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Abstract. We calculate the heat capacity of electrons as a function of the electron density and temperature in two-direction double-barrier resonant-tunnelling structures. The strength of the barrier potential increases in one direction, so that the system becomes 2D; the heat capacity as a function of the electron density goes to a step-like shape, which is similar to the one in the DOS. From 2D to 1D, the heat capacity reflects the peaks in the DOS with increasing electron density, and becomes a sawtooth-like shape in 1D. However, an asymmetric peak in the DOS makes two peaks in the heat capacity because the available DOS in thermal excitations becomes smaller as the chemical potential approaches the peak in the DOS. The heat capacity shows a linear dependence on the temperature in 3D and 2D, but not in 1D even at low temperatures. It exhibits a $\sqrt{T}$ dependence when the chemical potential is located near a pole in the DOS.

With the development of nanoscale fabrication techniques there has been growing interest in low-dimensional structures, such as quantum wells, quantum wires and quantum dots [1]. A quantum-well structure consists of two heterojunctions with different energy gaps; it freezes the motion of electrons perpendicular to the heterojunction interface and electrons are confined within it. In this structure the electronic density of states is characterized by a staircase-type shape. The confinement of one more direction confines the electrons to move only along the remaining direction; this is called a quantum wire, and the density of states has a sawtooth-type shape as a function of energy. In general, the dimension of the quantum structures is designated by its density of states (DOS). The intermediate DOS, such as that in between two and three dimensions (3D) or one and two dimensions (2D), was studied using the two-direction double-barrier resonant-tunnelling structure [2, 3]. It is known that crossovers of the DOS occur as the strength of the confining potential increases.

The physical quantities related to the DOS are interesting in quantum structures. One of the thermal equilibrium properties, the heat capacity, is being extensively studied both experimentally and theoretically because it strongly depends upon details of the electronic structure [4–6]. In this paper, we study the heat capacity for various confining potentials in the two-direction double-barrier resonant-tunnelling structure and show the behaviour of the heat capacity in intermediate dimensions as a function of the electron density.

For the calculation of heat capacities we use the local DOS of the quantum-well region in two-direction double-barrier resonant-tunnelling structures. In such structures the local DOS in the quantum-well region changes from 3D to 1D behaviour by adjusting the strength of

the barrier potential. The crossovers of the DOS can be derived by the following potential:

$$V(y, z) = V_0[\delta(y + b) + \delta(y - b)] + V_1[\delta(z + a) + \delta(z - a)] \tag{1}$$

where the confining barriers are located at $\pm a$ in the z direction and $\pm b$ in the y direction. The strength of the barrier potential is approximately related to the real potential parameter by

$$V_i = d_i \Delta V_i \qquad i = 0, 1 \tag{2}$$

where d_i is the width of the barrier and ΔV_i is the conduction band offset between two materials forming heterojunctions.

The DOS in the quantum-well region is calculated by the effective mass Hamiltonian

$$H = -\frac{\hbar^2}{2m^*} \nabla^2 + V(y, z). \tag{3}$$

A method of solving the above equation and the results were discussed in [2, 3]. The cross sectional DOS in the two-direction double-barrier resonant-tunnelling structure is given by

$$\rho(\epsilon) = \frac{2m^* l_x}{\pi^3 \hbar^2} \int_0^{b\eta} \mathrm{d}p \left(F_e(p) + F_o(p) + [F_e(p) - F_o(p)] \frac{\sin(2p)}{2p} \right)$$
$$\times \int_0^{a[\eta^2 - (p/b)^2]^{1/2}} \mathrm{d}q \frac{G_e(q) + G_o(q) + [G_e(q) - G_o(q)] \sin(2q)/2q}{[\eta^2 - (q/a)^2 - (p/b)^2]^{1/2}} \tag{4}$$

where

$$F_e(p) = \frac{p^2}{p^2 + U_1^2 \cos^2 p - U_1 \sin 2p} \tag{5}$$

$$F_o(p) = \frac{p^2}{p^2 + U_1^2 \sin^2 p + U_1 \sin 2p} \tag{6}$$

$$G_e(q) = \frac{q^2}{q^2 + U_0^2 \cos^2 q - U_0 \sin 2q} \tag{7}$$

$$G_o(q) = \frac{q^2}{q^2 + U_0^2 \sin^2 q + U_0 \sin 2q} \tag{8}$$

where $\eta^2 = 2m^* \epsilon / \hbar^2$, $U_1 = 2m^* V_1 b / \hbar^2$ and $U_0 = 2m^* V_0 b / \hbar^2$. Here the DOS is calculated in a box with the dimensions $l_x \times 2a \times 2a$, where l_x is the length of sample in the x direction and b is taken to be the same as a. Figure 1 shows the calculated DOS for various values of U_0 and U_1. For $U_1 = 0$, a square-root-type three-dimensional DOS changes continuously as U_0 increases, ultimately into the staircase pattern at $U_0 = \infty$ which represents the 2D structure. The variation of the DOS is displayed in figure 1(b), in which U_0 varies from zero to infinity at a fixed $U_1 = \infty$. In this case the DOS approaches a 1D sawtooth shape as $U_0 \rightarrow \infty$.

The heat capacity at a temperature T is given by

$$c_v = \frac{\mathrm{d}E_{\text{tot}}}{\mathrm{d}T} = \frac{\mathrm{d}}{\mathrm{d}T} \int_0^\infty \epsilon f(\epsilon) \rho(\epsilon) \, \mathrm{d}\epsilon \tag{9}$$
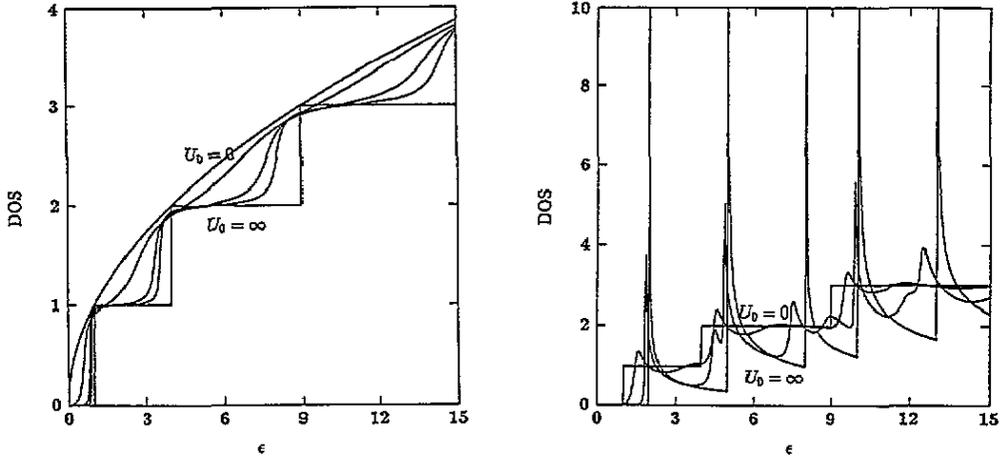
Figure 1. The crossover behaviour of the density of states plotted as a function of energy. The density of states and energies are in units of $2m^*bl_x/\pi\hbar^2$ and $\pi^2\hbar^2/8m^*a^2$ respectively. In (a), $U_0 = 0, 3, 10, 16, \infty$ for $U_1 = 0$, while in (b) $U_0 = 0, 2, 12, \infty$ for $U_1 = \infty$.

where E_{tot} is the total energy of electrons and $f(\epsilon)$ is the Fermi–Dirac distribution function. Here we consider only the heat capacity contributed by electrons. Other effects such as phonons are neglected to test the crossover of the heat capacity. Through a simple argument the above equation is simplified as

$$c_v = k_B(l_2 - l_1^2/l_0) \tag{10}$$

where

$$l_r = \int_0^\infty \frac{e^z z^r}{(1 + e^z)^2} \rho(\epsilon)\, d\epsilon. \tag{11}$$

In the above $z = \beta(\epsilon - \mu)$, $\beta = 1/k_B T$ and μ is the chemical potential. Here l_2 reflects the increase in the total energy by the transition of electrons near μ to the upper levels when the temperature is raised by a small amount. It is noted that the second term in (10) is negative and represents the decrease of the total energy as the temperature increases, associated with the temperature dependence of the chemical potential. The chemical potential is uniquely determined by the number of electrons. If we define a dimensionless electron density n such as $n = Na^3/V$, where N is the total number of electrons in a volume $V = 4abl_x$, the chemical potential μ is calculated through the relation

$$n = \frac{a^3}{V} \int_0^\infty \frac{1}{1 + e^{\beta(\epsilon - \mu)}} \rho(\epsilon)\, d\epsilon. \tag{12}$$

This equation is solved numerically for any temperature and dimensionless electron density.

We study the variation of the heat capacity for various U_0 and U_1 as a function of electron density n. Figure 2(a) shows the heat capacities calculated for $U_0 = 0, 3, 10, 16, \infty$ and $U_1 = 0$. We find that the heat capacity changes from a saturated form to a staircase-like shape as U_0 increases. As a whole, the electron-density dependence of the heat capacity is similar to the DOS which is a function of energy. It is known that in the 3D system the heat capacity is given by

$$c_v = \tfrac{1}{3}\pi^2 k_B^2 T \rho(\epsilon_F) = \tfrac{1}{6} V k_B^2 T \left(\frac{2m^*}{\hbar^2}\right)^{2/3} \sqrt{\epsilon_F} \tag{13}$$
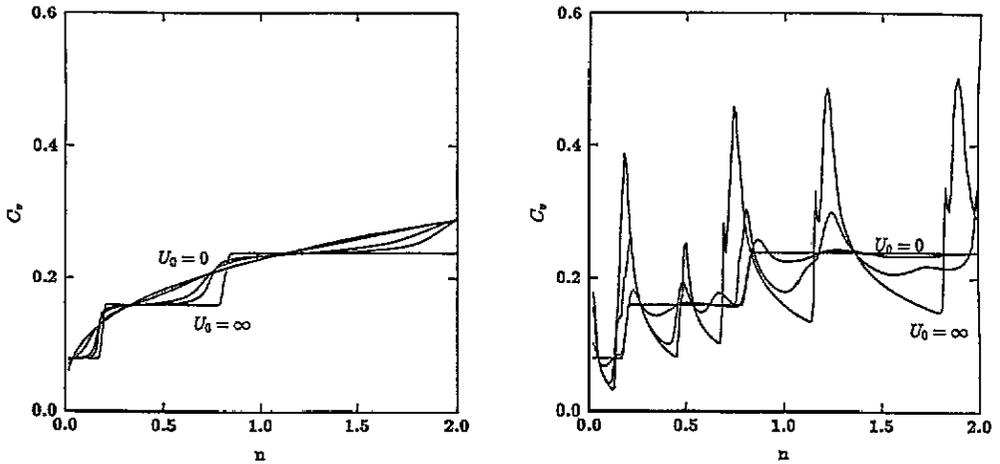
Figure 2. The crossover behaviour of the heat capacity drawn as a function of dimensionless electron density. The heat capacities are in units of $\pi k_B b l_x/4a^2$. U_0 and U_1 are the same as in figure 1.

where ϵ_F is the Fermi energy, i.e. the chemical potential at $T = 0$. Since the Fermi energy is given by $\epsilon_F = (\hbar^2/2m^*a^2)(3\pi^2n)^{2/3}$, the heat capacity in the 3D system is proportional to $n^{1/3}$. Our results at $T = 4\,\mathrm{K}$ almost exhibit a $n^{1/3}$ dependence for $U_0 = U_1 = 0$.

For $U_1 = 0$ the height of the DOS becomes smaller as U_0 increases, as shown in figure 1(a), so that in the full range of energy, the heights of the DOS have the largest values at $U_0 = 0$ and $U_1 = 0$. However, the calculated heat capacity shows behaviour deviating somewhat from the DOS; the heat capacity in the 2D system has larger values in some regions of n than in 3D. This results from the fact that, for a fixed electron density n, the chemical potential in the 3D system is different to that of the 2D system at the same temperature; in the 3D system the Fermi energy is given by $\epsilon_F = (24n/\pi)^{2/3}$ in local units, $E_0 = \pi^2\hbar^2/8m^*a^2$, while in the 2D system $\epsilon_F = 16n/\pi + 1$, considering only the first subband.

Figure 2(b) shows the crossover of the heat capacity for the cases $U_0 = 0, 2, 12, \infty$, with $U_1 = \infty$ as a function of n. It is found that the sawtooth-like DOS gives rise to a larger value for the heat capacity than the staircase-like DOS. Overall, the calculated heat capacities exhibit shapes similar to those of the DOS except for the split peaks in the 1D system. When the chemical potential passes through each pole of the sawtooth in the DOS, a set of double peaks is generated in the heat capacity. This behaviour is due to the asymmetry of peaks in the DOS. In this case, the smaller peak appears when the chemical potential is located at the lower side of a pole in the DOS. In contrast, the larger peak appears when the chemical potential is located at the upper side of a pole in the DOS. Since the magnitude of the heat capacity is directly related to the thermal excitations of electrons, it is required for a large value to have abundant available states of both the empty upper levels and the filled levels lower than μ within the range of several k_BT from μ. As μ approaches a pole in the DOS, the heat capacity increases due to the increase of empty upper levels and then decreases when μ lies very near a pole due to the decrease of filled lower levels; it then again starts to increase when μ passes a pole due to the increase of filled lower levels. Thus, the heat capacity in the 1D system exhibits a sawtooth with sets of double peaks. For the 1D heat capacity, the heights of sawtooth-like peaks near $n = 0$ and $n = 0.5$ are rather smaller than the others, as shown in figure 2. This is due to the fact that the levels responsible for these

peaks have different degeneracies from the others. Since the energy levels for the barrier height $U_0 = U_1 = \infty$ are given by

$$E(k_x, m, l) = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\pi^2 \hbar^2}{8m^*}\left(\frac{m}{a^2} + \frac{l}{b^2}\right) \qquad m, l = 1, 2, 3, 4, \ldots \qquad (14)$$

they are doubly degenerate unless $l = m$ in the case of $a = b$.
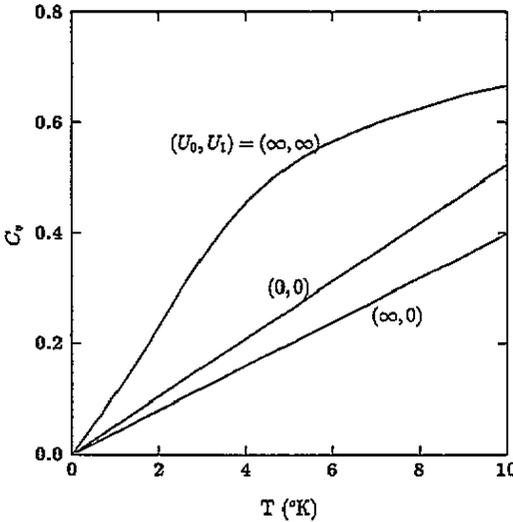
Figure 3. The heat capacities are drawn as a function of temperature for $n = 0.75$.

The sawtooth-like DOS in the 1D structure exhibits a non-linear temperature dependence of the heat capacity. In figure 3, the heat capacities for the 1D to 3D electrons are plotted as a function of temperature for $n = 0.75$. In the 3D and 2D structures they increase linearly with temperature, as expected from the Sommerfeld expansion for a smooth DOS, $c_v = \pi^2 k_B^2 \rho(\epsilon_F)T/3$. In the 1D structure, however, the heat capacity shows a non-linear variation with T. This result implies that the Sommerfeld expansion cannot be applied to the pole region of the sawtooth-type DOS. When the chemical potential lies at a pole in the DOS, the heat capacity can be shown to have a $\sqrt{T}$ dependence. To see this, we assume that there is a single sawtooth in the DOS. Let the sawtooth start from $\epsilon = 0$ and the chemical potential be also at $\epsilon = 0$. Then l_r becomes

$$l_r = \int_0^\infty d\epsilon \frac{e^z}{(1 + e^z)^2} z^r \frac{D_0}{\sqrt{\epsilon}} \qquad (15)$$

where D_0 is a normalized constant. Defining s_r as

$$s_r = \int_0^\infty dz \frac{e^z}{(1 + e^z)^2} z^r \frac{D_0}{\sqrt{z}} \qquad (16)$$

the heat capacity in this case can be expressed as

$$c_v = k_B^{2/3}(s_2 - s_1^2/s_0)\sqrt{T} \qquad (17)$$

exhibiting a square-root dependence on temperature. However, in reality, as shown in figure 3, the heat capacities in 1D depend on temperature linearly in some temperature region and on $\sqrt{T}$ in the other regions since μ also changes with temperature.

In conclusion, we have found that the heat capacities in various intermediate dimensions vary with electron density in a similar fashion to the density of states at fixed temperatures. However, in the 1D structure the heat capacity exhibits two peaks that result from a single asymmetric peak in the density of states. In this case, the heat capacity shows a $\sqrt{T}$ dependence when the chemical potential lies near a pole of the density of states, while it varies almost linearly with temperature for the chemical potential located in the smooth region of the density of states. Further experimental tests are suggested to determine the dimensional and temperature variation of the heat capacity.

Acknowledgments

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