

The problem of the difference between the kinetic energy of an electron in the constrained box obtained from the uncertainty relationship and that derived from the Schrödinger equation -- 2017.01.28 --

Let us determine the kinetic energy of electrons trapped in the wall of infinite potential by the Heisenberg's uncertainty relationship, $\Delta p \cdot \Delta x \geq \frac{\hbar}{2}$.

Even in one dimension the conclusion may not change essentially, so we discuss this case. The kinetic energy (T) of an electron with mass m and velocity u is $(1/2)mu^2$. It is rewritten in terms of momentum ($p = mu$) and becomes $(1/2m)p^2$. Let us calculate the kinetic energy using "ambiguity of momentum" (Δp).

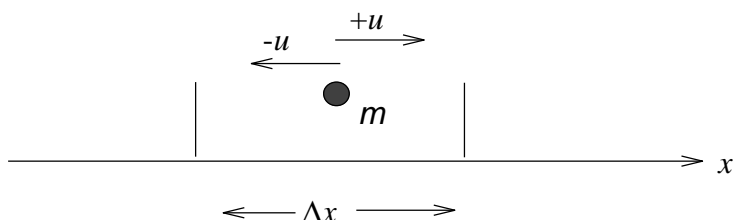


Fig. 1. The particle that moves within region Δx .

The range of movement is defined as Δx , and the momentum includes ambiguity Δp (that is, it is in the range of $p \pm \Delta p$ as p is the correct value). The mean value of the square of p ($\overline{p^2}$) is obtained by averaging the momentum including ambiguity. Since the particles cause rightward motion and leftward motion occur with the same probability, the momentum is averaged to 0 ($\overline{p} = 0$).

$$(\Delta p)^2 = (p - \overline{p})_{aver}^2 = \overline{p^2}$$

Using the above relationship, the average energy (\overline{E}) is,

$$\overline{E} = \frac{1}{2m}(\Delta p)^2$$

This is put into the uncertainty relationship.

$$\Delta p \cdot \Delta x \geq \frac{\hbar}{2} \quad \Rightarrow \quad \Delta p \geq \frac{\hbar}{2\Delta x}$$

$$\overline{E} \geq \frac{\hbar^2}{8m(\Delta x)^2}$$

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Next, we seek the energy of an electron in the same box from the Schrödinger equation. This is given by solving the next equation,

$$E\psi(x) = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x)$$

If the size of the box is set Δx , then,

$$E(n_x) = (n_x^2) \frac{\hbar^2}{8m\Delta x^2} \quad 2$$

is given.

Compare 1 and 2 equations. When $n_x = 1$, The energy by Eq.1 is small by the factor of $1/4\pi^2$. Where does this difference come from?

Recently, Ozawa has shown that the uncertainty relationship so far is incomplete and submitted a new one (Ozawa's inequality).¹⁾ The inequality is,

$$\Delta x \cdot \Delta p + \Delta x' \cdot \Delta p + \Delta x \cdot \Delta p' \geq \frac{\hbar}{2} \quad 3$$

$\Delta x'$ and $\Delta p'$ are the intrinsic quantum fluctuation of particles. Since these terms in the left expression are not included, is Eq. 1 small? If so, the intrinsic quantum fluctuation may be derived from the difference between 1 and 2 equations.

- 1) Ozawa, Masanao (2003), "Universally valid reformulation of the Heisenberg uncertainty principle on noise and disturbance in measurement", *Physical Review A* **67** (4).