QUANTUM VERSUS CLASSICAL MECHANICS IN SOLIDS AND GASES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 1.18.

The de Broglie wavelength of a particle, which is the wavelength of an idealized free particle which has a precise momentum p and thus a completely indeterminate position, is

$$\lambda=\frac{h}{p} \tag{1}$$

In general, quantum mechanics is needed to describe systems in which the de Broglie wavelength of the constituent particles is larger than some characteristic size of the system itself. For example, if the wavelength of a free electron (that is, an electron not bound to a particular atom) in a solid is greater than the average spacing between atoms, then quantum mechanics is needed to describe these electrons. If the wavelength is much smaller than the size of the system, the wave nature of a particle isn't noticeable and we can get away with using classical mechanics.

In statistical mechanics, the average energy of each particle in a system is $\frac{1}{2}k_BT$ per degree of freedom of the particle, where k_B is Boltzmann's constant and T is the temperature in kelvins. For a single particle such as an electron, there are three degrees of freedom (one per coordinate direction) so its average energy is

$$E=\frac{p^2}{2m}=\frac{3}{2}k_BT \tag{2}$$

Combining this with the definition of the de Broglie wavelength above, we get

$$\lambda=\frac{h}{\sqrt{3mk_BT}} \tag{3}$$

so the condition for quantum mechanics to apply is that $\lambda>d$ where d is the size of the system.

Example 1. Solids. Using the typical lattice spacing of $d = 3 \times 10^{-10}$ m for a solid, what is the maximum temperature at which we need to use quantum mechanics to describe free electrons in such a solid? For quantum mechanics to apply, we need

$$d < \frac{h}{\sqrt{3mk_BT}} \tag{4}$$

$$T < \frac{h^2}{3mk_Bd^2} \tag{5}$$

We have the values (in SI units)

$$h = 6.626 \times 10^{-34} \tag{6}$$

$$m = 9.1 \times 10^{-31} \tag{7}$$

$$k_B = 1.38 \times 10^{-23} \tag{8}$$

$$d = 3 \times 10^{-10} \tag{9}$$

so we get

$$T < 1.29 \times 10^5 \text{ K} \tag{10}$$

so electrons most definitely need to be described quantum mechanically.

For the atomic nuclei in a solid, the critical temperature is much lower. For sodium, with an atomic mass of about 23 atomic mass units (where 1 amu $= 1.66 \times 10^{-27}$ kg), we have

$$T < 3.1 \text{ K} \tag{11}$$

Example 2. The ideal gas. The ideal gas law is

$$PV = Nk_BT \tag{12}$$

where P is the pressure, V is the volume and N is the number of gas molecules. We can get an estimate of d by calculating the average volume per molecule v:

$$v = \frac{V}{N} \tag{13}$$

$$d = v^{1/3} \tag{14}$$

$$= \left(\frac{k_BT}{P}\right)^{1/3} \tag{15}$$

Therefore, the condition for quantum mechanics to apply to an ideal gas is

$$\left(\frac{k_BT}{P}\right)^{1/3} < \frac{h}{\sqrt{3mk_BT}} \tag{16}$$

$$T < \frac{h^{6/5}P^{2/5}}{k_B(3m)^{3/5}} \tag{17}$$

For helium at atmospheric pressure we have

$$P = 10^5\text{N m}^{-2} \tag{18}$$

$$m = 4\times\left(1.66\times10^{-27}\right)\text{ kg} \tag{19}$$

$$T < 2.92\text{ K} \tag{20}$$

This is actually below the boiling point of helium (4.55 K) so whenever helium is a gas, we don't need quantum mechanics to describe it.

For hydrogen atoms (protons) in outer space, $d = 1$ cm and $T = 3$ K. In this case, the critical temperature is given by 5 with $m = 1.66\times10^{-27}$ kg:

$$T < \frac{h^2}{3mk_Bd^2} = 6.4\times10^{-14}\text{ K} \tag{21}$$

Definitely no quantum mechanics needed here.