Thermopower oscillations of a quantum-point contact

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Abstract

Oscillations in the thermopower of a quantum-point constriction in the absence and presence of a magnetic field are discussed.

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In addition to the quantized conductance steps discovered by van Wees et al.[1] and Wharam et al.[2] in split-gate constrictions of a two-dimensional electron gas (2DEG), Molenkamp et al.[3] reported very recently on oscillations in the transverse voltage of a conducting channel in a high mobility 2DEG. They related these oscillations to the thermopower of a quantum-point contact.

On the theoretical side, while the electrical properties of quantum point contacts have received wide interest,[4-14] much less attention has been paid so far to the analysis of the thermal and thermoelectric properties of such systems.

Streda,[15] using an approach that goes back to work by Sivan and Imry,[16] outlines a calculation of the thermopower oscillations of a ballistic quantum point contact as the number of one-dimensional subbands at the point contact is changed. He assumes a transverse parabolic confining potential, a longitudinal transmission coefficient through the constriction that is a step function of energy, and zero magnetic field.

However, as pointed out by Büttiker,[14] since constrictions in the experiments are usually electrostatically induced, with a pair of split gates, the confining potential must be a smooth function of the coordinates in every direction, and consequently the bottleneck of the constriction forms a saddle.

The aim of the present work is to analyze the thermopower of a quantum point contact for the realistic case of a saddle-point constriction, give simple criteria for its observability, and study the effect of a magnetic field perpendicular to the 2DEG.

The linear response expressions for the chemical potential (μ) and temperature (θ) dependent two-terminal conductance $G(\mu,\theta)$ and thermopower $S(\mu,\theta)$ for transport from one equilibrium electron reservoir to another, along a multichannel lead are given by[16]

$$G(\mu,\theta) = \frac{2e^2}{h} \sum_i \int_{E_i^T}^{\infty} dE \left(-\frac{df}{dE}\right) T_i(E) \tag{1}$$

$$S(\mu,\theta) = \frac{1}{e\theta} \frac{L_1(\mu,\theta)}{L_o(\mu,\theta)} = \frac{k_B}{e} \frac{\sum_i \int_{E_i^T}^{\infty} dE \left(-\frac{df}{dE}\right) T_i(E) \left(\frac{E-\mu}{k_B\theta}\right)}{\sum_i \int_{E_i^T}^{\infty} dE \left(-\frac{df}{dE}\right) T_i(E)} \tag{2}$$

with E_i^T being the transverse energy associated with the ith channel in the lead, T_i the transmission probability from all channels into channel i,

$$T_i = \sum_j T_{ij} \tag{3}$$

f the Fermi-Dirac distribution function, and e the electronic charge ($e = -|e|$). The sum over i runs over all occupied channels.

The model used for the derivation of equations (1) and (2) assumes that the thermalization of electrons, by inelastic scattering, and the corresponding Joule heating occurs only in the outside reservoirs and not in the system itself.

In reference 16 the lower limit of the integrals in equations

(1) and (2) was subsequently replaced by zero, under the assumption that no transverse level falls in the range of a few $k_B\theta$ around μ. However, this is the more interesting situation for the analysis that follows, so we conserved the lower limit E_1^T.

It is already possible to make a few qualitative considerations about $G(\mu,\theta)$ and $S(\mu,\theta)$ from the general expressions (1) and (2), for the case of transmission about a quantum point contact. In the case of a lead which is non-uniform along the direction of current flow (as is the case for a realistic constriction) the transmission coefficient T_1 is changed by unity within a finite energy range E^L.

Accordingly a schematic drawing of the different contributions to the integrand of equation (2) is shown in Fig. 1. The parameters were chosen such that $\Delta E^T > E^L > k_B\theta$ where ΔE^T is the transverse subband splitting, but the argument that follows is also valid for the case $\Delta E^T > k_B\theta > E^L$.

Taking into account that the lower integration limit is E_1^T, clearly the result is essentially zero if $\mu - E_1^T$ is a few $k_B\theta$ away from E_1^T, with a maximum contribution when $\mu \simeq E_1^T$. It should be expected as a consequence that the thermopower of a quantum-point constriction will have oscillations as function of μ, with peak values when $\mu \simeq E_1^T$ and a width of a few $k_B\theta$.[15]

In accordance with these considerations the condition for the observation of well pronounced oscillations in the thermopower of a quantum-point contact is approximately given by

$$\Delta E^{T} > \text{a few } k_B\theta \tag{4}$$

These qualitative arguments can be put on a more firm basis assuming that $k_B\theta \ll E^L$. It is then permissible to expand the transmission coefficient T_i around μ, in equations (1) and (2), with the following result (for the thermopower):

$$S(\mu,\theta) \simeq \frac{1}{e\theta}\left[\frac{L_1^{(0)}}{L_0^{(0)}} + \frac{1}{L_0^{(0)}}\left(\frac{L_0^{(0)}L_1^{(1)} - L_0^{(1)}L_1^{(0)}}{L_0^{(0)}}\right) + \ldots\right] \tag{5}$$

where

$$L_0^{(0)} = \sum_i T_i(\mu)\; f(E_i) \tag{6}$$

$$L_0^{(1)} = k_B\theta \sum_i T_i'(\mu) \left\{\left(\frac{E_i-\mu}{k_B\theta}\right)\left[f(E_i)-1\right] - \ln f(E_i)\right\} \tag{7}$$

$$L_1^{(0)} = k_B\theta \sum_i T_i(\mu) \left\{\left(\frac{E_i-\mu}{k_B\theta}\right)\left[f(E_i)-1\right] - \ln f(E_i)\right\}. \tag{8}$$

$$L_1^{(1)} = (k_B\theta)^2 \sum_i T_i'(\mu) \left[\frac{\pi^2}{6} + \left(\frac{E_i-\mu}{k_B\theta}\right)^2 f(E_i) - \int_0^{(E_i-\mu)/k_B\theta} \frac{2x\,dx}{1+e^x}\right] \tag{9}$$

where $T_i'(\mu) = \frac{d\,T_i(E)}{dE}\Big|_{E=\mu}$.

It should be pointed out that equation (5) is <u>not</u> a typical

Sommerfeld expansion, in that the coefficients $L_0^{(0)}$, $L_0^{(1)}/(k_B\theta)$, $L_1^{(0)}/(k_B\theta)$, and $L_1^{(1)}/(k_B\theta)^2$ are temperature dependent; the superscript only indicates the order of the expansion of T_1 around μ.

The first term in (5), $L_1^{(o)}/e\theta L_o^{(o)}$ is a new contribution to the thermopower, that gives rise to the above mentioned oscillations, with peak values when $\mu = E_1$ and is exponentially small when $|\mu-E_1| >> k_B\theta$.

The second term, when $|\mu-E_1| >> k_B\theta$, reduces to the result usually quoted for the thermopower[16] $\frac{1}{e\theta}\frac{L_1^{(1)}}{L_o^{(o)}}$ (note that in this limit $L_o^{(1)}$ and $L_1^{(o)}$ are exponentially small).

Close to one of its peak values ($\mu \simeq E_1$) the expansion (5) simplifies considerably

$$S(\mu\simeq E_1,\theta) \simeq \frac{k_B}{e}\left[\frac{T_1(E_1)\ln 2}{1+\frac{1}{2}\,T_1(E_1)} + \frac{T_1'(E_1)}{\left(1+\frac{1}{2}\,T_1(E_1)\right)}\left(\frac{\pi^2}{6} - \frac{(\ln 2)^2 T_1(E_1)}{1+\frac{1}{2}\,T_1(E_1)}\right)(k_B\theta)+\ldots\right] \tag{10}$$

and linear temperature corrections are obtained to the quantized values given by the first term.

While the discussion until now has been completely general, with no assumptions about the particular geometry of the quantum-point contact, in order to make a quantitative calculation of the thermopower of a quantum-point constriction, a model should be adopted for the transmission coefficient T_1 (or equivalently, for the constriction potential $V(x,y)$).

As mentioned above, a realistic quantum-point contact may be modeled by a constriction that close to its bottleneck forms a saddle; expanding the constriction potential around its saddle point[14]

$$V(x,y) = V_o - \frac{1}{2} m\omega_x x^2 + \frac{1}{2} m\omega_y y^2 \qquad (11)$$

where x and y correspond to the longitudinal and transverse directions, respectively, ω_x and ω_y are convenient parametrizations of the respective curvatures, and V_o refers to the value of the constriction potential at the saddle point (it will be taken as the origin of energy in the following).

Fortunately the quantum mechanical problem of transmission and reflection at the constriction potential described by equation (11) can be exactly solved without[17] and with [18] a magnetic field (perpendicular to the x-y plane).

According to these results, the transmission probability at the saddle is given by

$$T_{ij} = \delta_{ij} \frac{1}{1+e^{-\pi\varepsilon_i}} \qquad (12)$$

where

$$\varepsilon_i = \frac{E-\Delta E^T(i+1/2)}{E^L} = \frac{E-E_i^T}{E^L} \qquad (13)$$

and

$$\Delta E^T = \frac{\hbar}{\sqrt{2}} \left[\left(\Omega^4 + 4\omega_x^2\omega_y^2\right)^{1/2} + \Omega^2\right]^{1/2} \qquad (14)$$

$$E^L = \frac{1}{2}\frac{\hbar}{\sqrt{2}}\left[\left(\Omega^4 + 4\omega_x^2\omega_y^2\right)^{1/2} - \Omega^2\right]^{1/2} \tag{15}$$

$$\Omega^2 = \omega_c^2 + \omega_y^2 - \omega_x^2 \tag{16}$$

$$\omega_c = \frac{eB}{mc} \tag{17}$$

In the limit of zero magnetic field $\Delta E^T \to \hbar\omega_y$ and $E^L \to \hbar\omega_x/2$, while when $\omega_c >> \omega_x$ and ω_y, $\Delta E^T \to \hbar\omega_c$, and $E^L \to \hbar\omega_x\omega_y/2\omega_c$. Using (12)- (17) Büttiker analyzed the conditions for the occurrence of well-pronounced steps in the zero-temperature two-terminal conductance, and the accuracy of its quantization.

The numerical evaluation of equations (1) and (2), with the saddle-point constriction transmission as given by (12) produces the results shown in Figures 2, 3 and 4. The two-terminal zero magnetic field resistance (left scale) and thermopower (right scale) are shown in Figure 2. The parameters are chosen such that condition (4) is fulfilled and consequently well-pronounced oscillations in the thermopower are obtained.

As already mentioned, the temperature dependence of the oscillations (width and peak value) is explained by the low-temperature expansion (5). It is interesting to point out that for the maximum temperature shown in Fig. 2 ($k_B\theta/\hbar\omega_x = 0.5$), while the resistance shows weak indication of quantization, it is still possible to have well-defined oscillations in the thermopower.

We display in Figure 3 the dependence of the resistance and thermopower on magnetic field. As discussed previously, the onset of each oscillation in the thermopower is related to the opening of a new channel for conduction. Because ΔE^T is an increasing function of B, the oscillations spread apart for increasing values of B.

The parameters chosen in Fig. 3 correspond to a situation where already for B = 0 the thermopower has well-pronounced oscillations (the essential effect of $B \neq 0$ being that of changing the distance between two successive oscillations). However, an interesting situation arises in connection with condition (4), because since ΔE^T is an increasing function of B, it is possible that $\Delta E^T(B=0) < k_B\theta$ while $\Delta E^T(B\neq 0) > k_B\theta$, with a crossover from a poor-oscillation regime to a well-developed oscillation regime.

Such an example of magnetic-field induced oscillation is shown in Fig. 4. For $\omega_y=\omega_x$ and $k_B\theta/\hbar\omega_x = 0.25$ the zero-field thermopower shows only an indication of oscillatory behavior. However, when $\omega_c=\omega_y$ the oscillations begin to grow and when $\omega_c=2\omega_y$ they are clearly visible. For $\omega_c=2\omega_y$, $\Delta E^T/\hbar\omega_x \simeq 2$ and the condition (4) is well fulfilled.

In summary, we have calculated the thermopower of a quantum point constriction. Our results show that the thermopower shows oscillations as a function of chemical potential μ, each time a new quantum channel is open for conduction. The amplitude of the oscillations is temperature dependent. Finally, the possibility of magnetic-field induced oscillations is suggested.

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19.- When many subbands are occupied, as is the case of Fig. 4 for large μ, the assumption of a parabolic confining potential in the transverse direction is not realistic. As self-consistent calculations show (S.E. Laux, D.J. Frank, and F. Stern, Surf. Sci. 196 101 (1988), C.R. Proetto (to be published)), in this situation the transverse potential becomes flat in the central region, and a better approximation would be a hard-wall potential.

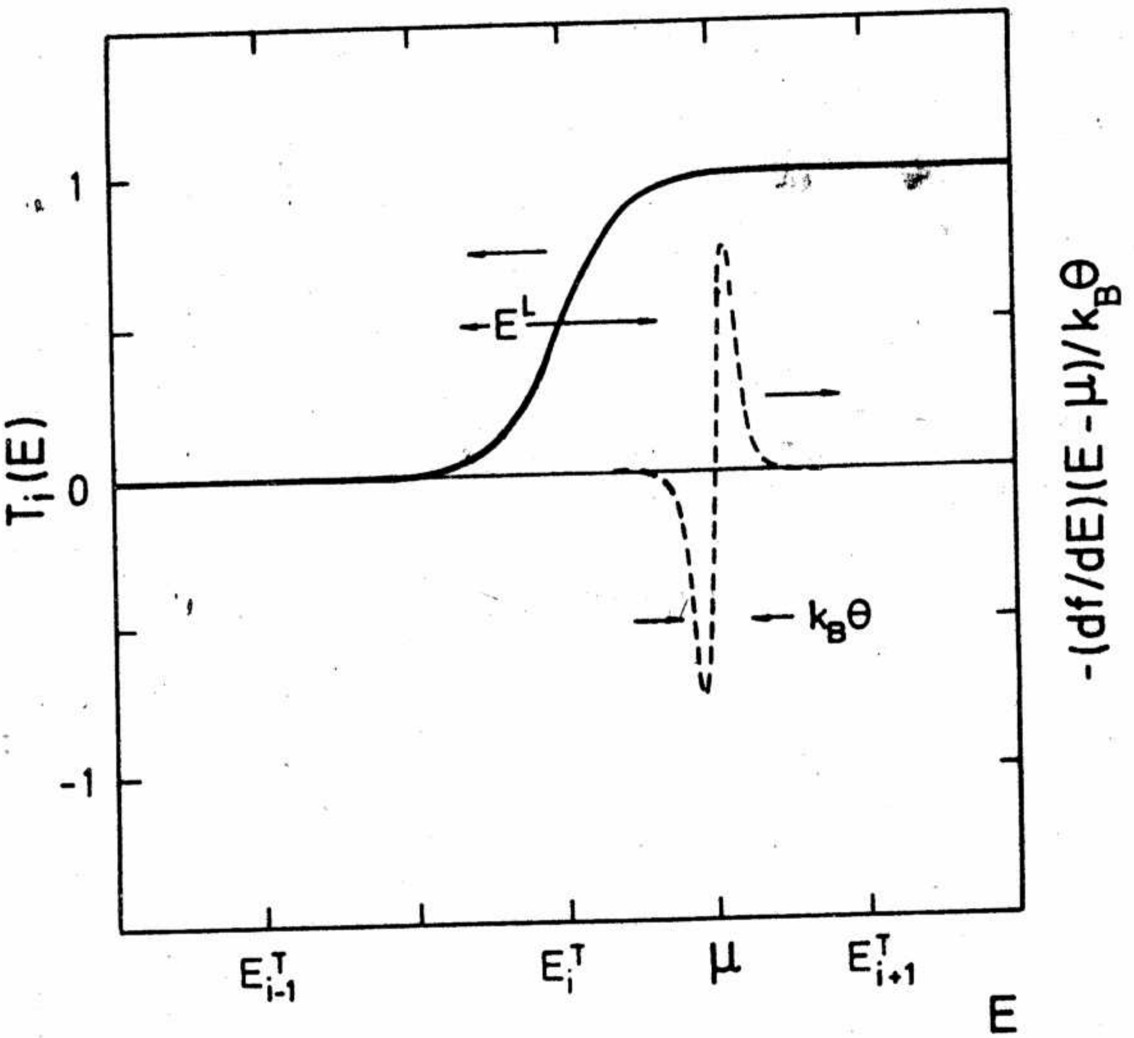
Figure Captions

Figure 1: Schematic drawing of the integrand in equation (2) which defines the thermopower.

Figure 2: Resistence (left scale) and thermopower (right scale) as function of chemical potential μ for a ratio of $\omega_y/\omega_x = 3$. Full line, $k_B\theta/\hbar\omega_x = 0.5$; dashed line, $k_B\theta/\hbar\omega_x = 0.25$; pointed line, $k_B\theta/\hbar\omega_x = 0.1$.

Figure 3: Resistence (left scale) and thermopower (right scale) as function of μ, in presence of magnetic field: full line, $\omega_c/\omega_x = 0$; dashed line, $\omega_c/\omega_x = 1$; pointed line $\omega_c/\omega_x = 2$. The ratio $\omega_y/\omega_x = 3$ and $k_B\theta/\hbar\omega_x = 0.1$.

Figure 4: Magnetic field-induced thermopower oscillations for $\omega_y/\omega_x = 1$ and $k_B\theta/\hbar\omega_x = 0.25$. Full line, $\omega_c/\omega_x = 0$; dashed line, $\omega_c/\omega_x = 1$; pointed line $\omega_c/\omega_x = 2$.



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E_{i-1}^T
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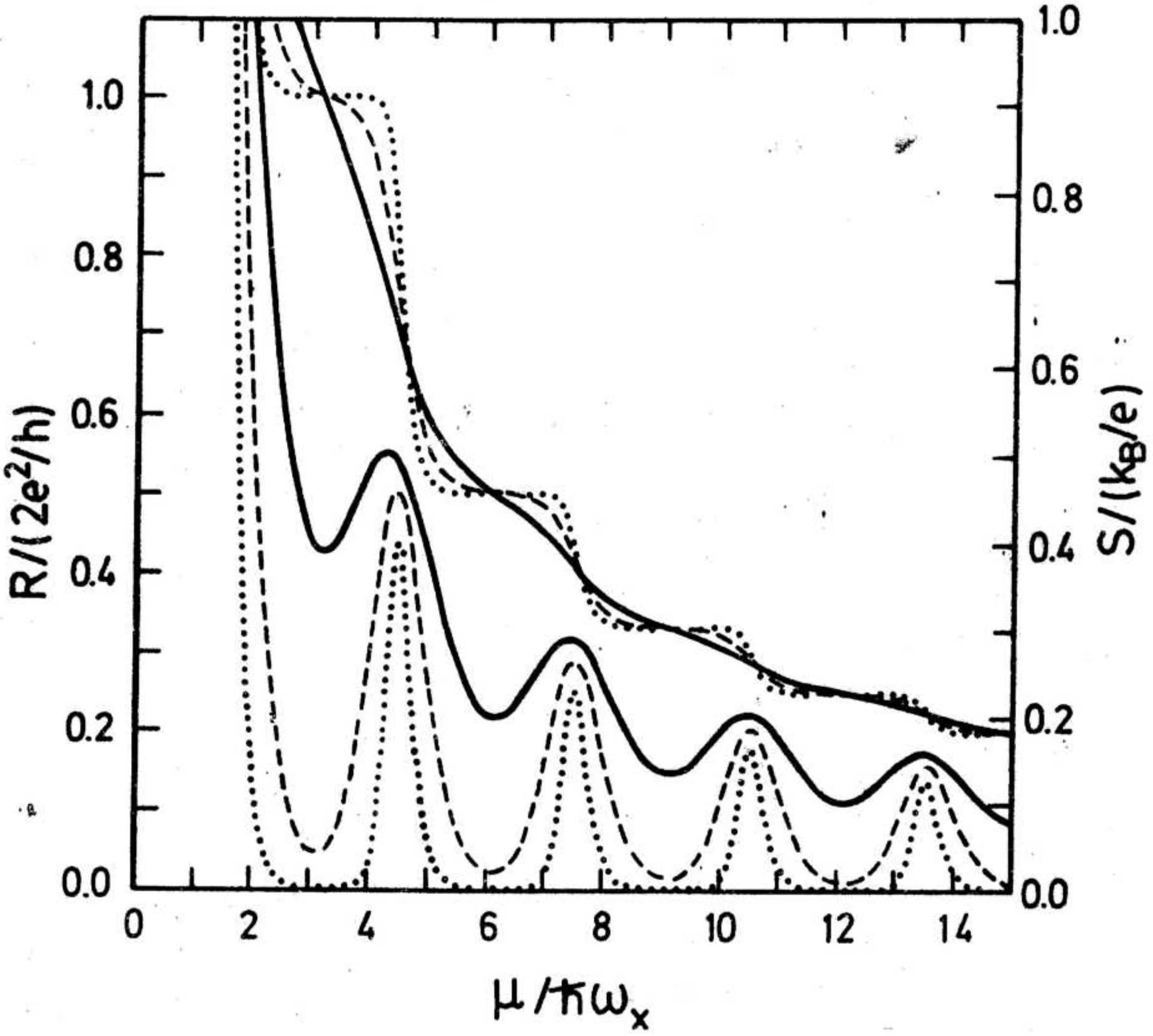
μ
E_{i+1}^T
E



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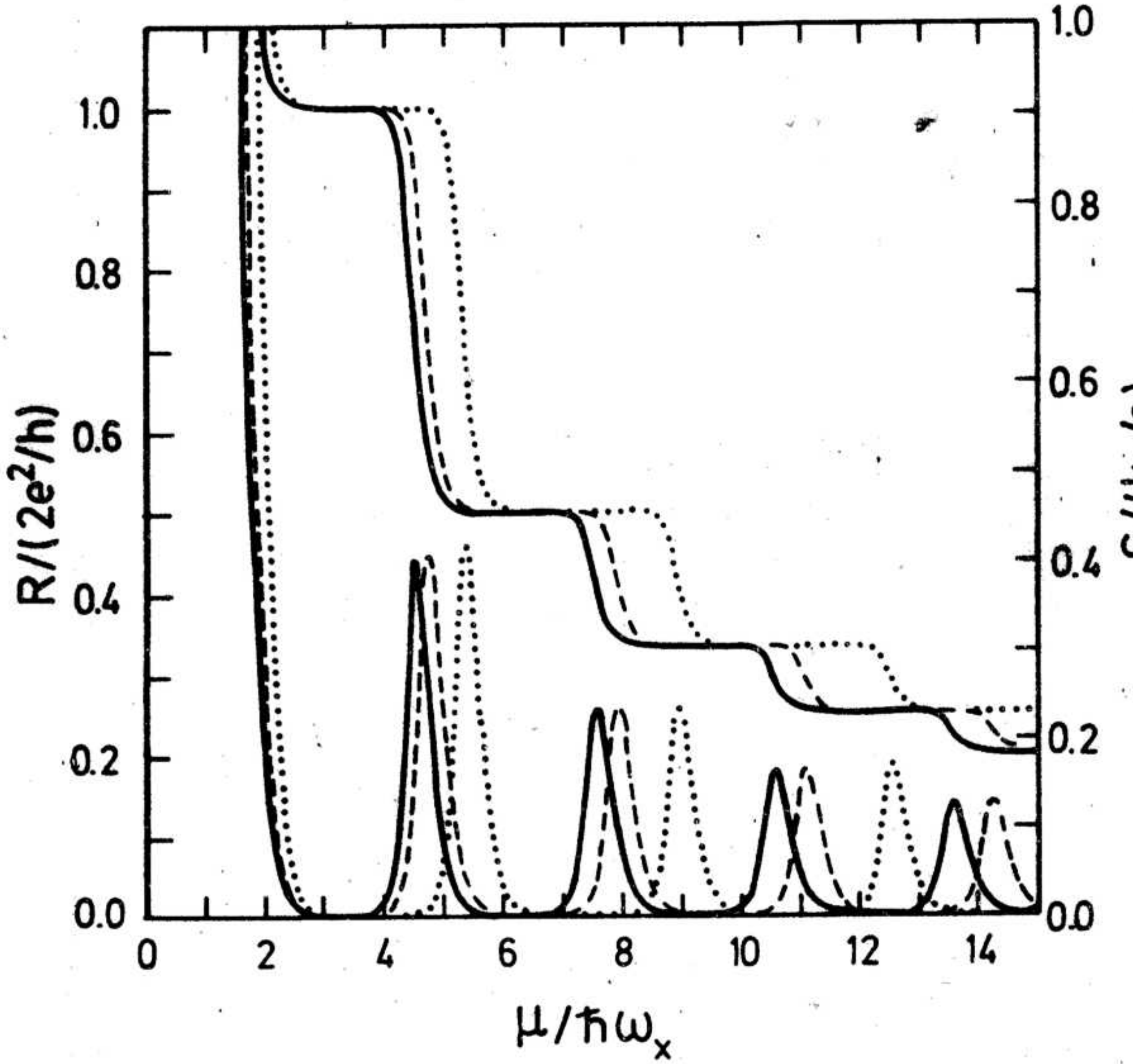

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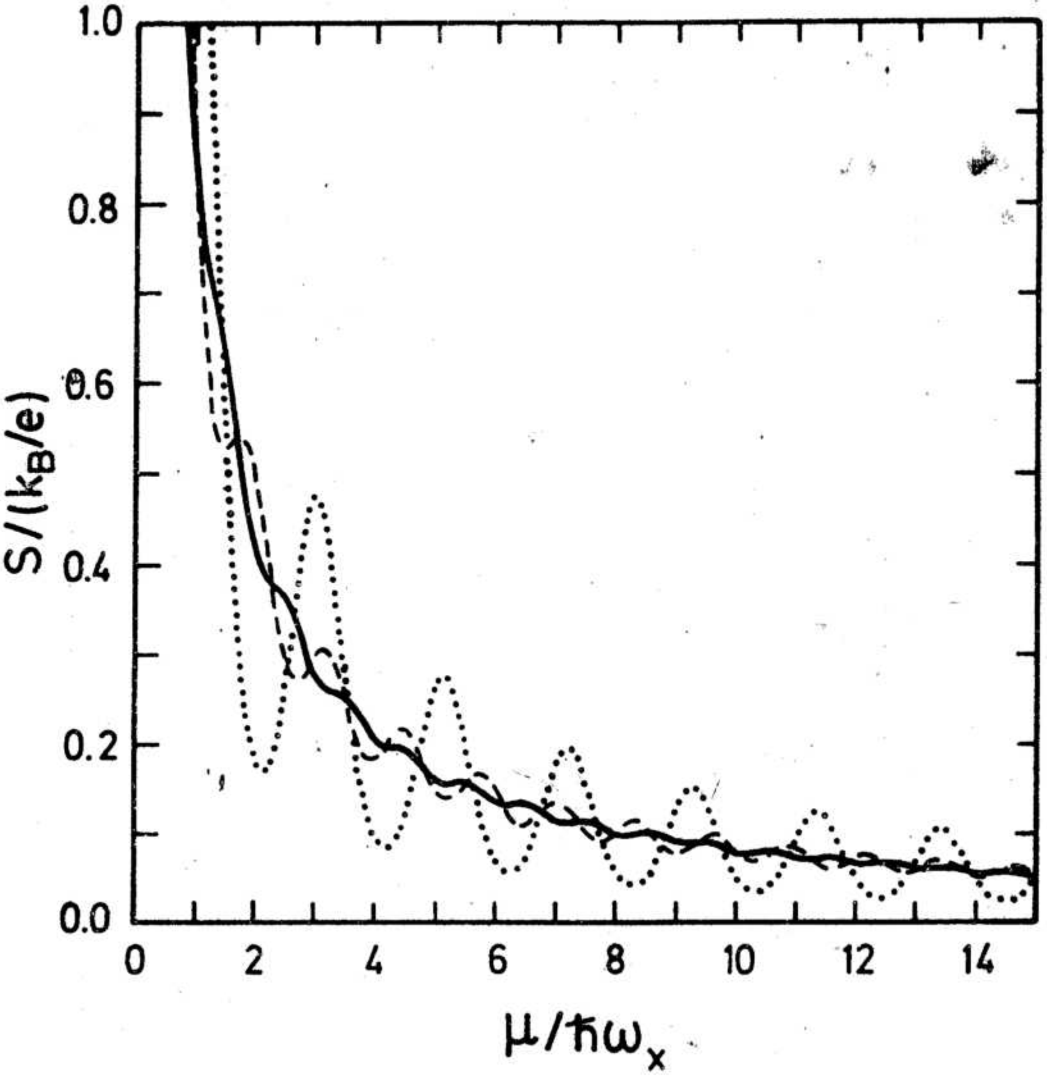

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