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

8th Nov 2021

Discuss on your table in AIR. When all teams finished a stage, make sure all students at your table understand the solution and agree on one by using the board.

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.

(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.

  (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.

  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:

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

  (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 *oversimply* 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).

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

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

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

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

(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.

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

$$\hat{H} = \frac{\Omega(t)}{2}\hat{\sigma}_x + \frac{\Delta E(t)}{2}\hat{\sigma}_z. \tag{3}$$

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).

(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?