Interaction enhanced thermopower in a Luttinger liquid

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The thermopower $S_L(T)$ of a finite Luttinger liquid (LL) wire containing an impurity and connected to leads of noninteracting electrons is calculated. It is shown that at low temperatures $k_B T \ll \Delta_L \simeq \hbar \mathbf{v}_F / gL$ (L is the length of the wire, $\mathbf{v}_F$ is the Fermi velocity of the electrons, and g is the correlation parameter of the LL), $S_L(T)$ is described by a Mott-type formula. However, at higher temperatures, that is, when $\Delta_L \leqslant k_B T \ll \varepsilon_F$, the expression for $S_L(T)$ contains an interaction-dependent factor. For strong interelectron interaction, the enhancement of the thermopower is large and it is much more pronounced for spinless electrons.

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Thermopower expresses the ability of a system of charged particles to generate an electromotive force when a temperature gradient is applied across the system. For noninteracting electrons the thermopower coefficient $S_0(T)$ can be represented by Mott's formula as a logarithmic derivative of the conductivity, σ, evaluated at the Fermi energy ε_F (see, e.g., Ref. 1),

$$S_0(T) \simeq -\frac{\pi^2}{3}\frac{k_B^2 T}{e}\left(\frac{\partial \ln \sigma(\varepsilon)}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_F}. \tag{1}$$

In ordinary metals, the conductivity is a smooth function of the energy near ε_F and the thermopower coefficient is very small,

$$S_0(T) \simeq -\frac{\pi^2}{3}\frac{k_B^2 T}{e\varepsilon_F}. \tag{2}$$

An appreciable value of the thermopower coefficient may develop in a system with a strong energy dependence of the electron scattering processes, such as, for example, in Kondo systems.[2] A change in the thermopower behavior may also take place in a ballistic wire (constriction) connecting bulk reservoirs, and the thermopower of such a wire may also be described by Eq. (1) with the conductance G replacing the conductivity,[3,4] that is,

$$S_W(T) \simeq -\frac{\pi^2}{3}\frac{k_B^2 T}{e}\left(\frac{\partial \ln G(\varepsilon)}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_F}. \tag{3}$$

In the following, we will refer to Eq. (3) as a Mott-type formula. In the classical limit (i.e., when the electron Fermi wavelength is much smaller than the constriction size), the conductance of the constriction is a smooth function of the energy and the above expression for the thermopower [Eq. (2)] maintains.[5] In a quantum wire, the thermopower exhibits a peaklike behavior both in two-dimensional[6] and three-dimensional[4] systems due to the steplike energy dependence of the electronic transmission probabilities. It is also known that in a Luttinger liquid (LL) with an impurity, the conductance for a strong repulsive interaction is a sharp function of the energy (that is, temperature or bias voltage) near ε_F (see Ref. 7 and a review in Ref. 8). Assuming the validity of Eq. (3) for *interacting* electrons, one would expect strong thermoelectric response in certain LL systems, such as long quantum wires or in carbon nanotubes. While the above simple local relation between the thermopower and conductivity does not hold for interacting particles, we show below that under certain conditions the thermopower of a LL wire can be expressed through the derivative of the conductance of noninteracting electrons multiplied by an interaction- and spin-dependent factor which takes large values for strong repulsive interactions.

In contrast to the ''diagonal'' transport coefficients (electric and thermal conductance) of a LL, the off-diagonal coefficients, which determine thermoelectric effects in a LL (i.e., the Seebeck and Peltier effects), remain largely unexplored. It is known (see, e.g., Ref. 8) that for an ideal (without impurities) LL, the dc conductance does not depend on the energy parameters (e.g., temperature and bias voltage) and the thermopower vanishes[9] as a direct consequence of the linearized spectrum of electrons in the LL model. However, consideration of the small electronic band curvature leads to a finite result for the thermopower[9] which is described by an expression analogous to Eq. (1) but renormalized by an interaction-dependent factor g^{-1}, where g is the correlation parameter of a spinless LL (see below). It has been noted also that the thermopower of a Hubbard chain in the vicinity of a Mott-Hubbard phase transition to a dielectric phase can be calculated using a Mott-type formula [see Eq. (3)] for noninteracting fermions.[10] This observation was exploited[11] in a derivation of the thermopower of a homogeneous infinite Hubbard chain in the limits when the Hubbard model could be mapped onto a model of spinless Dirac fermions.

For noninteracting electrons, the thermopower in the linear-response regime can be represented as a ratio of the L and G transport coefficients $S(T,\mu) = -L(T,\mu)/G(T,\mu)$, where G is the electric conductance and L is the cross-transport coefficient which connects the electric current to the temperature difference. Both these coefficients can be calculated using the formalism developed in Ref. 5 and adapted in Ref. 12 to the Landauer scheme.[13] In this approach, the transport coefficients are expressed through a transmission probability $t_j(\varepsilon)$ for an electron to arrive at the drain electrode in the jth channel as

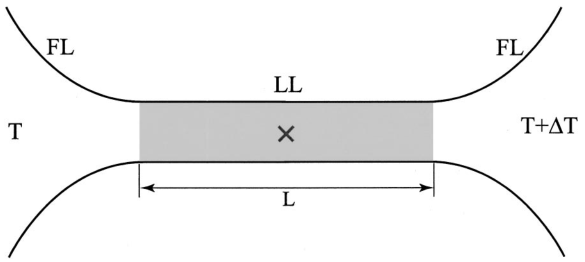

FIG. 1. A schematic of a Luttinger liquid (LL) nanowire of length L connected to Fermi liquid (FL) reservoirs held at different temperatures. The impurity (denoted by X) is placed in the middle of the LL wire.

$$G(T,\mu)=G_0\sum_{j=1}^{N}\int_0^\infty d\varepsilon\left(-\frac{\partial f_F}{\partial\varepsilon}\right)t_j(\varepsilon) \tag{4}$$

and

$$L(T,\mu)=G_0\frac{k_B}{h}\sum_{j=1}^{N}\int_0^\infty d\varepsilon\left(-\frac{\partial f_F}{\partial\varepsilon}\right)\frac{\varepsilon-\mu}{k_BT}t_j(\varepsilon). \tag{5}$$

Here $G_0=e^2/h$ is the conductance quantum for each spin direction, $f_F(\varepsilon-\mu)$ is the Fermi-Dirac distribution function of the electrons in the leads, and μ is the chemical potential.

Equations (4) and (5) cannot be applied to an infinite LL where the electrons are not the propagating particles and the conventional scattering problem is ''ill-defined.'' A general approach for calculating transport coefficients in a system of strongly interacting particles is the Kubo formalism, which as aforementioned has been used for calculation of the thermopower for a Hubbard chain.[11] With the Kubo approach it is difficult to calculate the thermopower for the entire range of external parameters (temperature, interaction strength, density of particles, etc.), and indeed the final analytic expressions for the desired quantities were derived[10,11] only in the limits when the Hubbard model can be mapped onto a model of noninteracting fermions for which a Mott-type expression for the thermopower [Eq. (3)] could be used.

To obtain results for the thermopower pertaining to transport properties of systems of strongly interacting electrons, and to consider thermoelectric effects for quantum wires which could be tested experimentally, we chose to invoke as a first step certain simplified (yet physically reliable) models of strongly interacting electron systems. Such physical models of charge transport in LL's with strongly interacting electrons were proposed in Ref. 14 and they were shown to yield the same results as those obtained from more conventional (and rigorous) treatments of LL effects.[7,15] In the following, we apply these ideas to study the thermopower in a LL connected to Fermi liquid (FL) leads with an impurity located in the middle of the wire.

For a LL connected to FL reservoirs with given temperatures and chemical potentials, one can make use of Eqs. (4) and (5), with $t_j(\varepsilon)$ regarded now as the probability of transmission of the electrons (in the jth channel) through the *effective* potential barrier formed by the LL part of the wire. Consider first a wire which is adiabatically connected to the leads (that is, a LL constriction, see Fig. 1). For this arrange-

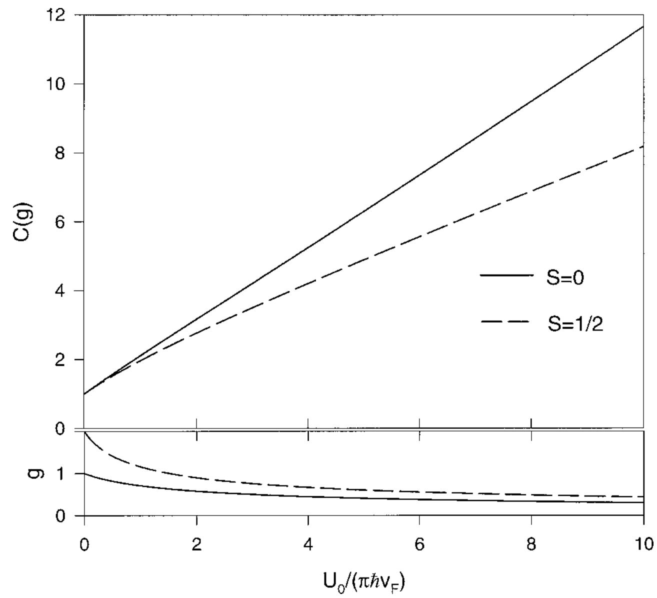

FIG. 2. The renormalization parameter $C(g)$ and the dimensionless electron interaction parameter g plotted as functions of the dimensionless electron-electron interaction strength, $U_0/(\pi\hbar v_F)$, for spinless and spin-$\frac{1}{2}$ electrons.

ment, the transmission coefficient is unity as long as we neglect the backscattering of the electrons by the confining potential. For a perfect wire, the backscattering effect is exponentially small for practically all values of the chemical potential, except at the narrow regions in the vicinity of the conductance jumps (steps) where an additional mode is converted from being an evanescent mode to becoming a propagating one. This physical picture results in a staircaselike behavior of the conductance as a function of the chemical potential and it is often modeled by abrupt jumps of the electron transmission coefficient from zero (reflected mode) to one (fully transmitted mode). For strongly interacting electrons, this simple model, which does not depend on the details of the *bare* scattering potential, may serve as an appropriate first approximation. Indeed, the transmission of electrons through a long but finite LL is determined by the effective scattering potential, which includes the effects of electron-electron interactions. For sufficiently long wires and for temperatures $k_BT\ll\varepsilon_F$, this effective potential quenches all modes whose bare transmission coefficients t_0 are not very close to unity (see discussion in Ref. 19). Since according to Eqs. (4) and (5) the thermopower $S(T,\mu)\propto\partial G/\partial\mu$, we observe that for a multimode LL constriction the thermopower vanishes on the conductance plateaus and it peaks at the conduction steprises as in the case of noninteracting electrons;[6] the ''oscillations'' of the thermopower in a LL are distinguished from those expected for noninteracting electrons (see, e.g., Ref. 16) by the shape of the thermopower peaks. Consequently, for strongly interacting electrons, a simple approximation where the (effective) transmission coefficient is modeled by a Heaviside step function could be a rather reliable procedure, and in this case the temperature behavior of the peaks will be universal (i.e., independent of the concrete shape of the confining potential).

To proceed with our calculation of the thermopower for a quantum wire with a single impurity, we require first an estimate for the electron transmission coefficient renormalized by the interelectron interaction (that is, the transmission coefficient of the LL piece of the electrical circuit). For a weak interaction, the renormalized transmission probability of a LL with an impurity has been evaluated in Ref. 17. When the interaction is not weak and the tunneling probability is small, one could use the semiclassical approximation developed in Ref. 14 (see also the review in Ref. 18). The above allows us to model the effective transmission coefficient as follows:[19]

$$t^{\text{eff}}(\varepsilon)=t_0(\varepsilon)\begin{cases}\left(\dfrac{\Delta_L}{\Lambda}\right)^{\alpha} & \text{for } |\varepsilon-\varepsilon_F|\ll\Delta_L\\[2mm] \left|\dfrac{\varepsilon-\varepsilon_F}{\Lambda}\right|^{\alpha} & \text{for } |\varepsilon-\varepsilon_F|\gg\Delta_L .\end{cases} \tag{6}$$

Here $t_0(\varepsilon)\ll 1$ is the bare transmission coefficient determined by the unrenormalized scattering potential (we restrict ourselves to a single-mode LL), $\Delta_L=\hbar v_F/gL$ is the characteristic low-energy scale (g is the LL correlation parameter, see below), and Λ is the cutoff energy which for a one-dimensional LL is of the order of the Fermi energy ε_F. The exponent α depends on the electron-electron interaction strength, U_0, and is different for spinless and spin-$\frac{1}{2}$ electrons (see, e.g., Ref. 20),

$$\alpha=2\left(\frac{1}{g}-1\right),\quad g=\left(1+\frac{U_0}{\pi\hbar v_F}\right)^{-1/2}\quad \text{for } s=0 \tag{7}$$

and

$$\alpha=\frac{2}{g_s}-1,\quad g_s=2\left(1+\frac{2U_0}{\pi\hbar v_F}\right)^{-1/2}\quad \text{for } s=\tfrac{1}{2}. \tag{8}$$

Note that the transmission probability t^{eff} in Eq. (6) results in an expression for the linear conductance which coincides (up to an irrelevant numerical constant) with that obtained in Ref. 21 via a renormalization-group calculation.

When evaluating Eq. (1) in the Landauer-Büttiker formalism, it is assumed that the transmission coefficient is a smooth function of the energy near ε_F. While this is an adequate approximation for a bare tunneling probability,

$$t_0(\varepsilon)\simeq t_0(\varepsilon_F)+(\varepsilon-\varepsilon_F)\left(\frac{\partial t_0}{\partial\varepsilon}\right)_{\varepsilon=\varepsilon_F}, \tag{9}$$

it is not so for the renormalized transmission coefficient given in Eq. (6). Hence, a simple local relation between the thermopower and the conductivity ceases to be valid for a LL with an impurity.

In a LL constriction, both of the transport coefficients given in Eqs. (4) and (5) are power-law functions of the temperature. By substituting Eqs. (6) and (9) into Eqs. (4) and (5), one readily obtains

$$G_{\text{LL}}(T)=G_0 t_0(\varepsilon_F)\begin{cases}\left(\dfrac{\Delta_L}{\Lambda}\right)^{\alpha}, & k_BT\ll\Delta_L\\[2mm] 2(1-2^{1-\alpha})\Gamma(1+\alpha)\zeta(\alpha)\left(\dfrac{k_BT}{\Lambda}\right)^{\alpha}, & \Delta_L\ll k_BT\ll\Lambda\end{cases} \tag{10}$$

and

$$L_{\text{LL}}(T)=G_0\left(\frac{\pi^2k_B^2T}{3e}\right)t_0'(\varepsilon_F)\begin{cases}\left(\dfrac{\Delta_L}{\Lambda}\right)^{\alpha}, & k_BT\ll\Delta_L\\[2mm] \dfrac{6}{\pi^2}(1-2^{-1-\alpha})\Gamma(3+\alpha)\zeta(2+\alpha)\left(\dfrac{k_BT}{\Lambda}\right)^{\alpha}, & k_BT\gg\Delta_L ,\end{cases} \tag{11}$$

where $\Gamma(x)$ and $\zeta(x)$ are the Gamma function and the Riemann zeta function, respectively.

From Eqs. (10) and (11), we conclude that at low temperatures $k_BT\ll\Delta_L$, the thermopower of a LL constriction with an impurity is not renormalized by the interelectron interactions, i.e.,

$$S_{\text{LL}}(T\ll\Delta_L/k_B)\simeq S_W^{(0)}(T), \tag{12}$$

and the thermopower coefficient, $S_W^{(0)}(T)$, is described by a Mott-type formula for noninteracting electrons, Eq. (3), with G being the corresponding (bare) conductance of the noninteracting electrons. This finding is not surprising, since at $k_BT\ll\Delta_L$ the noninteracting electrons in the leads determine the transport properties of the LL constriction. However, at temperatures $k_BT\gg\Delta_L$, the thermopower, being still a linear function of temperature, undergoes a strong multiplicative renormalization,

$$S_{\text{LL}}(T\gg\Delta_L/k_B)\simeq C_s(g)S_W^{(0)}(T),$$

$$C_s(g)=\frac{3}{\pi^2}\frac{1-2^{-1-\alpha}}{1-2^{1-\alpha}}\frac{\zeta(\alpha+2)}{\zeta(\alpha)}(\alpha+1)(\alpha+2). \quad (13)$$

Note that unlike the electric conductance $G_{\mathrm{LL}}(T)$ and the cross coefficient $L_{\mathrm{LL}}(T)$, the thermopower $S_{\mathrm{LL}}(T)$ does not depend on the cutoff parameter and therefore the interaction- and spin-dependent factor $C_s(g)$ cannot be absorbed into a redefinition of Λ.

For noninteracting electrons $C_s(g=1)=1$ and the Mott-type formula [Eq. (3)] holds (as it should) for all temperatures $k_BT \ll \varepsilon_F$. In the limit of strong interaction $U_0 \gg \pi\hbar v_F$, we have

$$C_{1/2}(g\ll 1)=6\frac{U_0}{\pi^3\hbar v_F}\gg 1, \quad C_0(g\ll 1)=2C_{1/2}(g\ll 1). \quad (14)$$

The numerical factor $C_s(g)$ is shown in Fig. 2 for a range of values of the electron-electron interaction strength U_0. We observe that the LL effects on the thermopower are most significant in the regime of strong interactions $U_0 \gg \pi\hbar v_F$, and that they are more pronounced for spinless particles than for spin-$\frac{1}{2}$ electrons.

Since for the thermopower the interaction dependence is factorizable, Eq. (13) can be readily generalized for the case of wires with dilute impurities where the average spacing between the impurities is sufficiently large so that the LL effects develop independent of each other and the impurities act incoherently. In this case the thermopower is still described by Eq. (13) at temperatures $k_BT > \hbar s\overline{n}$, where $\overline{n}$ is the mean concentration of the impurities and s is the sound velocity. We also note that for a junction made of a perfect LL wire of length L connected to leads through a potential barrier at the contacts, the thermopower is described for temperatures $k_BT \gg \Delta_L$ by Eq. (13) with the total (bare) conductance $G^0=G_1^0G_2^0/(G_1^0+G_2^0)$, where G_1^0 and G_2^0 are the (bare) conductances of the contacts.

The Peltier coefficient of a LL wire (defined as the ratio between the heat and electric currents in the absence of a temperature gradient across the system) obeys in the linear response regime ($eV \ll k_BT$) the Thompson relation $\Pi_{\mathrm{LL}} = -k_BTS_{\mathrm{LL}}$. Consequently, the linear Peltier coefficient can be also described using Eqs. (12)–(14).

In conclusion, we note that the efficiency of a thermoelectric system is characterized by the dimensionless parameter ZT, where $Z=S^2G/K=S^2/TL_0$ is the so-called figure of merit, K is the thermal conductance, and L_0 is the Lorentz number (see, e.g., Ref. 22). Since at ''high'' temperature in a LL constriction with an impurity the thermopower coefficient $S\sim 1/g^2$ [see Eqs. (13) and (14) and Eqs. (7) and (8)] and $L_0 \sim g$,[23] the parameter $ZT\sim 1/g^5$ may be rather large. The latter suggests that the LL systems considered here may be of interest for certain thermoelectric applications.

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[1] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, 1986).
[2] A. A. Abrikosov, *Fundamentals of the Theory of Metals* (Elsevier, Amsterdam, 1988).
[3] E. N. Bogachek, A. G. Shkorbatov, and I. O. Kulik, Fiz. Nizk. Temp. **15**, 278 1989 [Sov. J. Low Temp. Phys. **15**, 156 (1989)].
[4] E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B **54**, R11 094 (1996).
[5] E. N. Bogachek, I. O. Kulik, and A. G. Shkorbatov, Fiz. Nizk. Temp. **11**, 1189 1985 [Sov. J. Low Temp. Phys. **11**, 656 (1985)].
[6] P. Streda, J. Phys.: Condens. Matter **1**, 1025 (1989).
[7] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992).
[8] J. Voit, Rep. Prog. Phys. **58**, 977 (1995).
[9] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **76**, 3192 (1996).
[10] H. J. Schulz, Int. J. Mod. Phys. B **5**, 57 (1991).
[11] C. A. Stafford, Phys. Rev. B **48**, 8430 (1993).
[12] U. Sivan and Y. Imry, Phys. Rev. B **33**, 551 (1986).
[13] R. Landauer, Philos. Mag. **21**, 863 (1970).
[14] L. I. Glazman, I. M. Ruzin, and B. I. Shklovskii, Phys. Rev. B **45**, 8454 (1992).
[15] A. Furusaki and N. Nagaosa, Phys. Rev. B **47**, 4631 (1993).
[16] H. van Houten, L. W. Molenkamp, C. W. J. Beenakker, and C. T. Foxon, Semicond. Sci. Technol. **7**, B215 (1992).
[17] D. Yue, L. I. Glazman, and K. A. Matveev, Phys. Rev. B **49**, 1966 (1994).
[18] M. P. A. Fisher and L. I. Glazman, in *Mesoscopic Electron Transport*, edited by L. L. Sohn *et al.* (Kluwer Academic Publishers, Dordrecht, 1997), p. 331.
[19] M. Jonson, P. Sandstrom, R. I. Shekhter, and I. V. Krive, Superlattices Microstruct. **23**, 957 (1998).
[20] K. A. Matveev and L. I. Glazman, Physica B **189**, 266 (1993).
[21] A. Furusaki and N. Nagaosa, Phys. Rev. B **54**, R5239 (1996).
[22] G. Mahan, B. Sales, and J. Sharp, Phys. Today **50 (3)**, 42 (1997).
[23] I. V. Krive, Fiz. Nizk. Temp. **24**, 498 1998 [Low Temp. Phys. **24**, 377 (1998)].