Onset of degeneracy in confined systems

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In this paper, we examine the onset of degeneracy in confined systems under the condition that the de Broglie wavelength λ_D of an electron is comparable to the size of the confinement. In quantum-well structures the ratio of the critical concentration in a confined system to that in a bulk at which the onset of degeneracy takes place is proportional to λ_D/d, where d is the thickness of the quantum well. For a quasi-one-dimensional system (area confinement), the critical concentration is found to be proportional to λ_D^2/A, where A is the area of the confinement, i.e., $A=\pi R_0^2$ in a cylindrical thin wire of radius R_0, $A=\pi\lambda^2$ in a magnetic field B with $\lambda=(\hbar c/eB)^{1/2}$, and $A=ab$ for a rectangular thin wire with transverse lengths a and b. The critical concentration for onset of degeneracy is found to increase with stronger confinement (smaller size) under quantum-confinement conditions.

In recent years, there has been an active interest in the study of microsystems which are limited by their size. An electron confinement in a magnetic field has been known for a long time.[1] There have been two regimes under active study—the classical regime and the quantum regime. In a classical regime, the de Broglie wavelength of an electron is much smaller than the radius of the orbit in which it is confined. In this regime, the semiclassical Boltzmann transport equation is adequate to describe the transport behavior of electrons. The statistical description of electrons can be given by a Fermi-Dirac distribution function. In a strongly degenerate system, the theoretical considerations show little effect of magnetic field on resistivity.[1] In a classical nondegenerate regime, a predicted quadratic dependence of the magnetoresistance on magnetic field appears to be consistent with several observations.[1] On the other hand, in a quantum regime, the de Broglie wavelength of an electron is comparable to the quantized radius of an electron in a magnetic field. A large deviations from the classical behavior have been observed in this regime.[2,3]

Similarly, a large number of classical studies have been presented[4] in thin films and thin wires. Nowadays, these studies are being extended[5–10] into the quantum regime with surprising new results. One of the outcome of these studies is the observation of a nonmetallic behavior in electronic transport in confined metallic systems.[11] A similar degenerate-nondegenerate transition is predicted[12,13] for electrons confined to a magnetic field and its experimental observation reported.[14,15] It is, therefore, of interest to evaluate the critical concentration at which onset of degeneracy takes place in confined systems.

The explicit relation which relates n_e, the electronic concentration per unit volume to the Fermi energy ζ is[12]

$$n_e=\Omega^{-1}\int_0^\infty N(\epsilon)\{1+\exp[(\epsilon-\zeta)/k_BT]\}^{-1}d\epsilon\ , \quad (1)$$

where Ω is the crystal volume. $N(\epsilon)$ is the density of states which for parabolic isotropic bands is given by

$$N(\epsilon)=[(2m^*)^{3/2}/2\pi^2\hbar^3]\epsilon^{1/2}\ , \quad (2)$$

where m^* is the effective electronic mass.

The criterion which we set for the onset of degeneracy is that the Fermi energy $\zeta=0$ in a *bulk* (infinite size) semiconductor.[16,17] The critical concentration $n_e^*(\infty,T)$ for the onset of degeneracy is then given by

$$n_e^*(\infty,T)=F_{1/2}/2\pi^2\lambda_D^3\ , \quad (3)$$

with

$$F_k=\int_0^\infty dx\,x^k[\exp(x)+1]^{-1}\ , \quad (4)$$

$$\lambda_D=\hbar/(2m^*k_BT)^{1/2}\ . \quad (5)$$

The values of F_k for half-integer values of k are tabulated by McDougall and Stoner[18] and by Beer,

Chase, and Choquard.[19] In particular, $F_{1/2}=0.678$. At $T=300$ K, this concentration is $n_e^*(\infty,300)=1.92\times10^{19}$ cm^{-3} and at $T=1$ K, its value drops to $n_e^*(\infty,1)=3.7\times10^{15}$ cm^{-3} for $m^*=m_e$, the free-electron mass. Equation (1) essentially shows that $\lambda\!\!\!^{-}_D\sim n_e^{1/3}$ for onset of degeneracy. The thermal de Broglie wavelength $\lambda\!\!\!^{-}_D$ of an electron at 1 K is $\lambda\!\!\!^{-}_D\sim2\times10^{-6}$ cm. This value of de Broglie wavelength will be still higher for an effective mass lower than m_e.

In a *quantum-well structure* with rigid boundaries, as is the case in a thin film of thickness d, the energy levels are quantized[7]:

$$\epsilon_{lk_xk_y}=l^2\epsilon_0+\hbar^2(k_x^2+k_y^2)/2m^*\ , \quad l=1,2,3,\ldots \tag{6}$$

with

$$\epsilon_0=\pi^2\hbar^2/2m^*d^2\ . \tag{7}$$

The quantum well thus exhibits a quasi-two-dimensional (QTD) character and the density of states $N(\epsilon)$ is given by

$$N(\epsilon)=(m^*A/\pi\hbar^2)[\sqrt{\epsilon/\epsilon_0}]\ , \tag{8}$$

where A is the surface area of the quantum well and [ ] represents the integer part only. Equation (8) contains a spin factor of 2. Obviously $N(\epsilon)=0$ for $\epsilon<\epsilon_0$. An appropriate criterion for onset of degeneracy is then $\zeta-\epsilon_0=0$. If this criterion is used in the size quantum limit (SQL, $\epsilon_0\gtrsim k_BT$ or $\lambda\!\!\!^{-}_D\gtrsim d$), the critical concentration $n_e^*(d,T)$ is obtained as

$$n_e^*(d,T)=(\ln2)m^*k_BT/d\pi\hbar^2\ , \tag{9}$$

which when compared to the bulk-limit value given by Eq. (3) is given by

$$n_e^*(d,T)/n_e^*(\infty,T)=[\pi\ln2/F_{1/2}](\lambda\!\!\!^{-}_D/d)=3.21\lambda\!\!\!^{-}_D/d\ . \tag{10}$$

If a metallic film of 100 Å is taken, $n_e^*(d,T)=6.42\times n_e^*(\infty,T)$. Therefore, the critical concentration for onset of degeneracy is increased by the confinement. This increase is even further enhanced in degenerate semiconductors with low effective mass. Equation (9) is now changed to $\lambda\!\!\!^{-}_D\sim n_s^{-1/2}$ where $n_s=n_ed$ is the surface carrier concentration per unit area.

In a *thin wire* of rectangular cross section, the electrons exhibit quasi-one-dimensional (QOD) character[10] with eigenvalues given by

$$\epsilon_{lpk_z}=l^2\epsilon_x+p^2\epsilon_y+\hbar^2k_z^2/2m^*,\quad l,p=1,2,3,\ldots \tag{11}$$

with

$$\epsilon_x=\pi^2\hbar^2/2m^*a^2\ , \tag{12}$$

$$\epsilon_y=\pi^2\hbar^2/2m^*b^2\ , \tag{13}$$

where $a\,(b)$ is the length of the wire in the x (y) direction, assuming the longitudinal direction of the wire parallel to the z axis ($L_z\gg a,b$). The density of states $N(\epsilon)$ is given by[10]

$$N(\epsilon)=[L_z(2m^*)^{1/2}/\pi\hbar]\times\sum_{lp}{}'(\epsilon-l^2\epsilon_x-p^2\epsilon_y)^{-1/2}\ , \tag{14}$$

where $\Omega=AL_z$ is the volume and $A=ab$ is the cross-section area of the wire. The prime on the summation indicates that $x^{-1/2}$ is zero if $x<0$. The suitable criterion $\zeta-\epsilon_x-\epsilon_y=0$ for the critical concentration gives the following expression:

$$n_e^*(A,T)/n_e^*(\infty,T)=2\pi(F_{-1/2}/F_{+1/2})(\lambda\!\!\!^{-2}_D/A)\ , \tag{15}$$

where $F_{-1/2}=1.072$ as obtained from tables.[18,19] It may be noted that the rectangular wire structure is not an ideal structure, but has now been realized experimentally by Sakaki.[20] For $m^*=0.067m_e$ appropriate to GaAs wires, $n_e^*(A,T)$ can be considerably larger than $n_e^*(\infty,T)$. But, even for metallic wires the right-hand side of Eq. (15) can be considerably larger than 1. For example, if $A=10^{-12}$ cm^2, $n_e^*(A,1)/n_e^*(\infty,1)\simeq40$. Equation (15) essentially indicates that the onset-of-degeneracy criterion is equivalent to $\lambda\!\!\!^{-}_D\sim n_l^{-1}$ where $n_l=n_eA$ is the linear electronic concentration per unit length.

In a *cylindrical thin wire* of radius R_0, the eigenvalues are given by[21]

$$\epsilon_{nmk_z}=\alpha_{nm}^2\epsilon_0+\hbar^2k_z^2/2m^*\ , \tag{16}$$

where α_{nm} is the mth zero of the Bessel function of the order n. Then, Eq. (15) is also valid for cylindrical thin wires provided $A=\pi R_0^2$ is used.

The interesting case of an electron confined to a *strong magnetic field* has been discussed in detail by Nag.[12] The appropriate criterion for onset of degeneracy is $\zeta-\epsilon_0=0$, where $\epsilon_0=\frac{1}{2}\hbar\omega_c=\hbar^2/2m^*\lambda^2$ is the lowest quantized energy in a magnetic field. Here, $\lambda=(\hbar/m^*\omega_c)^{1/2}=(\hbar c/eB)^{1/2}$ is the quantized radius of the cyclotron orbit in a magnetic field of strength B with cyclotron frequency $\omega_c=eB/m^*c$. The result, in

the magnetic-quantum limit ($\hat{\lambda}_D \gtrsim \lambda$), is given by

$$n_e^*(A,T)/n_e^*(\infty,T)=\pi^{3/2}(F_{-1/2}/F_{+1/2})(\hat{\lambda}_D^2/A)\ , \tag{17}$$

where $A=\pi\lambda^2$ is the cross-section area of the orbit. The statistics of electrons in a magnetic field have been discussed by Nag[12] whose conclusion is similar to that predicted by Eq. (17) that the material becomes less degenerate when a magnetic field is applied. The availability of strong magnetic fields available from superconducting magnets makes it easier for us to check the confinement effect given by Eq. (17). This should give us a useful clue to explain the magnetoresistance in metals with spherical energy surfaces whose satisfactory explanation lacks in the published literature. Whether or not a metal-semiconductor transition is feasible by the criterion (17) is yet to be seen by future investigations.

To conclude, we have shown above that the critical concentration for onset of the degeneracy is enhanced by the quantum confinement effect. This means that the systems which are ordinarily degenerate in bulk configuration may become nondegenerate under strong confinement conditions.

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