

PHY 303, I-Semester 2023/24, Tutorial 7 solution

8th Nov 2021

Stage 1 (catch-up) Among the topics below and past tutorials, decide on the most important and/or interesting topic you want to learn better and do that one first.

Stage 2 (Hydrogen atom to periodic table) Review the allowed electronic quantum states of the Hydrogen atom from the lecture, their energies and the ranges and constraints on quantum numbers.

Solution: See week 10.

(a) Then checkout the Hydrogen part of the app: <http://www.falstad.com/qmatom/> that we had earlier looked at for 1D quantum problems.

(i) Switch the top menu to “complex orbitals (physics)” and keep it there. Starting from the lowest energy state, see the visualisation and connect it with the equations for wavefunctions provided in the lecture. Checkout also the highest available (Rydberg) states.

Solution: See screenshots below, these correspond to examples 34 and 35 in the lecture, please read those and link to screenshots.

(ii) For each state, think about the underlying/corresponding state of “classical motion” of an electron that corresponds to the quantum mechanical standing wave, as we had done in example 13 for the 1D square well potential. Also think about the expected probability current.

Solution: Take the entire following discussion with a grain of salt. It can give helpful intuition in some cases, but rigorously there is no fixed electron position: (a) For $|1s0\rangle$ we have zero angular momentum but, due to the HUP, some nonzero fluctuations of momentum (momentum uncertainty). Nonzero momentum but zero angular momentum, classically corresponds to linear motion through the origin. While being careful with this picture, think of the $|1s0\rangle$ as the electron going on straight lines through the origin, equally in all possible 3D directions. (b) $|2s0\rangle$ follows the same picture, except that the “standing wave” of electronic motion (motion fluctuations) through the origin now went to the next higher wavenumber, such that it has one (radially symmetric) node. (d,e) Here we have non-zero angular momentum, pointing as much as possible up or down the z-axis. Classically this would imply circular or elliptical motion

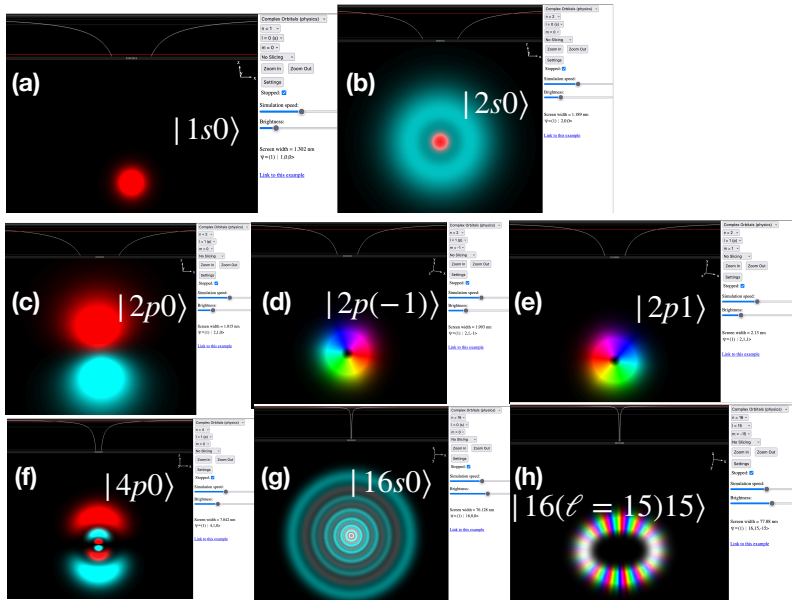


Figure 1: Visualisation of Hydrogen wavefunctions for the states indicated. The intensity of the shading is related to probability density (up to some cutoff, i.e. not to scale). Red implies ”+” sign of the wavefunction, cyan ”-”. Rainbow colors indicate a continuously varying complex phase.

around the nucleus. Quantum mechanically this is expressed by the $e^{\pm i\varphi}$ component of the wavefunction. (c) Zero z -component implies an angular momentum lying in the xy plane, let’s say along x , which classically implies orbital motion e.g. in the yz plane. However we do not know in which direction in the xy plane the angular momentum is pointing, so we have to superimpose all such orbits, which gives something as the $|2p_0\rangle$.

You can find the app documentation [here](#) .

(b) (bonus/advanced) We can very crudely understand the [periodic table](#) from the Hydrogen atom with the following assumptions/facts:

(i) We can redo our calculation for Hydrogen assuming the nucleus of a heavier atom with charge $-Ze$ and would then find an energy:

$$E_n = -Z^2 \frac{\mathcal{R}}{n^2}, \quad (1)$$

- (ii) Due to the Pauli exclusion principle (week 12), two electrons (one spin up, one spin down) can fill each Hydrogen state. We say that all electrons with a given principal quantum number n form a “shell” .
- (iii) Let us *oversimplify* the effect of electron-electron interactions as follows: All electrons in shells below the outer one ($n < n_{\text{outer}}$, let their number be N_{inner}) screen the nucleus, such that electrons in the outermost shell

feel an effective charge $Z' = Z - N_{\text{inner}}$. Electrons within the outermost shell do no screen but also do not interact with each other.

- (iv) Screening is not quite as effective for electrons in an s-state (why?), hence those will have a slightly lower energy than p electrons in heavy atoms.

Based on these assumptions, discuss how you can understand the first three periods of the periodic table, in particular the features that elements in the same column have very similar ionisation energies (which is low for Alkali's, high for noble gases).

Solution: (later)

Stage 3 (Q-bit for a quantum computer) Review spin in the lecture notes. Particular consider spin $s = 1/2$, which is the simplest case, since it allows only two different basis states for the description of the spin direction. We can map these onto “logical states” $|0\rangle \leftrightarrow |\downarrow\rangle$ and $|1\rangle \leftrightarrow |\uparrow\rangle$, which form a “quantum bit” or q-bit.

- (i) Convince yourself that $|\Psi\rangle = c_0|0\rangle + c_1|1\rangle$, with $|c_0|^2 + |c_1|^2 = 1$ is the most general quantum state for the q-bit, and discuss on your table why you can write this as

$$|\Psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\varphi}|1\rangle, \quad (2)$$

for $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$, without loss of generality.

Solution: We know from section 4.7.2 that $|0\rangle$ and $|1\rangle$ are a basis of the spin-1/2 Hilbertspace, hence $|\Psi\rangle = c_0|0\rangle + c_1|1\rangle$ is the most general state. For this to be normalised we require $|c_0|^2 + |c_1|^2 = 1$. Let us write both coefficients in polar representation $c_{0,1} = a_{0,1}e^{i\varphi_{0,1}}$, with $a_{0,1} > 0 \in \mathbb{R}$ and $0 \leq \varphi_{0,1} \in \mathbb{R} \leq 2\pi$. Normalisation then reduces to $a_0^2 + a_1^2 = 1$. We can parametrise all positive real numbers fulfilling this relation through an angle θ and setting $a_0 = \cos\frac{\theta}{2}$ and $a_1 = \sin\frac{\theta}{2}$, with $0 \leq \theta \leq \pi$.

The state then reads

$$|\Psi\rangle = \cos\frac{\theta}{2}e^{i\varphi_0}|0\rangle + \sin\frac{\theta}{2}e^{i\varphi_1}|1\rangle = e^{i\varphi_0} \left(\cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{\underbrace{i(\varphi_1 - \varphi_0)}_{\equiv \varphi}}|1\rangle \right) \quad (3)$$

We know the global phase $e^{i\varphi_0}$ does not matter (section 1.6.1) and we can re-name the relative phase between the $|1\rangle$ and $|0\rangle$ state into φ as shown, and then reached the form Eq. 2.

- (ii) Which outcomes can you find when measuring the q-bit, and with which probability?

Solution: The only two possible answers are $m_s = 1/2$ or $m_s = -1/2$ (or you may call this 0 and 1). As usual the probability for each can be found as $p_{0/1} = |c_{0/1}|^2$ from the mod-square of the coefficients attached to the corresponding eigenstate.

- (iii) Discuss how you can visualize any state of the form Eq. 2 as a point on a unit sphere, then represent $|0\rangle$, $|1\rangle$, $(|0\rangle + |1\rangle)/\sqrt{2}$, $(|0\rangle - |1\rangle)/\sqrt{2}$ in this way.

Solution: We have seen in the preceding step, that the state is parametrised by two angles $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$. These can also be used to parametrise the position on the surface of a unit sphere (i.e. use 3D spherical polar coordinates fixing $r = 1$). Using this, the 4 states listed above can be distinguished as shown in Fig. 2. This representation of a spin-1/2 is very popular in many fields, and called the Bloch sphere.

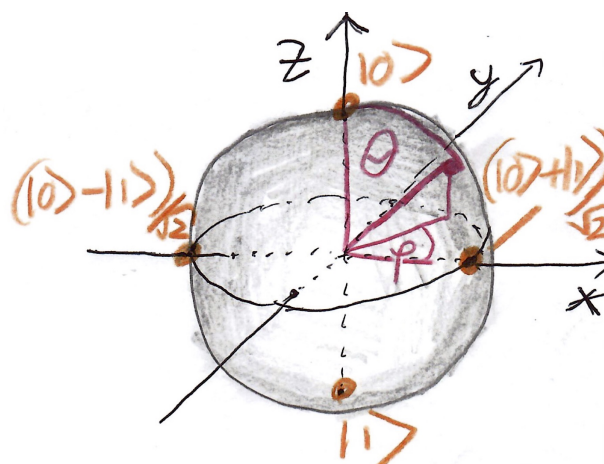


Figure 2: Bloch sphere representation of quantum states as discussed in the text.

- (iv) In terms of Pauli matrices (see lecture), a sufficiently general Hamiltonian for a q-bit can be written as:

$$\hat{H} = \frac{\hbar\Omega(t)}{2}\hat{\sigma}_x + \frac{\Delta E(t)}{2}\hat{\sigma}_z. \quad (4)$$

Discuss the physical meaning of the two terms. Suppose you can control their prefactors in time as indicated, how can this Hamiltonian be used to reach any desired q-bit state? (Such an operation realizes a single q-bit gate).

Solution: The second term implies an energy difference between the $|\uparrow\rangle$

and $|\downarrow\rangle$ state (in a preview of QM-II, this could be for example due to the interaction of the magnetic moment associated with the spin with an external magnetic field along the z-axis.) The first term could be either the same, but for a magnetic field along the x-axis, or some external coupling that changes $|\uparrow\rangle$ into $|\downarrow\rangle$, e.g. resonant electromagnetic radiation between the two states.

This can be seen as follows: Suppose there is only the first term, let us set $\Omega(t) = \Omega = \text{const}$, and we start in $|0\rangle$. This can be written as

$$|0\rangle = |\downarrow\rangle \stackrel{\text{Eq. 4.114}}{=} \frac{1}{\sqrt{2}} (|\leftarrow\rangle - |\rightarrow\rangle). \quad (5)$$

In time this will evolve as

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}} (|\leftarrow\rangle e^{i\frac{\Omega}{2}t} - |\rightarrow\rangle e^{-i\frac{\Omega}{2}t}). \quad (6)$$

which provides a probability to be in $|0\rangle$ of

$$\begin{aligned} p_0 = |\langle 0 | \Psi(t) \rangle|^2 &= \left| \frac{1}{\sqrt{2}} \left(\underbrace{\langle 0 | \leftarrow \rangle}_{=1} e^{i\frac{\Omega}{2}t} - \underbrace{\langle 0 | \rightarrow \rangle}_{=-1} e^{-i\frac{\Omega}{2}t} \right) \right|^2 \\ &= \cos^2 \left(\frac{\Omega}{2}t \right). \end{aligned} \quad (7)$$

Since $p_1 = 1 - p_0$ we can write that as $p_1 = \sin^2 \left(\frac{\Omega}{2}t \right)$. Since action of the first term thus changes the probability to be in either state $|0\rangle$ or $|1\rangle$, we conclude that it induces transitions between the two states. Comparison with Eq. 2 shows that we can control θ , identifying this with $\theta = \Omega t$.

Controlling φ works via the second term in the Hamiltonian (by itself), simply using the fact that $|0\rangle$ and $|1\rangle$ are eigenstates of that part of the Hamiltonian. Which means as long as only the second term is present.

$$\begin{aligned} |\Psi(t)\rangle &= c_0(0)e^{i\Delta E/2/\hbar t} |0\rangle - c_1(0)e^{-i\Delta E/2/\hbar t} |1\rangle \\ &= e^{i\Delta E/2/\hbar t} (c_0(0)|0\rangle - c_1(0)e^{-i\Delta E/\hbar t} |1\rangle). \end{aligned} \quad (8)$$

We can now control $\varphi = -\Delta E t/\hbar$. Note that we can use the time-independent formalism since we assume the first and last term to be switched on and off but then kept constant.

- (v) (bonus/advanced). To realize a quantum computer, we also require 2 q-bit gates. Discuss which are the basis states for a system of 2 q-bits and how you would generalise the truth table for a classical AND (OR, XOR, ETC.) operation to the quantum case. Why do these truth tables fully specify a 2 q-bit quantum gate? Why does a q-bit carry (much) more information than a classical bit?

Solution: (later)