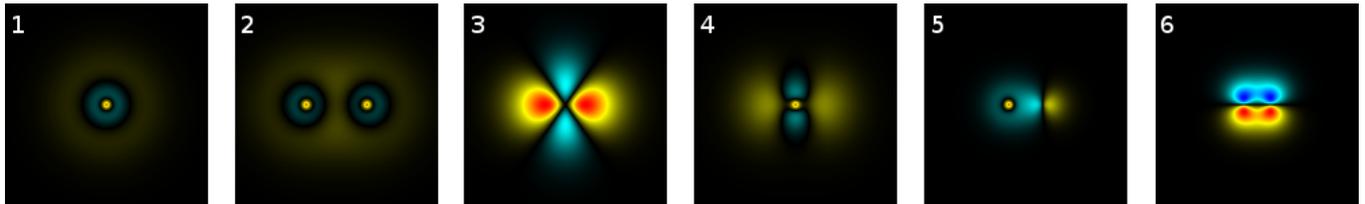


ph237 Quantum Physics workshop 3 (RW)

1. The shape of wave functions

Match the following cross sections of the xz plane of various states of the hydrogen atom with the descriptions below. Some are pure atomic states, some are hybrid states, and some are molecular states. To distinguish them, see if there is one nucleus or two, and how many radial and planar nodes you can detect.

One image and one description do not match; provide a sketch of the wave function that is not pictured and a description of the one shown in the surplus picture.



- A- a pure 3s state
- B- a pure 3d state
- C- a hybrid 3sd state
- D- an antibonding $2\sigma_{sp}$ state
- E- a bonding $2\pi_{pp}$ state
- F- a bonding $3\sigma_{ss}$ molecular state

2. Pick and mix - approximate solutions of complicated quantum systems

In order to describe a cold molecule ion (*i.e.* an ionised hydrogen molecule) near $T=0$ K as a quantum-mechanical system, several of the fundamental, analytically solvable quantum systems may be superimposed.

- (a) Which “ingredient” fundamental systems are best used for this purpose? In which order are they invoked?
- (b) Choose a suitable reference frame and sketch the geometry of the system and its position in the reference frame. Let d be the bond length.
- (c) Plot the potential against each of the three coordinates of your chosen reference frame (keeping the other coordinates constant).
- (d) Explain how the treatment of the system would change if the temperature was higher.

3. Perturbation - the anharmonic oscillator

Mathematical techniques to derive Schrödinger solutions (*i.e.* eigenfunction/eigenvalue pairs) for new systems from solutions for known systems include the variation and perturbation techniques.

- (a) Explain the difference between the harmonic and the anharmonic oscillator models. Illustrate the need for the anharmonic correction by reference to the vibration states of a linear two-atom molecule.
- (b) Calculate the 1st order energy correction

$$E_n^{(1)} = \int_{-\infty}^{\infty} \psi_n^{(0)*} \hat{H}_1 \psi_n^{(0)} dx$$

of the anharmonic oscillator. Use the perturbation

$$\hat{H}_1 = cx^3 + dx^4$$

for this purpose.

Note:

$$\int_0^{\infty} x^{2n} e^{-bx^2} dx = \frac{1 \cdot 3 \cdots (2n-1)}{2^{n+1}} \sqrt{\frac{\pi}{b^{2n+1}}}$$

(c) The 1st order term in perturbation theory is

$$(E_m^{(0)} - E_n^{(0)}) \int \psi_m^{(0)*} \psi_n^{(1)} dx = E_n^{(1)} \int \psi_m^{(0)*} \psi_n^{(0)} dx - \int \psi_m^{(0)*} \hat{H}_1 \psi_n^{(0)}$$

The energy correction calculated above comes from the $m = n$ case. What is the physical significance of the $m \neq n$ case?

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