Reply to "Comment on 'Wave-scattering formalism for thermal conductance in thin wires with surface disorder"

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We confirm the analysis given by Menezes *et al.* in their comment [M. G. Menezes, J. Del Nero, R. B. Capaz, and L. G. C. Rego, Phys. Rev. B **81**, 117401 (2010)]. Hence, one heat conductance expression derived by us is actually equivalent to the one in a previous paper by Rego and Kirczenow [L. G. C. Rego and G. Kirczenow, Phys. Rev. Lett. **81**, 232 (1998)]. In addition, a rather detailed derivation of our heat conductance formula for a one-mode case is now given.

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The preceding Comment by Menezes *et al.*¹ compared two expressions for the heat conductance of a ballistic quantum wire between two reservoirs. One expression is from the seminal work by Rego and Kirczenow² and the other is independently derived by us in studies of heat conductance in disordered thin wires.³ Reference 1 showed that these two expressions are both correct and in fact equivalent to each other but with different definitions of the so-called dilogarithm function. As such, the observed discrepancy between the two expressions, recently reported in Ref. 3 as a side result, is due to a misunderstanding. We are glad that this issue is now settled. We emphasize, as the authors of Ref. 1 agree, that all other findings in Ref. 3 are not affected.

The dilogarithm function in general takes complex values and so it should be treated with care. Remarkably, when discussing our result, Ref. 1 used a different treatment than ours. Hence, it is still of considerable interest to explicitly show how we derived Eq. (16) in Ref. 3 using a rather standard definition of the dilogarithm function, ^{4,5}

$$\operatorname{Li}_{2}(z) \equiv \int_{z}^{0} \frac{\ln(1-t)}{t} dt. \tag{1}$$

In particular, adopting the same notation as in Ref. 3 (but without scaling the temperature etc.), the heat conductance for a general throughput is given by

$$\kappa = \frac{\hbar^2}{k_B T^2} \sum_{\alpha} \frac{1}{2\pi} \int_0^{\infty} G_{\alpha}(w) \frac{w^2 \exp(\hbar w/k_B T)}{[\exp(\hbar w/k_B T) - 1]^2} dw.$$
 (2)

For a single-mode case with the throughput function G(w) = 0 for w < a and G(w) = 1 for $w \ge a$, we obtain

$$\kappa = \frac{k_B^2 T}{h} \left[\frac{\pi^2}{3} - \int_0^{x_0} \frac{x^2 e^x}{(e^x - 1)^2} dx \right],\tag{3}$$

with

$$x_0 \equiv \frac{\hbar a}{k T}.$$
 (4)

The second term in Eq. (3) can be evaluated by using integration by parts twice, i.e.,

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$$\int_{0}^{x_{0}} \frac{x^{2} e^{x}}{(e^{x} - 1)^{2}} dx = -\frac{x_{0}^{2} e^{x_{0}}}{e^{x_{0}} - 1} + 2x_{0} \ln(e^{x_{0}} - 1)$$
$$-2 \int_{1}^{e^{x_{0}}} \frac{\ln(t - 1)}{t} dt, \tag{5}$$

where we have introduced a change in integration variables in the last term of Eq. (5). Using⁶

$$\operatorname{Li}_{2}(z) = \frac{\pi^{2}}{6} - \int_{1}^{z} \frac{\ln(t-1)}{t} dt - i\pi \ln(z), \tag{6}$$

the last term in Eq. (5) can be rewritten as

$$-2\int_{1}^{e^{x_0}} \frac{\ln(t-1)}{t} dt = -2\left\{\frac{\pi^2}{6} - \Re[\text{Li}_2(e^{x_0})]\right\}. \tag{7}$$

With Eqs. (5) and (7), Eq. (3) finally leads to

$$\kappa = \frac{k_B^2 T}{h} \left\{ \frac{x_0^2 e^{x_0}}{(e^{x_0} - 1)} - 2x_0 \ln(e^{x_0} - 1) + \frac{2\pi^2}{3} - 2\Re[\text{Li}_2(e^{x_0})] \right\}.$$
(8)

As pointed out in Ref. 1, Eq. (8) derived above is equivalent to Eq. (5) in Ref. 1.

Considering the current wide interest in heat conduction studies and the importance of Ref. 2, the detailed derivations and the clarifications made here and in Ref. 1 should be useful.

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- ¹M. G. Menezes, J. Del Nero, R. B. Capaz, and L. G. C. Rego, Phys. Rev. B **81**, 117401 (2010).
- ²L. G. C. Rego and G. Kirczenow, Phys. Rev. Lett. **81**, 232 (1998).
- ³G. B. Akguc and J. B. Gong, Phys. Rev. B **80**, 195408 (2009).
- ⁴L. Lewin, *Polylogarithms and Associated Functions* (North-Holland, New York, 1981).
- ⁵R. Morris, Math. Comput. **33**, 778 (1979).
- ⁶http://en.wikipedia.org/wiki/Polylogarithm#Dilogarithm