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Practice for Qualifying Exams

Problem Source: **CMU Qualifying Exam August 2002**

This problem considers electrons confined to a box of length a with a square well potential

$$V(x) = \begin{cases} 0 & \{0 \le x \le a\} \\ \infty & otherwise \end{cases}$$

In addition to the confining potential, a strong magnetic field ensures that all electrons have parallel spins. Neglect interactions between electrons.

(a) Write down the complete set of single-particle wave functions $\psi_n(x)$, properly normalized, and give their energies.

These are the well-known solutions to the particle in the box problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x\right) \quad E_n = \frac{\hbar^2}{2m}\frac{\pi^2 n^2}{a^2}$$

(b) Write down the properly normalized two-electron ground state wave function $\psi_0(x_1, x_2)$ in terms of the single-electron wave functions $\psi_n(x)$, and give its energy.

The antisymmetric combination of these two wave functions (assuming both electrons are forced to be in the down state) is

$$\psi_0(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right]\left|--\right\rangle$$

with energy $E = E_1 + E_2 = 5\frac{\hbar^2\pi^2}{2ma^2}$

(c) Calculate the electronic density of states $D(E)$, the number of single-particle states per unit energy per length of box. Work in the limit of large box length a, so that the energies of the single particle states are effectively continuous.

$$D(E) = \frac{\partial}{\partial a}\frac{n(E)}{E}$$

$$n(E) = \frac{a}{\hbar\pi}\sqrt{2mE}$$

$$D(E) = \frac{\partial}{\partial a}\left[\frac{a}{\hbar\pi}\sqrt{\frac{2m}{E}}\right] = \sqrt{\frac{2m}{\hbar^2\pi^2 E}}$$

(d) Calculate the total kinetic energy per electron *(I assume this means in the ground state)*. **Your answer should be expressed as a function of the density of electrons** $\rho = \frac{N_e}{a}$**, where** N_e **is the number of electrons in the box. Work in the limit of large box length a, so that the energies of the single particle states are effectively continuous.**

In this ground state, exactly one particle occupies each available energy state. Then,

$$N_e = a\int_0^{E_{\max}} D(E)dE = 2a\sqrt{\frac{2mE_{\max}}{\hbar^2\pi^2}}$$

Solving this, I have

$$E_{\max} = \frac{\hbar^2\pi^2}{2m}\left(\frac{1}{2}\frac{N_e}{a}\right)^2 = \frac{\hbar^2\pi^2}{8m}\rho^2$$

Now,

$$\langle E\rangle = a\int_0^{E_{\max}} ED(E)dE = \frac{2}{3}a\sqrt{\frac{2m}{\hbar^2\pi^2}}(E_{\max})^{\frac{3}{2}}$$

What I want, though, is

$$\frac{\langle E\rangle}{N_e} = \frac{2}{3}\frac{a}{N_e}(E_{\max})^{\frac{3}{2}} = \frac{2}{3}\rho\sqrt{\frac{2m}{\hbar^2\pi^2}}\left(\frac{\hbar^2\pi^2}{8m}\rho^2\right)^{\frac{3}{2}} = \frac{\hbar^2\pi^2}{24m}\rho^4$$