell/2}^{-\sqrt{\frac{m\omega}{\hbar}}\ell/2} dy \, e^{-y^{2}} \simeq C \, e^{-\frac{m\omega\ell^{2}}{4\hbar}} , \qquad (1.37)$$

where C is some numerical constant of the order of 1. Note that  $\frac{m\omega\ell^2}{4\hbar} = \frac{\pi\ell}{2\hbar}\sqrt{mV_0}$  so that

$$P = C \exp\left(-\frac{\pi\ell}{2\hbar}\sqrt{mV_0}\right), \qquad (1.38)$$

which is to be compared with the tunnel probability given in the lecture of

$$P_{\text{tunnel}} \simeq \exp\left(-\frac{2}{\hbar} \int_{x_1}^{x_2} \mathrm{d}x \sqrt{2mV(x)}\right),$$
 (1.39)

with  $\int_{x_1}^{x_2} dx \sqrt{2mV(x)} \simeq \ell \sqrt{2mV(x)}$ . The expectation value of the position operator is

$$\langle X \rangle = \int_{-\ell}^{\ell} dx \, x \, |\varphi_{R,0}(x)|^2 = \int_{-\ell}^{\ell} dx \, x \, |\varphi_0(x - \frac{\ell}{2})|^2 = \int_{-3\ell/2}^{\ell/2} dx \, (x + \frac{\ell}{2}) |\varphi_0(x)|^2$$

$$\simeq \int_{-\infty}^{\infty} dx \, (x + \frac{\ell}{2}) |\varphi_0(x)|^2 = 0 + \frac{\ell}{2} \int_{-\infty}^{\infty} dx \, |\varphi_0(x)|^2 = \frac{\ell}{2} \,, \tag{1.40}$$

where in the last line one used that  $\int_{-\infty}^{\infty} dx \, x |\varphi_0(x)|^2 = 0$  since the integrand is odd.

6) That the harmonic approximation around  $x_L = -\frac{\ell}{2}$  gives totally analogous results is obvious. For the "off-diagonal" matrix element of X one has

$$\langle \varphi_{L,0} | X | \varphi_{R,0} \rangle = \int_{-\ell}^{\ell} \mathrm{d}x \, x \, \varphi_0 \left( x + \frac{\ell}{2} \right) \varphi_0 \left( x - \frac{\ell}{2} \right) , \qquad (1.41)$$

which vanishes since the integrand is odd and one integrates over an even interval.

7) We have already seen that P was similar to the tunnel probability given in the lecture. Then the tunnel amplitude should be  $\sqrt{P}$ . The off-diagonal elements in the Hamiltonian induce transition amplitudes between the corresponding basis states, and by the Schrödinger equation, an off-diagonal element  $H_{12}$  should correspond to a transition amplitude per unit time (times  $\hbar$ ), i.e. a transition amplitude times a frequency times  $\hbar$ . So  $H_{12} \sim \hbar \omega \sqrt{P}$  seems to be quite reasonable to start with.

8) We have

$$H_0 = \frac{\hbar\omega}{2} \left( \mathbf{1} + a\sigma_x \right) \,, \tag{1.42}$$

where  $\sigma_x$  is the Pauli matrix. Then the eigenvectors of  $\sigma_x$  also are the eigenvectors of  $H_0$ . Hence

eigenvectors : 
$$|\varphi_{\pm}\rangle = \frac{1}{\sqrt{2}} (|\varphi_{R,0}\rangle \pm |\varphi_{L,0}\rangle)$$
 , eigenvalues :  $\frac{\hbar\omega}{2} (1 \pm a)$  . (1.43)

Obviously also

$$|\varphi_{R,0}\rangle = \frac{1}{\sqrt{2}} (|\varphi_{+}\rangle + |\varphi_{-}\rangle) \quad , \quad |\varphi_{L,0}\rangle = \frac{1}{\sqrt{2}} (|\varphi_{+}\rangle - |\varphi_{-}\rangle) .$$
 (1.44)

9) The normalisation condition is  $|c_{+}|^{2} + |c_{-}|^{2} = 1$ . We have

$$|\psi(t)\rangle = e^{-i\omega t/2} \left( c_{+} e^{-i\omega at/2} |\varphi_{+}\rangle + c_{-} e^{i\omega at/2} |\varphi_{-}\rangle \right)$$
(1.45)

10) At t=0 we have  $|\psi(0)\rangle = |\varphi_{R,0}\rangle$ . Then  $c_+=c_-=\frac{1}{\sqrt{2}}$  and

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-i\omega t/2} \left( e^{-i\omega at/2} |\varphi_{+}\rangle + e^{i\omega at/2} |\varphi_{-}\rangle \right)$$

$$= \frac{1}{2} e^{-i\omega t/2} \left( \left( e^{-i\omega at/2} + e^{i\omega at/2} \right) |\varphi_{R,0}\rangle + \left( e^{-i\omega at/2} - e^{i\omega at/2} \right) |\varphi_{L,0}\rangle \right)$$

$$= e^{-i\omega t/2} \left( \cos \frac{\omega at}{2} |\varphi_{R,0}\rangle - i \sin \frac{\omega at}{2} |\varphi_{L,0}\rangle \right), \qquad (1.46)$$

and

$$\mathcal{P}_{R\to L}(t) = |\langle \varphi_{L,0} | \psi(t) \rangle|^2 = \sin^2 \frac{\omega a t}{2} . \tag{1.47}$$

11) The expectation value of X at time t can be written as

$$\langle X \rangle(t) \equiv \langle X \rangle_{\psi(t)} = \langle \psi(t) | X | \psi(t) \rangle$$

$$= \left( \cos \frac{\omega a t}{2} \langle \varphi_{R,0} | + i \sin \frac{\omega a t}{2} \langle \varphi_{L,0} | \right) X \left( \cos \frac{\omega a t}{2} | \varphi_{R,0} \rangle - i \sin \frac{\omega a t}{2} | \varphi_{L,0} \rangle \right)$$

$$= \cos^{2} \frac{\omega a t}{2} \langle \varphi_{R,0} | X | \varphi_{R,0} \rangle - i \cos \frac{\omega a t}{2} \sin \frac{\omega a t}{2} \langle \varphi_{R,0} | X | \varphi_{L,0} \rangle$$

$$+ i \cos \frac{\omega a t}{2} \sin \frac{\omega a t}{2} \langle \varphi_{L,0} | X | \varphi_{R,0} \rangle + \sin^{2} \frac{\omega a t}{2} \langle \varphi_{L,0} | X | \varphi_{L,0} \rangle$$

$$(1.48)$$

Using (1.18) and (1.19) we have  $\langle \varphi_{R,0} | X | \varphi_{R,0} \rangle = \langle X \rangle_{R,0} \simeq \frac{\ell}{2}$  and  $\langle \varphi_{L,0} | X | \varphi_{L,0} \rangle = \langle X \rangle_{L,0} \simeq -\frac{\ell}{2}$ , and by (1.20)  $\langle \varphi_{L,0} | X | \varphi_{R,0} \rangle = 0$ , so that

$$\langle X \rangle(t) = \frac{\ell}{2} \left( \cos^2 \frac{\omega a t}{2} - \sin^2 \frac{\omega a t}{2} \right) = \frac{\ell}{2} \cos \omega a t .$$
 (1.49)

This is consistent with (1.47) since  $\mathcal{P}_{R\to L} = 1$  if  $\frac{\omega at}{2} = (n + \frac{1}{2})\pi$ , i.e.  $\omega at = (2n + 1)\pi$ . These are exactly the values when  $\langle X \rangle = -\frac{\ell}{2} = x_L$ .

12)

$$H_{\rm spin} = -\frac{e}{m}\vec{B}\cdot\vec{S} = -\frac{\hbar e}{2m}\vec{B}\cdot\vec{\sigma} = -\frac{\hbar eB_0}{2m}\sigma_z = -\hbar\omega_c\sigma_z \quad , \quad \omega_c = \frac{eB_0}{2m} \ . \tag{1.50}$$

Recall that

$$|x:\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle) \quad , \quad |\pm\rangle = \frac{1}{\sqrt{2}}(|x:+\rangle \pm |x:-\rangle)$$
 (1.51)

After the measurement at t=0 the spin state is  $|\chi(0)\rangle = |x:+\rangle$ . Since the eigenstates of the spin Hamiltonian are the  $|\pm\rangle$ , one must write  $|\chi(0)\rangle$  in this basis :  $|\chi(0)\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ . Then

$$|\chi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{i\omega_c t} |+\rangle + e^{-i\omega_c t} |-\rangle \right) . \tag{1.52}$$

The probability to measure  $-\frac{\hbar}{2}$  along the x-axis is

$$\mathcal{P}(x:-\frac{\hbar}{2}) = |\langle x:-|\chi(t)\rangle|^2 = \frac{1}{4} |(\langle +|-\langle -|)(e^{i\omega_c t}|+\rangle + e^{-i\omega_c t}|-\rangle)|^2 = \frac{1}{4} |e^{i\omega_c t} - e^{-i\omega_c t}|^2$$

$$= \sin^2 \omega_c t . \tag{1.53}$$

13) A more exact writing of the combined Hamiltonian is  $H = H_0 \otimes \mathbf{1} + \mathbf{1} \otimes H_{\text{spin}}$ . The basis of eigenvectors of H is

$$|\varphi_{+}\rangle \otimes |+\rangle , \quad |\varphi_{+}\rangle \otimes |-\rangle , \quad |\varphi_{-}\rangle \otimes |+\rangle , \quad |\varphi_{-}\rangle \otimes |-\rangle , \tag{1.54}$$

with corresponding eigenvalues (in this order)

$$E_{1} = \frac{\hbar\omega}{2}(1+a) - \hbar\omega_{c} , \quad E_{2} = \frac{\hbar\omega}{2}(1+a) + \hbar\omega_{c} , \quad E_{3} = \frac{\hbar\omega}{2}(1-a) - \hbar\omega_{c} , \quad E_{4} = \frac{\hbar\omega}{2}(1-a) + \hbar\omega_{c} .$$
(1.55)

With a > 0 and  $\omega$ ,  $\omega_c > 0$ , the lowest possible energy is  $E_3 = \frac{\hbar\omega}{2}(1-a) - \hbar\omega_c$ .

14) If at t=0 the electron is measured on the right, it's spatial state is  $|\varphi_{R,0}\rangle$ . If its spin along the x-direction is measured to be  $+\frac{\hbar}{2}$  then it's spin state is (as before)  $|x:+\rangle = \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle)$ . Hence,

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|\varphi_{+}\rangle + |\varphi_{-}\rangle) \otimes \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle)$$

$$= \frac{1}{2} (|\varphi_{+}\rangle \otimes |+\rangle + |\varphi_{+}\rangle \otimes |-\rangle + |\varphi_{-}\rangle \otimes |+\rangle + |\varphi_{-}\rangle \otimes |-\rangle). \tag{1.56}$$

Then to get the state at time t, each eigenstate must be multiplied with  $e^{-iE_nt/\hbar}$ . This gives

$$|\psi(t)\rangle = \frac{1}{2} \left( e^{-iE_{1}t/\hbar} |\varphi_{+}\rangle \otimes |+\rangle + e^{-iE_{2}t/\hbar} |\varphi_{+}\rangle \otimes |-\rangle + e^{-iE_{3}t/\hbar} |\varphi_{-}\rangle \otimes |+\rangle + e^{-iE_{4}t/\hbar} |\varphi_{-}\rangle \otimes |-\rangle \right)$$

$$= \frac{e^{-i\omega t/2}}{2} \left( e^{-i\frac{\omega a}{2}t + i\omega_{c}t} |\varphi_{+}\rangle \otimes |+\rangle + e^{-i\frac{\omega a}{2}t - i\omega_{c}t} |\varphi_{+}\rangle \otimes |-\rangle + e^{i\frac{\omega a}{2}t + i\omega_{c}t} |\varphi_{-}\rangle \otimes |+\rangle + e^{i\frac{\omega a}{2}t - i\omega_{c}t} |\varphi_{-}\rangle \otimes |-\rangle \right)$$

$$(1.57)$$

If at time t the spin is measured in the x-direction and found to be  $-\frac{\hbar}{2}$  the state gets projected

with  $P(x:-\frac{\hbar}{2})=|x:-\rangle\langle x:-|=\frac{1}{\sqrt{2}}|x:-\rangle(\langle +|-\langle -|))$ . This gives

$$P(x:-\frac{\hbar}{2}) |\psi(t)\rangle = \frac{e^{-i\omega t/2}}{2\sqrt{2}} \left( e^{-i\frac{\omega a}{2}t + i\omega_c t} |\varphi_{+}\rangle \otimes |x:-\rangle - e^{-i\frac{\omega a}{2}t - i\omega_c t} |\varphi_{+}\rangle \otimes |x:-\rangle + e^{i\frac{\omega a}{2}t + i\omega_c t} |\varphi_{-}\rangle \otimes |x:-\rangle - e^{i\frac{\omega a}{2}t - i\omega_c t} |\varphi_{-}\rangle \otimes |x:-\rangle \right)$$

$$= \frac{e^{-i\omega t/2}}{2\sqrt{2}} \left( e^{-i\frac{\omega a}{2}t} \left( e^{i\omega_c t} - e^{-i\omega_c t} \right) |\varphi_{+}\rangle + e^{i\frac{\omega a}{2}t} \left( e^{i\omega_c t} - e^{-i\omega_c t} \right) |\varphi_{-}\rangle \right) \otimes |x:-\rangle$$

$$= \frac{ie^{-i\omega t/2} \sin \omega_c t}{\sqrt{2}} \left( e^{-i\frac{\omega a}{2}t} |\varphi_{+}\rangle + e^{i\frac{\omega a}{2}t} |\varphi_{-}\rangle \right) \otimes |x:-\rangle$$

$$(1.58)$$

This projected state is not normalised. It's norm is  $\sin \omega_c t$  and dividing by its norm and dropping the overall phase, we get the state

$$\left|\widetilde{\psi}(t)\right\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\frac{\omega a}{2}t} \left|\varphi_{+}\right\rangle + e^{i\frac{\omega a}{2}t} \left|\varphi_{-}\right\rangle\right) \otimes \left|x:-\right\rangle$$

$$= \frac{1}{2} \left(\left(e^{-i\frac{\omega a}{2}t} + e^{i\frac{\omega a}{2}t}\right) \left|\varphi_{R,0}\right\rangle + \left(e^{-i\frac{\omega a}{2}t} - e^{i\frac{\omega a}{2}t}\right) \left|\varphi_{L,0}\right\rangle\right) \otimes \left|x:-\right\rangle$$

$$= \left(\cos\frac{\omega a}{2}t \left|\varphi_{R,0}\right\rangle - i\sin\frac{\omega a}{2}t \left|\varphi_{L,0}\right\rangle\right) \otimes \left|x:-\right\rangle . \tag{1.59}$$

Then

$$\langle X \rangle_{\widetilde{\psi}(t)} = \frac{\ell}{2} \left( \cos^2 \frac{\omega a}{2} t - \sin^2 \frac{\omega a}{2} t \right) = \frac{\ell}{2} \cos \omega at . \tag{1.60}$$

15) The probability to find any of the 4 possible energy eigenvalues is equal to  $|\frac{1}{2}|^2 = \frac{1}{4}$ , according to (1.57). Now the projection is simply on the eigenstate of the full Hamiltonian with eigenvalue  $E_3$ , so that up to a phase the normalised state is

$$\left|\widehat{\psi}(t_1)\right\rangle = \left|\varphi_-\right\rangle \otimes \left|+\right\rangle ,$$
 (1.61)

Since this is an eigenstate of the Hamiltonian any further time evolution only multiplies it with a phase. Since  $|+\rangle = \frac{1}{\sqrt{2}} \left( |x:+\rangle + |x:-\rangle \right) = \frac{1}{\sqrt{2}} \left( |y:+\rangle + |y:-\rangle \right)$ , any of the proposed spin measurements has probability  $\frac{1}{2}$ .

# Problem 2: A particle in a Mexican hat potential

1) To show that  $L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$  is symmetric, we need to show that  $(L_z \psi, \chi) = (\psi, L_z \chi)$ . Since  $\psi$  and  $\chi$  are in  $L^2(\mathbf{R}) \otimes L^2(S^1)$  we have in particular that they are periodic in  $\phi$ . For  $L_z$  to be defined, we need that it acts on functions that are differentiable in  $\phi$ . Let's try  $\mathcal{D}(L_z) = L^2(\mathbf{R}) \otimes C^1(S^1)$ . Periodicity in  $\phi$  (absence of a boundary of the circle) implies that we can freely integrate by parts. Then

$$(L_z \psi. \chi) = \int_{-\infty}^{\infty} dr \int_{0}^{2\pi} d\phi \left(\frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi\right)^* \chi = \int_{-\infty}^{\infty} dr \int_{0}^{2\pi} d\phi \frac{\partial}{\partial \phi} \psi^* \left(-\frac{\hbar}{i}\right) \chi$$
$$= \int_{-\infty}^{\infty} dr \int_{0}^{2\pi} d\phi \psi^* \left(+\frac{\hbar}{i}\right) \frac{\partial}{\partial \phi} \chi = (\psi, L_z \chi) , \qquad (1.62)$$

and  $L_z$  is symmetric. There is no additional requirement on the domain of definition for  $L_z^{\dagger}$  and then  $L_z$  is self-adjoint. This example was actually discussed in the lecture notes (although without the radial part but which here is only spectator). The eigenvalue problem is

$$\widehat{L}_z \phi_k(\phi) \equiv \frac{\hbar}{i} \frac{\partial}{\partial \phi} f_k(\phi) = \alpha_k f_k(\phi) \quad \Rightarrow \quad f_k(\phi) \simeq e^{i\alpha_k \phi/\hbar} \ . \tag{1.63}$$

Periodicity imposes  $\alpha_k = \hbar k$  with  $k \in \mathbf{Z}$ , so that the orthonormal eigenfunctions are

$$f_k(\phi) = \frac{1}{\sqrt{2\pi}} e^{ik\phi} \quad , \quad \alpha_k = \hbar k \ .$$
 (1.64)

Then with  $\langle \phi | k \rangle_{\text{angular}} = f_k(\phi)$  we also have  $L_z | k \rangle_{\text{angular}} = \hbar k | k \rangle_{\text{angular}}$ . Then  $H_{\phi} = \frac{1}{2mr_0^2} L_z^2$ , so that

$$H_{\phi} |k\rangle_{\text{angular}} = \frac{\hbar^2 k^2}{2mr_0^2} |k\rangle_{\text{angular}}$$
 (1.65)

2) We obviously define  $\widehat{P}_r = \frac{\hbar}{i} \frac{\partial}{\partial r}$  and then  $\langle r | P_r | \psi \rangle = \widehat{P}_r \langle r | \psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial r} \psi$ . The "position" operator R should correspond to  $\widehat{R} = r - r_0$ , i.e.  $\langle r | R | \psi \rangle = \widehat{R} \psi(r) = (r - r_0) \psi(r)$ . Then  $[\widehat{R}, \widehat{P}_r] = \frac{\hbar}{i} [r - r_0, \frac{\partial}{\partial r}] = \frac{\hbar}{i} (-1) = i\hbar$  which translates into  $[R, P_r] = i\hbar \mathbf{1}$ .

With  $\gamma = \sqrt{\frac{\hbar}{m\omega}}$  we define

$$a = \frac{1}{\sqrt{2}} \left( \frac{R}{\gamma} + i \frac{\gamma P_r}{\hbar} \right) \quad , \quad a^{\dagger} = \frac{1}{\sqrt{2}} \left( \frac{R}{\gamma} - i \frac{\gamma P_r}{\hbar} \right)$$
 (1.66)

so that  $[a, a^{\dagger}] = \frac{1}{2\hbar}(-i[R, P_r] + i[P_r, R]) = \mathbf{1}$ . Then as in the lecture

$$|n\rangle_{\text{radial}} = \frac{(a^{\dagger})^n}{\sqrt{n!}} |0\rangle_{\text{radial}} \quad , \quad a |0\rangle_{\text{radial}} = 0 \quad , \quad H_r |n\rangle_{\text{radial}} = \hbar\omega \left(n + \frac{1}{2}\right) |n\rangle_{\text{radial}} \quad .$$
 (1.67)

3) The  $|n\rangle_{\text{radial}} \otimes |k\rangle_{\text{angular}} \equiv |n,k\rangle$  with  $n=0,1,2,\ldots$  and  $k\in \mathbf{Z}$  clearly constitute a basis of the full Hilbert space and

$$H |n, k\rangle \equiv (H_r \otimes \mathbf{1} + \mathbf{1} \otimes H_{\phi}) |n\rangle_{\text{radial}} \otimes |k\rangle_{\text{angular}} = (H_r |n\rangle_{\text{radial}}) \otimes |k\rangle_{\text{angular}} + |n\rangle_{\text{radial}} \otimes (H_{\phi} |k\rangle_{\text{angular}})$$

$$= \left(\hbar\omega(n + \frac{1}{2}) + \frac{\hbar^2 k^2}{2mr_0^2}\right) |n\rangle_{\text{radial}} \otimes |k\rangle_{\text{angular}}. \tag{1.68}$$

So this is indeed an eigenbasis of H with eigenvalues

$$E_{n,k} = \hbar\omega(n + \frac{1}{2}) + \frac{\hbar^2 k^2}{2mr_0^2} . {1.69}$$

For generic  $\omega$  these eigenvalues are non-degenerate.

4) Now we take  $H_2 = -\frac{1}{mr_0^3}RL_z^2$  with matrix elements

$$\langle nk | H_{2} | n'k' \rangle = -\frac{1}{mr_{0}^{3}} \langle n | R | n' \rangle \langle k | L_{z}^{2} | k' \rangle = -\frac{1}{mr_{0}^{3}} \frac{\gamma}{\sqrt{2}} \langle n | (a + a^{\dagger}) | n' \rangle \langle \hbar k' \rangle^{2} \delta_{kk'}$$

$$= -\frac{\hbar^{2}k^{2}}{mr_{0}^{3}} \frac{\gamma}{\sqrt{2}} (\sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1}) \delta_{kk'}$$
(1.70)

To first order in perturbation theory the eigenvalues  $E_{n,k}$  change by an amount

$$E_{n,k}^{(1)} = \langle nk | H_2 | nk \rangle = 0 ,$$
 (1.71)

since  $\langle nk | H_1 | n'k' \rangle$  vanishes for n = n'. At second order in perturbation theory we have

$$E_{n,k}^{(2)} = -\sum_{(n',k')\neq(n,k)} \frac{\left| \langle nk| H_2 | n'k' \rangle \right|^2}{E_{n'k'} - E_{n,k}} = -\sum_{n'=n\pm 1} \frac{\left| \langle nk| H_2 | n'k \rangle \right|^2}{E_{n'k} - E_{n,k}}$$

$$= -\left(\frac{\hbar^2 k^2}{m r_0^3} \frac{\gamma}{\sqrt{2}}\right)^2 \left[\frac{n+1}{\hbar \omega} + \frac{n}{(-\hbar \omega)}\right] = -\left(\frac{\hbar^2 k^2}{m r_0^2}\right)^2 \frac{\gamma^2}{2 r_0^2} \frac{1}{\hbar \omega} = -\left(\frac{\hbar^2 k^2}{m r_0^2}\right)^2 \frac{1}{2m \omega^2 r_0^2} . (1.72)$$

5) Clearly  $H_1 = -\frac{q\mathcal{E}}{2}(r_0 + R)(e^{i\widehat{\phi}} + e^{-i\widehat{\phi}})$  where  $\widehat{\phi}$  is such that  $\langle \phi | \widehat{\phi} | \psi \rangle = \phi \psi(\phi)$ . We have  $R = \frac{\gamma}{\sqrt{2}}(a + a^{\dagger})$  and then

$$\langle nk|H_1|n'k'\rangle = -\frac{q\mathcal{E}}{2}\langle n|\left(r_0 + \frac{\gamma}{\sqrt{2}}(a+a^{\dagger})\right)|n'\rangle \langle k|\left(e^{i\widehat{\phi}} + e^{-i\widehat{\phi}}\right)|k'\rangle . \tag{1.73}$$

Now,

$$\langle n | \left( r_0 + \frac{\gamma}{\sqrt{2}} (a + a^{\dagger}) \right) | n' \rangle = r_0 \delta_{nn'} + \frac{\gamma}{\sqrt{2}} \left( \sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1} \right) , \qquad (1.74)$$

and

$$\langle k | \left( e^{i\widehat{\phi}} + e^{-i\widehat{\phi}} \right) | k' \rangle = \int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi} \ e^{-ik\phi} \left( e^{i\widehat{\phi}} + e^{-i\widehat{\phi}} \right) e^{ik'\phi} = \delta_{k,k'+1} + \delta_{k,k'-1} \ . \tag{1.75}$$

Putting things together we get

$$\langle nk | H_1 | n'k' \rangle = -\frac{q\mathcal{E}}{2} \left[ r_0 \delta_{nn'} + \frac{\gamma}{\sqrt{2}} \left( \sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1} \right) \right] \left[ \delta_{k,k'+1} + \delta_{k,k'-1} \right] . \tag{1.76}$$

6) To first order in perturbation theory the eigenvalues  $E_{n,k}$  change by an amount

$$E_{n,k}^{(1)} = \langle nk | H_1 | nk \rangle = 0 ,$$
 (1.77)

since  $\langle nk | H_1 | n'k' \rangle$  vanishes for k = k'. At second order in perturbation theory we have

$$E_{n,k}^{(2)} = -\sum_{(n',k')\neq(n,k)} \frac{\left| \langle nk| H_1 | n'k' \rangle \right|^2}{E_{n'k'} - E_{n,k}}$$
(1.78)

There are 6 terms contributing to the sum, namely (n', k') being (n, k+1), (n, k-1), (n+1, k+1), (n+1, k-1), (n-1, k+1), (n-1, k-1). This leads to

$$E_{n,k}^{(2)} = -\frac{q^2 \mathcal{E}^2}{4} \left[ \frac{r_0^2}{\frac{\hbar^2 (2k+1)}{2mr_0^2}} + \frac{r_0^2}{\frac{\hbar^2 (-2k+1)}{2mr_0^2}} + \frac{\frac{n+1}{2}\gamma^2}{\frac{\hbar\omega + \frac{\hbar^2 (2k+1)}{2mr_0^2}}{\hbar\omega + \frac{\hbar^2 (2k+1)}{2mr_0^2}}} + \frac{\frac{n+1}{2}\gamma^2}{\hbar\omega + \frac{\hbar^2 (-2k+1)}{2mr_0^2}} + \frac{\frac{n}{2}\gamma^2}{-\hbar\omega + \frac{\hbar^2 (2k+1)}{2mr_0^2}} + \frac{\frac{n}{2}\gamma^2}{-\hbar\omega + \frac{\hbar^2 (-2k+1)}{2mr_0^2}} \right] . (1.79)$$

Recall that  $\gamma^2 = \frac{\hbar}{m\omega}$  and introduce the dimensionless quantity  $\eta = \frac{\gamma^2}{r_0^2}$ . Then one can rewrite this as

$$E_{n,k}^{(2)} = -\frac{mq^2 \mathcal{E}^2 r_0^4}{2\hbar^2} \left[ \frac{1}{2k+1} + \frac{1}{-2k+1} + \frac{\frac{n+1}{2}\eta}{\frac{2}{\eta} + 2k+1} + \frac{\frac{n+1}{2}\eta}{\frac{2}{\eta} - 2k+1} + \frac{\frac{n}{2}\eta}{-\frac{2}{\eta} + 2k+1} + \frac{\frac{n}{2}\eta}{-\frac{2}{\eta} - 2k+1} \right]$$

$$= \frac{mq^2 \mathcal{E}^2 r_0^4}{\hbar^2} \left[ \frac{1}{4k^2 - 1} + \frac{\frac{n+1}{2}(2+\eta)}{4k^2 - (1+\frac{2}{\eta})^2} + \frac{\frac{n}{2}(2+\eta)}{4k^2 - (1-\frac{2}{\eta})^2} \right]. \tag{1.80}$$