

## Comment on “Wave-scattering formalism for thermal conductance in thin wires with surface disorder”

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In their calculations based on the Landauer transport equation, Akguc and Gong [Phys. Rev. B **80**, 195408 (2009)] obtained an expression for the heat conductance of a quantum wire valid in the ballistic regime and in the limit of vanishing temperature difference between reservoirs. Their result appears to be different from the one reported in the previous paper of Rego and Kirczenow [Phys. Rev. Lett. **81**, 232 (1998)], which led them to argue that their new result was the correct one. We show here that, in fact, both results are correct since different definitions for the dilogarithm function were used in those papers. Hence, comparisons between these two results should be done with care.

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In order to obtain an expression for the heat conductance of a quantum wire between reservoirs with different temperatures in the ballistic regime, both papers of Akguc and Gong (AG) (Ref. 1) and Rego and Kirczenow (RK) (Ref. 2) have a common starting point: the Landauer transport equation for the heat flux

$$\dot{Q} = \sum_{\alpha} \int_0^{\infty} \frac{dk}{2\pi} \hbar \omega_{\alpha}(k) v_{\alpha}(k) (\eta_R - \eta_L) \zeta_{\alpha}(k), \quad (1)$$

where  $\hbar \omega_{\alpha}(k)$  is the phonon energy,  $v_{\alpha}(k)$  its velocity,  $\zeta_{\alpha}(k)$  is a transmission coefficient, and  $\eta_i(\omega) = [e^{\hbar \omega / k_B T_i} - 1]^{-1}$ , with  $i=L, R$ , is the phonon occupation number in each reservoir. Setting  $\zeta_{\alpha}(k)=1$  in the ballistic regime and using  $\kappa = \dot{Q} / \Delta T$  for the conductance, with  $\Delta T = T_R - T_L$ , RK obtained in the limit  $\Delta T \rightarrow 0$  the expression

$$\frac{\kappa}{\frac{k_B^2 T}{h}} = \frac{\pi^2}{3} N_{\alpha} + \sum_{\alpha'} \left\{ \frac{\pi^2}{3} + 2 \operatorname{dilog}(e^{x_0}) + \frac{x_0^2 e^{x_0}}{e^{x_0} - 1} \right\}, \quad (2)$$

where  $N_{\alpha}$  is the number of modes with zero cutoff frequency (massless modes),  $N_{\alpha'}$  is the number of modes with nonzero cutoff frequency  $\omega_{\alpha'}(0)$ , and  $x_0 = \hbar \omega_{\alpha'}(0) / k_B T$  with  $T = (T_R + T_L) / 2$  is the average temperature of the reservoirs. For a single-mode with nonzero cutoff frequency, this expression becomes

$$\frac{\kappa}{\frac{k_B^2 T}{h}} = \frac{\pi^2}{3} + 2 \operatorname{dilog}(e^{x_0}) + \frac{x_0^2 e^{x_0}}{e^{x_0} - 1}. \quad (3)$$

Here, and in Eq. (2), the function  $\operatorname{dilog}(z)$  known as the dilogarithm function is defined as the integral<sup>3</sup>

$$\operatorname{dilog}(z) = \int_1^z \frac{\ln t}{1-t} dt. \quad (4)$$

This definition associated with the “dilog” notation is the one adopted, for example, in the software MAPLE.<sup>4</sup> Note that

$\operatorname{dilog}(e^{x_0})$  is a real function for all values of  $x_0$  and since  $\operatorname{dilog}(1)=0$  for  $x_0=0$ , the correct limit of high temperatures or zero cutoff frequency is obtained.

On the other hand, by first taking the limit  $\Delta T \rightarrow 0$  on the expression for  $\kappa$  and then evaluating the resulting integral, AG obtained the result for a single mode with nonzero cutoff frequency as

$$\frac{\kappa}{\frac{k_B^2 T}{h}} = \frac{x_0^2 e^{x_0}}{e^{x_0} - 1} - 2x_0 \ln(1 - e^{x_0}) + \frac{2\pi^2}{3} - 2\operatorname{Li}_2(e^{x_0}). \quad (5)$$

Here, the function  $\operatorname{Li}_2(z)$  is also known as the dilogarithm function, but when used with this notation, it is defined in a slightly different form as<sup>5</sup>

$$\operatorname{Li}_2(z) = \int_z^0 \frac{\ln(1-t)}{t} dt. \quad (6)$$

This definition and notation for the dilogarithm function is the one adopted, for example, in the MATHEMATICA software.<sup>6</sup> It is associated with the more general polylogarithm function  $\operatorname{Li}_n(z)$ , defined as a power series<sup>5</sup> that has the integral representation of Eq. (6) for  $n=2$ . This function is different from the  $\operatorname{dilog}(z)$  function defined earlier. In fact, from Eq. (4) we obtain an important relation between the definitions,

$$\operatorname{dilog}(z) = \operatorname{Li}_2(1-z). \quad (7)$$

Note that  $\operatorname{Li}_2(e^{x_0})$  is a complex function, but its imaginary part is canceled by the one of  $\ln(1 - e^{x_0})$  in Eq. (5), so we can drop the real part on  $\operatorname{Li}_2$  of Eq. (6) of AG’s paper by flipping their logarithmic argument, as we did above. Note also that  $\operatorname{Li}_2(1) = \pi^2 / 6$  for  $x_0=0$ , so AG’s expression (5) also satisfies the correct limit of high temperatures or zero cutoff frequency. However, AG noted the “clear” difference between Eqs. (3) and (5) and stated that RK’s expression, Eq. (3), was wrong. They pointed out some differences between the expressions, but apparently they were not aware that the  $\operatorname{dilog}(z)$  function in RK’s paper is not the same function as

$\text{Li}_2(z)$  they used. This fact led them to incorrect conclusions, such as the one in Fig. 4b of their paper, where RK's expression is plotted after the wrong substitution  $\text{dilog}(z)=\text{Li}_2(z)$  and therefore a physically incorrect result is obtained, where the conductance does not even go to zero as  $T$  goes to zero.

In fact, there is a "reflection" property of the  $\text{Li}_2(z)$  function<sup>5</sup>

$$\text{Li}_2(z) + \text{Li}_2(1-z) = \frac{\pi^2}{6} - \ln(z)\ln(1-z) \quad (8)$$

that allows us to establish a relation between the expressions of RK and AG. By setting  $z=e^{x_0}$  and using Eq. (7), we can see that RK's expression leads to AG's expression and vice versa, so both results are correct when compatible definitions

are considered, as should be expected from the high-temperature or zero cutoff limits we discussed above.

Finally, we remark that extra care must be taken when referring to "the" dilogarithm function. In fact, due to historical reasons, there are several definitions for this function in the literature<sup>5</sup> other than the two we discussed here. Therefore, authors should be aware of that when comparing their results with others in the literature. We emphasize, however, that the comparison between RK and AG represents a small portion of AG's paper and most of the results of the latter paper are sound and important.

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<sup>4</sup><http://www.maplesoft.com/>

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<sup>6</sup><http://mathworld.wolfram.com/>