Four-Terminal Thermal Conductance of Mesoscopic Dielectric Systems

Qing-feng Sun, Ping Yang, and Hong Guo
Center for the Physics of Materials and Department of Physics, McGill University, Montreal, PQ, Canada H3A 2T8
(Received 19 February 2002; published 3 October 2002)

A four-terminal thermal conductance formula for a mesoscopic dielectric system with arbitrary central scattering region is derived. Similar to four-terminal electric conductance, the four-terminal thermal conductance also has a set of Onsager relations. In the temperature $T \to 0$ limit, in contrast to the two-terminal thermal conductance which is a monotonic function of T and tends to zero, the four-terminal thermal conductance is nonmonotonic and tends to ∞. We also find that temperatures of the two terminals without thermal flux become very close to each other at low temperatures. Rather different behaviors are found for systems satisfying fractional exclusion statistics.

DOI: 10.1103/PhysRevLett.89.175901 PACS numbers: 66.70.+f, 44.10.+i, 63.22.+m

Recently, the low-temperature heat transport in a mesoscopic dielectric system in which the wavelength of thermal phonons can be comparable to the geometrical size of the system has attracted much attention both experimentally [1–3] and theoretically [4–9]. Based on scattering theory as in the electron transport problem, a two-terminal Landauer formula for thermal flux has been derived [4,5,7]. The universal quantum of thermal conductance $\frac{\pi^2 k_B^2 T}{3h}$ has been predicted [4] and experimentally observed [1]. For a mesoscopic dielectric system, four-terminal measurements of thermal conductance $\kappa_{ij,kl}$ should be experimentally feasible [10], in which two terminals i, j carry thermal flux to and from the scattering region while temperatures are measured at the other two terminals k, l which are at local equilibrium with the dielectric device. A four-terminal measurement is interesting as it can, in principle, exclude effects of contact thermal resistance. Theoretically, $\kappa_{ij,kl}$ provide physical understanding of how energy flux is partitioned among the multiple leads. Unlike its electric counterpart which is given by the Landauer-Büttiker conductance formula [11,12], to the best of our knowledge the physics associated with the four-terminal quantity $\kappa_{ij,kl}$ has not been investigated before, and it is the subject of this paper.

In a two-terminal thermal transport at the limiting temperature $T \to 0$ where the phonon number associated with transport tends to zero, the two-terminal thermal conductance has a universal behavior regardless of the property of the dielectric scattering region: it tends to zero and the thermal resistance tends to infinity. This is different from electric transport in which two-terminal electric conductance may take any finite value depending on the scattering region. It is an interesting problem to understand the properties of the four-terminal quantity $\kappa_{ij,kl}$, and, in particular, if it also has a universal tendency at the $T \to 0$ limit. Our investigation suggests that the four-terminal quantity $\kappa_{ij,kl}$ is nonmonotonic in T, unlike its two-terminal counterpart κ_{ij}; $\kappa_{ij,kl}$ indeed has a universal behavior in the zero temperature limit, but it tends to infinity instead of tending to zero, and the Onsager relations $\kappa_{ij,kl} = \kappa_{kl,ij}$ and $\kappa^{-1}_{ij,kl} + \kappa^{-1}_{il,jk} + \kappa^{-1}_{ik,lj} = 0$ hold.

Consider a four-terminal dielectric system shown in Fig. 1. The terminals are connected to thermal reservoirs at equilibrium with temperatures T_i where $i = 1, 2, 3, 4$, respectively. The terminal wires are assumed to be perfect and phonons coming from reservoirs are not scattered inside the wires. Phonon scattering occurs only in the scattering region which may have an arbitrary shape involving defects, rough surfaces, etc. Consider coherent transport, and we define phonon transmission coefficient $T_{ji,nm}(\omega)$ for the process where an incident phonon with energy $\hbar\omega$ from terminal i at phonon mode m is scattered to terminal j at mode n. From time-reversal invariance, the transmission coefficient has the property $T_{ji,nm}(\omega) = T_{ij,mn}(\omega)$. Generalizing the two-terminal derivation of Ref. [5], the multiterminal expression for energy flux, $\dot{Q}_i$, can be derived by quantizing the classical energy flux. Such a derivation is tedious but straightforward, and we obtain flux $\dot{Q}_i$ from terminal i flowing into the center scattering region to be [4,5,7,11]

$$\dot{Q}_i = \sum_{j(j\neq i)} \sum_{m,n} \int_{\max(\omega_{im},\omega_{jn})}^{+\infty} \frac{d\omega}{2\pi} \hbar\omega [n_i - n_j] T_{ji,nm}(\omega),$$

where $n_i(\omega) = [\exp(\hbar\omega/k_B T_i) - 1]^{-1}$ is the Bose-Einstein distribution function of the phonons in the ith reservoir, and ω_{im} is the cutoff frequency of mode m in

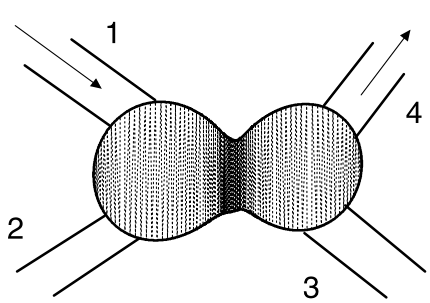

FIG. 1. Schematic diagram for the four-terminal system with an arbitrary scattering region.

terminal wire i. For $\omega < \omega_{jn}$, the incident phonon cannot be scattered to mode j, n, and for $\omega < \omega_{im}$, there does not exist incident phonons from the mode im. Therefore the integration begins from $\max(\omega_{im}, \omega_{jn})$. In the following, we measure temperature T_i from a common background value T taken as the lowest of the four T_i's. We further assume that the differences between T_i's are so small that only linear thermal conductance will be studied. Then the distribution function $n_i(\omega)$ can be expanded as $n_i(\omega) = n(\omega) + \Delta T_i \frac{d}{dT} n(\omega)$, here ΔT_i is the temperature difference $T_i - T$. The thermal flux can now be rewritten as $\dot{Q}_i = \sum_{j(j\neq i)} \kappa_{ij}(\Delta T_i - \Delta T_j)$, with

$$\kappa_{ij} = \sum_{m,n} \int_{\max(\omega_{im},\omega_{jn})}^{+\infty} \frac{d\omega}{2\pi} \hbar\omega T_{ij,mn} \frac{dn(\omega)}{dT} = \int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega T_{ij} \frac{dn(\omega)}{dT}. \quad (1)$$

Here $T_{ij}(\omega) = \sum_{m,n} \theta(\omega - \omega_{im})\theta(\omega - \omega_{jn})T_{ij,mn}(\omega)$ is the total transmission coefficient from terminal j to terminal i, and κ_{ij} is the two-terminal thermal conductance. From time-reversal invariance, we see $T_{ij}(\omega) = T_{ji}(\omega)$ and $\kappa_{ij}(T) = \kappa_{ji}(T)$. Moreover, one can exactly prove that the two-terminal thermal conductance $\kappa_{ij}(T)$ is a monotonic function of temperature T [13], a result that is very different from electric conductance which is not monotonic in both temperature and bias. At the low-temperature limit $T \to 0$, thermal conductance $\kappa_{ij}(T)$ tends to zero as $\sim T$.

In the following we solve the four-terminal thermal conductance $k_{ij,kl}$. Letting the terminals i and j carry flux $\dot{Q}$ to and from the scattering region and letting the other terminals k and l keep zero thermal flux, we measure temperatures T_k and T_l [12]. From $\dot{Q}_k = \dot{Q}_l = 0$, the temperature difference ratio $\alpha_{ij,kl}$ and $\kappa_{ij,kl}$ can be obtained without difficulty:

$$\alpha_{ij,kl} \equiv \Delta T_{ij}/\Delta T_{kl} = [\kappa_{kl}(\kappa_{ik} + \kappa_{il} + \kappa_{kj} + \kappa_{lj}) + (\kappa_{ik} + \kappa_{jk})(\kappa_{il} + \kappa_{jl})]/D, \quad (2)$$

$$\kappa_{ij,kl} \equiv \dot{Q}_i/\Delta T_{kl} = [\kappa_{ij}\kappa_{kl}(\kappa_{ik} + \kappa_{il} + \kappa_{kj} + \kappa_{lj}) + \kappa_{kl}(\kappa_{ik} + \kappa_{il})(\kappa_{jk} + \kappa_{jl}) + \kappa_{ij}(\kappa_{ik} + \kappa_{jk})(\kappa_{il} + \kappa_{jl}) + \kappa_{ik}\kappa_{il}\kappa_{kj}\kappa_{lj}(\kappa_{ik}^{-1} + \kappa_{il}^{-1} + \kappa_{kj}^{-1} + \kappa_{lj}^{-1})]/D, \quad (3)$$

where $D \equiv \kappa_{ik}\kappa_{lj} - \kappa_{il}\kappa_{kj}$, and $\Delta T_{ij} = T_i - T_j$. The four-terminal quality $\kappa_{ij,kl}$ has several general features. First, from its definition we have $\kappa_{ij,kl} = -\kappa_{ij,lk} = -\kappa_{ji,kl} = \kappa_{ji,lk}$. Second, from time-reversal invariance we have the reciprocity relation $\kappa_{ij,kl} = \kappa_{kl,ij}$ and $\kappa_{ij,kl}^{-1} + \kappa_{il,jk}^{-1} + \kappa_{ik,lj}^{-1} = 0$. The reciprocity relation indicates that if one exchanges the roles of terminals for thermal flux and for temperature measurements, the four-terminal thermal conductance is the same. On the other hand, the temperature difference ratios $\alpha_{ij,kl}$ do not satisfy similar Onsager relations. It is also worth mentioning that if $\kappa_{ik}\kappa_{jl} = \kappa_{il}\kappa_{jk}$, the four-terminal "thermal bridge" will reach equilibrium and the temperature difference ΔT_{kl} between two terminals k and l is always zero regardless how large a thermal flux passing through the other two terminals i and j. In such a situation quantities $\kappa_{ij,kl}$ and $\alpha_{ij,kl}$ will tend to infinity. As a comparison, for an electric four-terminal system, if the scattering matrix takes the Breit-Wigner form, the four-terminal electric bridge reaches equilibrium in which the voltage difference between the two voltage terminals is zero [14].

In the rest of this paper, we consider a specific two-dimensional four-terminal mesoscopic dielectric system, shown in the inset of Fig. 2(a), in which four semi-infinite wires parallel to the x axis are coupled to the center region with sizes b and L. Our goal is still on general properties of the four-terminal tensor $\kappa_{ij,kl}$. We permit different widths for the four-terminal wires so that the system does not have a mirror symmetry; therefore we clearly demonstrate that the characteristics of $\kappa_{ij,kl}$ are not originated from the geometric symmetry. We consider a scalar model of elasticity [7] where the displacement field $u(x, y)$ satisfies the wave equation: $c^2\nabla^2 u(x, y) + \omega^2 u(x, y) = 0$, where c is the sound velocity. If the coupling between three different components of the displacement vector field is small enough, the scalar wave model is a good model. We assume that incident phonon at mode n comes from terminal $i = 1$. Noting the free boundary condition, the wave functions $u(x, y)$ in the four-terminal region I-V are written as follows:

$$u_I(x, y) = \Psi_{1n}(y)e^{ik_{1n}x} + \sum_m r_{11,mn}\Psi_{1m}(y)e^{-ik_{1m}x},$$

$$u_{II}(x, y) = \sum_m t_{21,mn}\Psi_{2m}(y)e^{-ik_{2m}x},$$

$$u_{III/IV}(x, y) = \sum_m t_{3/41,mn}\Psi_{3/4m}(y)e^{ik_{3/4m}x},$$

$$u_V(x, y) = \sum_\alpha [a_{\alpha n}\Psi_\alpha(y)e^{ik_\alpha x} + b_{\alpha n}\Psi_\alpha(y)e^{-ik_\alpha x}],$$

where, $\Psi_{im}(y)$ $(m = 0, 1, 2, ...)$ and $\Psi_\alpha(y)$ $(\alpha = 0, 1, 2, ...)$ are orthonormal transverse wave functions in terminal i and center region V, respectively. k_{im} and k_α are the corresponding wave vectors with $\omega^2 = c^2k_{im}^2 + \omega_{im}^2 = c^2k_\alpha^2 + \omega_\alpha^2$, in which $\omega_{im} = \frac{m\pi c}{a_i}$ and $\omega_\alpha = \frac{\alpha\pi c}{L}$ are cutoff energies of modes im and α. $r_{11,mn}$ and $t_{j1,mn}$ $(j = 2, 3, 4)$ are reflection and transmission amplitudes; $a_{\alpha n}$ and $b_{\alpha n}$ are constants to be determined. We calculate these constants by matching boundary conditions. After solving $r_{11,mn}$ and $t_{j1,mn}$ $(j = 2, 3, 4)$, the reflection and transmission coefficients can be obtained straightforwardly, $R_{11,mn}(\omega) = \theta(\omega - \omega_{1m})|r_{11,mn}(\omega)|^2 k_{1m}/k_{1n}$ and $T_{j1,mn}(\omega) = \theta(\omega - \omega_{jm})|t_{j1,mn}(\omega)|^2 k_{jm}/k_{1n}$. Here the function $\theta(\omega - \omega_{jm})$ is because the outgoing wave vector κ_{jm} is imaginary at $\omega < \omega_{jm}$, so that this wave cannot

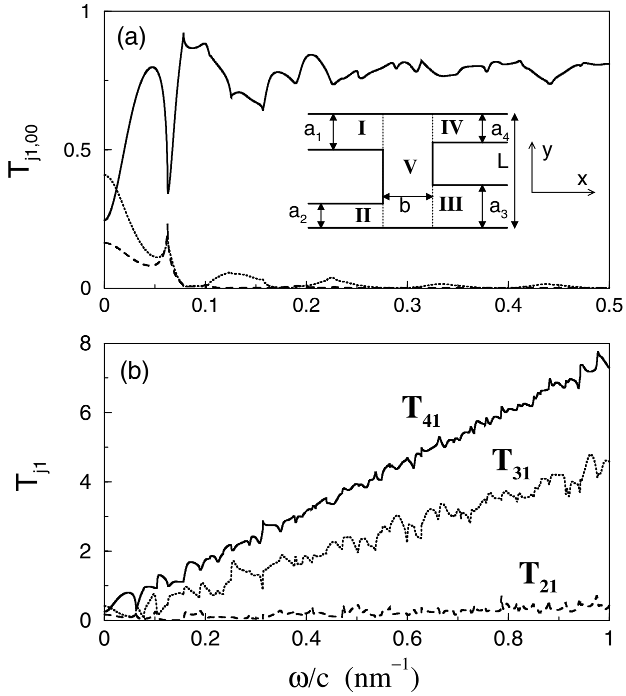

FIG. 2. Transmission coefficient $T_{j1,00}$ (a) and T_{j1} (b) versus incident phonon frequency ω. In (a), the dashed line is for $T_{21,00}$; the dotted line is for $T_{31,00}$; and the solid line is for $T_{41,00}$. Inset in (a) is a plot for a specific four-terminal system. Other parameters: $a_1 = 40$ nm, $a_2 = 20$ nm, $a_3 = 50$ nm, $a_4 = 30$ nm, $L = 100$ nm, $b = 30$ nm, and $c = 5000$ m/s.

propagate. The transmission coefficient of incident phonons from terminals 2, 3, and 4 can be solved in exactly the same fashion. Thermal conductance κ_{ij} and $\kappa_{ij,kl}$ can then be obtained from Eqs. (1) and (3), respectively.

Figure 2 shows the transmission coefficient $T_{j1,00}(\omega)$ for the incident wave coming from terminal 1 in mode 0, and the total transmission coefficient T_{j1}. They all exhibit rather complicated oscillating behavior. $T_{j1,m0}(\omega)$ must be less than unity, with $\sum_{j,m} T_{j1,m0}(\omega) + \sum_m R_{11,m0}(\omega) = 1$. $T_{ji}(\omega)$ can be greater than unity, due to the opening of higher modes at larger ω. At large ω, $T_{41,00}$ is much larger than other components of $T_{j1,00}$ [Fig. 2(a)]. Because the wavelengths of thermal phonons become very short at large ω, ballistic phonon transmission is observed in which the direct transport from terminal 1 to terminal 4 is clearly the easiest and therefore the largest [see the inset of Fig. 2(a)].

In the following we investigate the small ω limit. At $\omega \to 0$, the transmission coefficient tends to $T_{ij} = T_{ij,00} = \frac{4a_i a_j}{a^2}$, and the reflection coefficient tends to $R_{ii} = R_{ii,00} = \frac{(a-2a_i)^2}{a^2}$ where $a = \sum_{i=1}^{4} a_i$. Note that they are dependent only on the width of the terminal and are independent of the scattering region sizes L and b. This is actually expected since at small ω, the wavelength of the phonon is large, and when it becomes much larger than the dimension of the scattering region, the displacement field $u(x, y)$ becomes essentially the same throughout. Similarly, for two-terminal mesoscopic systems at the $\omega \to 0$ limit, we have $T_{12} = \frac{4a_1a_2}{a^2} = 1$ and $R_{11} = \frac{(a-2a_1)^2}{a^2} = 0$ $(a_1 = a_2)$, also independent of the scattering region [4,6].

Next, we investigate κ_{ij} by plotting κ_{ij} and κ_{ij}/T in Fig. 3 and its inset. κ_{ij} is a monotonic function of temperature T. At high temperature, e.g., $T > 1$ K, $\kappa_{ij} \sim T^2$. At low temperature, e.g., $T < 0.1$ K, $\kappa_{ij} \sim T$. In some temperature ranges, κ_{ij} may also exhibit a T^δ scaling with $\delta < 1$, e.g., κ_{13} in the range of $0.2 < T < 0.5$ K. These results are consistent with previous works for two-terminal systems [4,6,8]. κ_{ij}/T versus T may exhibit nonmonotonic behavior and it can have a minimum at $T \neq 0$ (see κ_{12}/T and κ_{13}/T, inset of Fig. 3). Similar results have been seen in the experiments of Schwab *et al.* [1]. Note, although here the two-terminal quantity κ_{ij} is actually measured between two terminals of a four-terminal device, it has the same property as that of a two-terminal device [1,4,6,8]. We emphasize, again, that at the $T \to 0$ limit in which the wavelength of incident phonons is much larger than the dimension of the scattering region, κ_{ij}/T tend to $[(4a_ia_j)/(a^2)][(\pi^2 k_B^2)/(3h)] = [(\pi^2 k_B^2)/(3h)]T_{ij}(0)$, which is dependent only on the width of the terminal and is independent from the shape of the scattering region. To put the magnitudes into perspective, if the linear size of the scattering region is 100 nm, phonons whose wavelength is 10 times larger correspond to a temperature scale $T = \frac{\hbar\omega}{k_B} = \frac{hc}{k_B\lambda} \approx 0.2$ K, which is experimentally realizable.

Next, we instigate the four-terminal quantity $\kappa_{ij,kl}$ which is shown in Fig. 4. Unlike the two-terminal quantity κ_{ij} which is monotonic, $\kappa_{ij,kl}$ is a nonmonotonic function of temperature T as indicated by one or more extremely small values. At high temperatures, $|\kappa_{ij,kl}|$ is proportional to T^2, similar to κ_{ij}. However, at the low-temperature limit ($T \to 0$), $|\kappa_{ij,kl}|$ does not tend to zero as κ_{ij} does; it tends to ∞ as T^{-1}, i.e., thermal resistance tends to vanish. This result is quite surprising indeed. From Eq. (3), $|\kappa_{ij,kl}|$ is in proportion to the two-terminal thermal conductance, therefore it apparently should go as

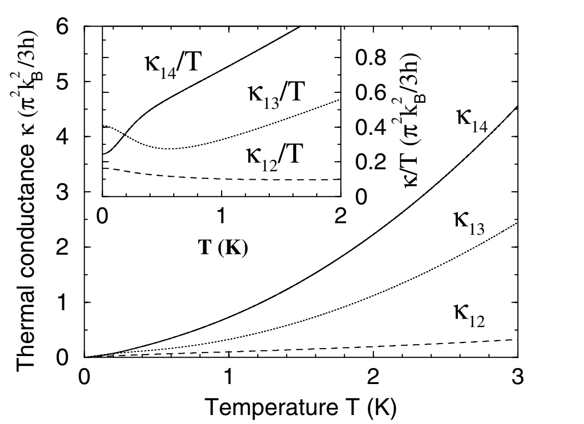

FIG. 3. Two-terminal thermal conductance κ_{ij} (main plot) and κ_{ij}/T (inset) vs temperature T. Other parameters are the same as those of Fig. 2.

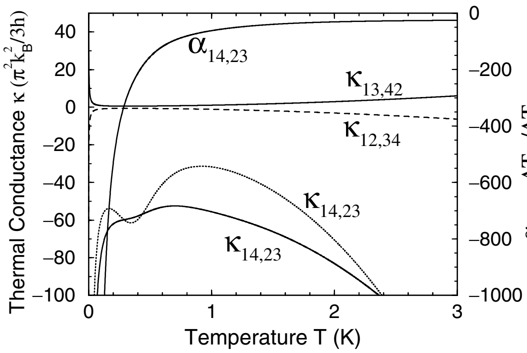

FIG. 4. Four-terminal thermal conductance $\kappa_{ij,kl}$ (left scale) and $\alpha_{14,23}$ (right scale) vs temperature T. The parameters of dotted curves ($\kappa_{14,23}$) are $a_1 = a_2 = a_3 = a_4 = 40$ nm; parameters of other curves are the same as those of Fig. 2.

T, not T^{-1}. However, at $T \to 0$, since κ_{ij} is proportional to $[(4a_i a_j)/(a^2)]T$, $\kappa_{ik}\kappa_{lj} = \kappa_{il}\kappa_{kj}$, and $D \to 0$. This means that the thermal bridge reaches equilibrium at $T \to 0$. Hence, the temperatures measured at the two temperature terminals k and l will be almost the same. This gives rise to $|\kappa_{ij,kl}| \to \infty$. To show more clearly the physical meaning of this result, we plot a temperature difference ratio $\alpha_{14,23} = \frac{\Delta T_{14}}{\Delta T_{23}}$ in Fig. 4. It clearly exhibits that at $T \to 0$, $|\alpha_{14,23}| \to T^{-2}$. In other words, at very low temperature, to have a finite ΔT_{14} so that there is a flux flowing between terminals 1 and 4, the temperature difference ΔT_{23} of the other two terminals with zero flux tends to vanish as $\sim T^2$. As a numerical example, at higher temperatures, e.g., $T = 3$ K for which $\alpha_{14,23} \approx 25$, hence to maintain $\Delta T_{14} \sim 0.5$ K, we obtain $\Delta T_{23} \approx 20$ mK which is an appreciable temperature difference. At lower temperature $T = 100$ mK we found $\alpha_{14,23} \sim 1500$; to maintain $\Delta T_{14} \sim 500$ mK the temperature difference ΔT_{23} is merely 0.33 mK, i.e., $T_2 \approx T_3$. Finally, it is important to note the following two points: (i) the result that $|\kappa_{ij,kl}| \to \infty$ at low temperature is independent from the shape of the scattering region; (ii) this result is very different from the behavior of four-terminal electric conductance which generally takes a finite value at $T = 0$ [12,14].

So far we have studied the general behaviors of κ_{ij} and $\kappa_{ij,kl}$ for multiterminal systems. It is an interesting theoretical problem to examine to see if these behaviors hold for fractional exclusion statistics (FES) [15]. This can be investigated by replacing the Bose-Einstein distribution $n(\omega)$ in Eq. (1) by the FES distribution function $n_g(\omega)$, with $n_g(\omega) = [W(\frac{\hbar\omega - \mu}{k_B T}) + g]^{-1}$ where μ is the particle chemical potential and $W(\tilde{\epsilon})^g[1 + W(\tilde{\epsilon})]^{1-g} = e^{\tilde{\epsilon}}$. For $g = 0$ or 1, $n_g(\omega)$ becomes the Bose-Einstein or Fermi-Dirac distribution, respectively. Following a similar line of derivation as discussed above, we find that the Onsager relations are still valid for FES. One can also prove that the monotonic behavior of κ_{ij} can survive only for $g = 0$, i.e., for the phonon system. For $g > 0$, our investigation indicates that κ_{ij} and $\kappa_{ij,kl}$ can be nonmonotonic or a monotonic function of T, depending on the specularity of each device. At the low-temperature limit, κ_{ij} tends to $\frac{\pi^2 k_B^2 T}{3h} T_{ij}(\mu)$ for all g. For $g > 0$, the thermal bridge may be in a nonequilibrium state, in that case $\kappa_{ij,kl}$ tends to zero as κ_{ij} does. When it is at equilibrium, $\kappa_{ij,kl}$ may tend to any value for $g > 0$. Therefore, the results for FES are quite different from the Bose-Einstein statistics in which $\kappa_{ij,kl}$ tends to ∞ at very low T.

In summary, we have examined the physical behavior of four-terminal thermal conductance for mesoscopic dielectric systems with arbitrary shapes of a scattering region. For the phonon system, κ_{ij} is a monotonic function of T and $\kappa_{ij,kl}$ is nonmonotonic. In the low-temperature limit, $|\kappa_{ij,kl}|$ tends to infinite as $\sim T^{-1}$; κ_{ij} tends to zero as $\sim T$; and the temperature difference of the two terminals without thermal flux tends to zero as $\sim T^2$. For fractional exclusion statistics ($g > 0$), κ_{ij} and $\kappa_{ij,kl}$ may be monotonic or a nonmonotonic function of T which is dependent on the special details of a device.

We gratefully acknowledge financial support from the Natural Science and Engineering Research Council of Canada, le Fonds pour la Formation de Chercheurs et l'Aide à la Recherche de la Province du Québec.

[1] K. Schwab, E. A. Henriksen, J. M. Worlock, and M. L. Roukes, Nature (London) **404**, 974 (2000).
[2] T. S. Tighe, J. M. Worlock, and M. L. Roukes, Appl. Phys. Lett. **70**, 2687 (1997).
[3] M. M. Leivo and J. P. Pekda, Appl. Phys. Lett. **72**, 1305 (1998); W. Holmes, J. M. Gildemeister, and P. L. Richards, *ibid.* **72**, 2250 (1998).
[4] L. G. C. Rego and G. Kirczenow, Phys. Rev. Lett. **81**, 232 (1998).
[5] M. P. Blencowe, Phys. Rev. B **59**, 4992 (1999).
[6] A. Kambili, G. Fagas, V. I. Fal'ko, and C. J. Lambert, Phys. Rev. B **60**, 15 593 (1999).
[7] D. E. Angelescu, M. C. Cross, and M. L. Roukes, Superlattices Microstruct. **23**, 673 (1998).
[8] B. A. Glavin, Phys. Rev. Lett. **86**, 4318 (2001); D. H. Santamore and M. C. Cross, *ibid.* **87**, 115502 (2001).
[9] A. Buldum, D. M. Leitner, and S. Ciraci, Europhys. Lett. **47**, 208 (1999).
[10] The devices of Refs. [1,2] were actually four terminal, although only two-terminal measurements were taken.
[11] M. Büttiker, IBM J. Res. Dev. **32**, 63 (1988); Phys. Rev. B **38**, 9375 (1988).
[12] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).
[13] In this work we have neglected phonon relaxation in the scattering region which is reasonable at low temperatures. At higher temperature, e.g., a few tens Kelvin or more, phonon-phonon scattering events become important. Especially, when umklapp processes are involved, κ_{ij} may be reduced as temperature is increased.
[14] M. Büttiker, Phys. Rev. B **38**, R12 724 (1988).
[15] L. G. C. Rego and G. Kirczenow, Phys. Rev. B **59**, 13 080 (1999); I. V. Krive and E. R. Mucciolo, *ibid.* **60**, 1429 (1999).