Decoupled heat and charge rectification as many-body effect in quantum wires

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We show that for a quantum wire with a local asymmetric scattering potential the principal channels for charge and heat rectification decouple and renormalise differently under electron interactions, with heat rectification generally being more relevant. The polarisation of the rectification results from quantum interference and is tuneable through external gating. Furthermore, for spin polarised or helical electrons and sufficiently strong interactions a regime can be obtained in which heat transport is strongly rectified but charge rectification is very weak.

Electronic technology relies significantly on the progressive miniaturisation of its components. Since this eventually leads to regimes in which quantum physics predominates, it is natural to ask if genuine quantum effects can lead to new functionality, even if quantum computing per se is not the target. This question is particularly interesting when electron interactions are taken into account. Interactions become increasingly important with the miniaturisation through the confinement of charges. They can be used then to generate many-body correlations that renormalise a device’s behaviour and offer the opportunity to design properties that are not achievable in conventional electronic setups. In this paper we present such an example in which interactions are tuned to decouple charge and heat rectification.

Rectification, the diode effect, is characterised by an asymmetric current-voltage relation. In a conventional diode this asymmetry is introduced by $p$ and $n$ type doped sides of a semiconductor junction. Although there is the electrostatic environment from the dopants the resulting physics is understood on the single electron level. A many-body variant can be obtained in a very different way. It was shown long ago that in a quantum wire as illustrated in Fig. 1 a local scattering potential $U(x)$ causes a strong renormalisation of the current-voltage relation through electron interaction $[1, 2]$. While the leading correction is independent of the potential’s form, sub-leading order are shape sensitive and a spatially asymmetric potential induces rectification $[3–5]$ which for strong interactions can become very large.

In this paper we investigate this scenario under the novel aspect of thermoelectric rectification where heat current is driven by a voltage $V$. In the nonlinear regime this is different from a temperature driven current which we do not consider. The thermoelectric response in quantum wires has been considered in various settings $[6–12]$ but for rectification our focus is entirely on the heat flow from backscattering which to our knowledge has not been investigated before. The many-body setup is also different from the usual approaches to heat rectification or thermal diodes that depend on an artful design of the system or the reservoirs $[13–33]$. With the tools of open quantum systems and quantum thermodynamics we derive an intuitive result that automatically incorporates the requirement of gauge invariance $[26, 27, 34, 35]$ and evaluate it through nonequilibrium perturbation theory. Remarkably the asymmetry of the heat current appears already at the leading current renormalisation such that through interactions it decouples from charge rectification and generally dominates.

In addition to normal electrons we consider effectively spinless (e.g. polarised or helical) conductors. For the latter we find that for strong interactions the heat asymmetry can become as large as the heat current itself whereas the charge asymmetry remains very small. This produces the novel phenomenon of a conductor that acts as a heat diode but not as a charge diode. Furthermore whether the heat transport is reduced for positive or negative bias depends on quantum interference and can be switched even through small changes of the impurity potential which can be created through local external gates.

Physics behind rectification — For a setup as in Fig. 1 the asymmetry responsible for current rectification is due to the local potential $U(x)$ alone. In an interacting system backscattering on $U(x)$ causes a strong renormalisation of transport $[1, 2]$. But the usually considered lead-
ing correction does not contribute to rectification because the asymmetry of \( U(x) \) does not enter. Rectification appears only at sub-leading orders in the renormalisation [3, 4] but for strong interactions they can create a pronounced diode effect.

In contrast, and quite remarkably, for energy or heat currents the dependence on the asymmetry of \( U(x) \) appears already at leading order. This is because \( U(x) \) takes in addition to the backscattering amplitude the role of a local change in chemical potential \( \mu(x) = \mu + U(x) \). Due to the latter \( U(x) \) the leading amplitude of the backscattered energy current contains a term in \( U^3 \) which, as we will see, can be written as \((U * U)_{2k_F}U_{2k_F}^* \) with \(*\) the convolution of the Fourier modes. This amplitude is complex and through its phase retains the signature of the spatial asymmetry. It thus takes the same role for heat rectification as the higher order terms for charge current rectification.

This decoupling of the renormalisation channels for charge and heat currents leads to different voltage \( V \) behaviour in the form of different power-law scalings. Since heat rectification arises at the most relevant order it usually dominates over charge rectification, and interactions can even be tuned such that heat rectification is strongly enhanced while charge rectification remains very small, both relative to their total currents. Such a device then operates as a good thermal diode without significant impact on charge rectification.

**Model and currents** — To quantitatively evaluate this physics we consider a one-dimensional quantum wire connected to reservoirs on each end. We consider \( V \) driven thermoelectric transport and thus the reservoirs do not have any specific form and their temperature is irrelevant as long as the dominant energy scale is set by \( V \). The quantum wire is described in terms of the Tomonaga-Luttinger model [36–39] in which the electron operators \( \psi(x) \) are split into right \( R \) and left \( L \) moving modes with momenta close to \(+k_F\) and \(-k_F\), respectively. With \( \psi_{R,L}(x) \) the corresponding field operators the Hamiltonian in the absence of the local potential becomes

\[
H = \int dx \sum_{\nu} \psi_{\nu}^\dagger(x)(\mu_{\nu} - v_i\hbar v_F  \partial_x)\psi_{\nu}(x) + \int dx dy \mathcal{V}(x-y)\psi_{\nu}^\dagger(x)\psi_{\nu}^\dagger(y)\psi(y)\psi(x),
\]

where \( \nu = R, L = +, - \), the integration is over the wire length, \( v_F \) is the Fermi velocity for the linearised dispersion, and \( \mathcal{V}(x-y) \) the (screened) electron interaction potential. Spin components are not written as all interactions are diagonal in spin but the influence of spin, including polarised and helical systems, will be discussed later. As shown in Fig. 1 (a) the system is in contact with reservoirs such that \( R \) movers are in equilibrium and share the chemical potential \( \mu_R \) with the reservoir on the left, and the \( L \) movers share the chemical potential \( \mu_L \) with the reservoir on the right. The contact to the reservoirs is adiabatic such that incoming particles are fully absorbed. The voltage drop is \( V = (\mu_R - \mu_L)/\epsilon \) where \( \epsilon \) is the electron charge. For \( \mu_R \neq \mu_L \) the Fermi momentum is adjusted to \( k_F^{R,L} = k_F + (\mu_R,L - \mu_0)/\hbar v_F \), where \( \mu_0 \) is the equilibrium chemical potential. The full field operator is \( \psi(x) = e^{ik_F^R x}\psi_R(x) + e^{-ik_F^L x}\psi_L(x) \). Interactions turn the elementary eigenmodes into collective density wave excitations [38, 39] but \( R \) and \( L \) movers remain decoupled if we exclude \( \pi/k_F \) being commensurate with the crystal lattice. We can thus write \( H = H_L + H_R \) with \( H_L \) containing only \( \nu \) movers.

Scattering on the local potential has the Hamiltonian

\[
H_U = \int dx \sum_{\nu,\nu'} U(x)e^{-i(\nu k_F^R - \nu' k_F^R)x}\psi_{\nu}^\dagger(x)\psi_{\nu'}(x),
\]

where the potential \( U(x) \) is non-zero only in a small region \( < \pi/k_F \) around \( x = 0 \) and we assume that it is spatially asymmetric, \( U(x) \neq U(-x) \). This potential takes two roles. For \( \nu = \nu' \) it describes forward scattering that can be added to \( H_0 \) by introducing a spatially dependent chemical potential as \( \mu_\nu(x) = \mu_\nu + U(x) \). For \( \nu \neq \nu' \) it introduces backscattering between \( R \) and \( L \) movers, and we call this part of the Hamiltonian \( H_b \). For a helical system (opposite spins bound to \( R, L \) movers) \( U \) is a magnetic impurity inducing both spin preserving forward and spin-flip backscattering.

Backscattering leads to a set of a relevant perturbations on electron transport [1, 2]. As mentioned, for charge current the leading term, proportional to \( |U_{2k_F}|^2 \), is insensitive to the shape of \( U(x) \) and sub-leading relevant contributions must be taken into account [3, 4]. To reveal the asymmetry the rectification particle current can be used, \( N_\nu^r = N_\nu(V) + N_\nu(-V) \), where the current \( N_\nu = \frac{\hbar}{2e} N_\nu \) measures the how the particle numbers \( N_\nu \) of \( \nu \) movers change through the backscattering. By particle conservation \( N_R = -N_L \).

Identifying heat or energy transfer is a bit more subtle. We have to consider \( R \) and \( L \) movers as thermodynamic subsystems that are brought into contact through the interface Hamiltonian \( H_0 \) as illustrated in Fig. 1 (b). The energy flow into system \( \nu \) is given by the change of the internal energy \( E_\nu = \text{Tr}_\nu\{H_\nu\rho_\nu\} \), where \( \text{Tr}_\nu \) is the trace over the degrees of freedom of subsystem \( \nu \) and \( \rho_\nu \) is the reduced density matrix obtained from the full density matrix \( \rho \) through \( \rho_{R,L} = \text{Tr}_{R,L}\{\rho\} \). If we put all time dependence in \( \rho \) and notice that we can write \( E_\nu = \text{Tr}\{H_\nu\rho\} \) with \( \text{Tr} \) the full trace we obtain

\[
\dot{E}_\nu = -\frac{i}{\hbar}\text{Tr}\{H_\nu[H_0,\rho]\} = -\frac{i}{\hbar}\text{Tr}\{[H_0, H_\nu]\rho\},
\]

where we have used the von Neumann equation for the time evolution of \( \rho \), the cyclic property of the trace, and \( [H_0, H_\nu] = 0 \). It should be noticed that \( \dot{E}_R + \dot{E}_L \) is not principally zero as for \( N_R + N_L \) but has a correction proportional to \( H_b \). In a standard thermodynamic setting
such a correction would be neglected due to the smallness of the surface-to-volume ratio. Here, however, $H_b$ takes an active role since it is the sole player for the rectification and its influence is strongly enhanced through the renormalisation by the electron interactions. Nevertheless in the steady state the net energy change of the interface vanishes, but $E_R = -E_L \neq 0$ is maintained whenever the reservoirs are out of equilibrium.

To identify the heat current $\dot{Q}_\nu$ through the interface $H_b$ we separate $E_\nu$ into heat and work fluxes. Applying the criterion that heat flux changes the entropy [40, 41] we would identify the full $E_\nu$ with the heat flux because $H_b$ mixes the $R$ and $L$ states. However, $H_b$ exchanges particles too such that for the grand canonical setting we have to split off the factor $\mu_\nu N_\nu$ as separate from the heat flux, which leads to $\dot{Q}_\nu = \dot{E}_\nu - \mu_\nu N_\nu$. This splitting is in particular necessary because it makes the heat flux independent of the gauge that fixes the origin of energy [26, 27, 34, 35]. Similarly to Eq. (3) we obtain

$$\dot{Q}_\nu = -\frac{i}{\hbar} \text{Tr} \{ [H_\nu - \mu_\nu N_\nu, H_b] \rho \}. \quad (4)$$

and the $\mu_\nu N_\nu$ term indeed removes the $\mu_\nu$ from the kinetic energy in Eq. (1).

**Noninteracting electrons** — Remarkably heat rectification occurs already for noninteracting electrons from quantum interference and this case provides a clear picture of the physics. Focusing on $\dot{Q}_R$ the standard anti-commutation relations yield

$$\dot{Q}_R = \frac{1}{\hbar} \int dx U(x) e^{i(k_F^L x + k_F^R x')} \times \text{Tr} \{ \psi_L^\dagger(x) U(x) - i\hbar v_F \partial_x \} \psi_R(x) \rho \} + \text{c.c.} \quad (5)$$

We shall drop the term in $\partial_x$ henceforth as it produces only a logarithmic correction to the amplitude and no rectification at the considered orders. Furthermore the $V$ dependence of $k_F^\nu$, in contrast to its role for $N_R^\nu$ [3, 4], just produces higher powers in $V$ and we set $k_F^L + k_F^R \approx 2k_F$.

Using the Keldysh nonequilibrium technique to expand $\rho$ in $U$ gives at leading order

$$\dot{Q}_R = -\frac{i}{\hbar^2} \int dx dx' U^2(x) U(x') e^{i2k_F(x-x')} \int_0^0 dt \times \langle \psi_L^\dagger(x, 0) \psi_R(x, 0), \psi_R^\dagger(x', t) \psi_L(x', t) \rangle \rangle + \text{c.c.}, \quad (6)$$

where $\psi_L$ evolves under $H_\nu$ and the expectation value is over the uncoupled $R$ and $L$ systems. Since $U(x)$ is non-zero only in a region $< \pi/k_F$ we can set the arguments of the field operators to $x, x' \approx 0$. The spatial integration then provides the Fourier transforms $U_k$ of $U(x)$ and $(U^2)_k = (U^\dagger U)_k$ of $U^2(x)$,

$$\dot{Q}_R = -\frac{i}{\hbar^2} (U^2)_k^* U_{2k_F} \int_0^0 dt \times \langle \{ \psi_L^\dagger(0, 0) \psi_R(0, 0), \psi_R^\dagger(0, t) \psi_L(0, t) \} \rangle + \text{c.c.} \quad (7)$$

To make the voltage dependence explicit we make a gauge transformation $\psi_\alpha(x, t) = e^{-i\mu_\nu \nu \partial_t / \hbar} \psi_\alpha(x, t)$, which sets the chemical potentials for both $R$ and $L$ movers to zero and gives rise to $e^{i(\mu_\nu \nu \partial_t / \hbar)} = e^{i e V t / \hbar}$ in Eq. (7). The time dependence of the remaining correlators $\langle \psi_L^\dagger(0, 0) \psi_R(0, 0) \rangle$ and $\langle \psi_L^\dagger(0, 0) \psi_L(0, 0) \rangle$ is $1/t$, set by the cutoff of the energy integration by the Fermi surface [42]. Temperature corrections can be neglected if $eV$ is larger than the thermal energy and the integrand becomes $e^{i e V t / \hbar} / t^2$. By going to dimensionless variables $y = |eV| t / \hbar$ we then see that $\dot{Q}_R$ scales as $|eV|$. This linear response result is expected since Eq. (7) is identical to the backscattering particle current $N_R$ except for the $U^2$ amplitude instead of $U$. If we introduce the constant $C$ to cover all invariant parameters we thus obtain

$$\dot{Q}_R = - (U^2)^*_k U_{2k_F} C |eV| \int_0^0 dy \frac{e^{i \text{sign}(V) y}}{y^2} + \text{c.c.} \quad (8)$$

The divergence at $y \to 0$ in the integral is a consequence from a constant density of states in the Tomonaga-Luttinger model approximation and requires a common cutoff by the true bandwidth. This cutoff could in principle produce a further $V$ dependence from the scaling $t \to y$ but the magnitude of currents is set by $V$ and has to vanish at $V = 0$. Therefore the cutoff must drop out with the commutators in Eq. (7) and any singularity can be neglected in the evaluation of the integral. For $N_R$ the first two factors in Eq. (8) would be $U_{2k_F} U_{2k_F}$ and the expression in front of the integral would be real. With the ‘c.c’ the integrand then becomes sign$(V) 2 \text{sin}(y) / y^2$ such that $N_R$ just changes sign but not magnitude with $V \to -V$. Charge rectification thus requires higher order corrections [3, 4].

For the heat current the first two factors are instead $(U^2)^*_k U_{2k_F}$. For a real symmetric potential $U(x) = U(-x)$ the Fourier components are real, and rectification remains absent. But for a spatially asymmetric potential $(U^2)^*_k U_{2k_F}$ is complex and can be written as $|U^2|_{2k_F} U_{2k_F} e^{i \alpha}$. The integrand then is $2 \text{sign}(V) \text{cos}(\alpha) \text{sin}(y) + \text{sin}(\alpha) \text{cos}(y) / y^2$. The term in $\text{sin}(\alpha)$ is invariant under the sign of $V$ showing that there is heat current rectification even for a noninteracting system. If we define $\dot{Q}_R = \dot{Q}_R(V) + \dot{Q}_R(-V)$ as the rectification heat current measuring the asymmetry between $\pm V$ bias, we have thus found that

$$\dot{Q}_R = \text{sign}(\alpha)|V| \ |U^2|_{2k_F} U_{2k_F} |C'| \quad (9)$$

where the constant $C'$ absorbs $C$ and the value of the remaining integration. An identical result holds for $\dot{Q}_L^r$ with $R \to L$ and $\alpha \to -\alpha$. For a helical system $\dot{Q}_L$ acquires a further minus sign since $U$ has to be a magnetic impurity and $L$ and $R$ movers carry opposite spins.

The phase $\alpha$ results from quantum interference and is thus very sensitive to the precise shape of $U(x)$, such that generally the sign of $\text{sin}(\alpha)$ is arbitrary. But this
sensitivity allows also tuning, and slight changes of \(U(x)\) as induced, for instance, through external gating can be sufficient to switch the polarity of the diode. In Fig. 2 we provide an example for \(U(x)\) being the sum of two Lorentzians (e.g. generated by two nearby impurities). Tuning the amplitudes of the Lorentzians even by just a few percent can completely reverse the polarity.

**Interacting electrons** — In one dimension the Fermi liquid is unstable under interactions. Elementary excitations are density waves and are better described as a Luttinger liquid [38, 39, 43]. Through bosonisation the latter provides a standard technique to compute correlation functions at arbitrary interaction strength. The correlators in Eq. (7) are then modified from \(1/t_1^2\) to \(1/t_1^\gamma\) [38, 39] where \(\gamma = 2K\) for the spinless and \(\gamma = K_e + K_s\) for the spinful case. The respective parameters \(K\) and \(K_{e,s}\) capture all interactions. \(K_{e,s} = 1\) is the noninteracting case, \(0 < K, K_e < 1\) encodes repulsive and \(K, K_e > 1\) attractive interactions. If spin SU(2) symmetry is preserved \(K_s = 1\) and broken (e.g. through spin-orbit interaction or fields) \(K_s > 1\). We exclude \(K_s < 1\) as it would represent an instability to spin density waves. The voltage dependence in Eq. (8) now becomes \(eVt^{-1}\) in agreement with the result for the backscattering current [1]. Since for repulsive interactions \(\gamma < 2\) this boosts the rectification current, \(\dot{Q}_e \sim |V|^{\gamma-1}\).

In comparison charge rectification \(\dot{N}_e = \dot{N}_e(V) + \dot{N}_e(-V)\) scales with \(|V|^\gamma\) where \(\gamma_c = \min(2K_e, 6K - 2)\) for spinless [3] and \(\gamma_c = \min(K_e + K_s, 4K_e, 3K_e + K_s - 2, 12K_e - 2)\) for spinful electrons [4]. Heat and charge rectification thus decouple, and since \(\dot{Q}_e \sim |V|^\gamma\) for different \(\gamma\), in which for \(\gamma < 1\) we smoothly interpolate to the strong coupling scaling \(\dot{Q}_e \sim |V|^{4/\gamma - 1}\) [1] across \(V^*\).

**Rectification efficiency** — For a good diode the ratio \(r = \dot{Q}_e(-V)/\dot{Q}_e(V)\) is either \(r \ll 1\) or \(r \gg 1\). In the Tomonaga-Luttinger model an exact calculation is tricky due to the required cutoffs. But Eq. (8) shows that \(r = [A\sin(\alpha) - B\cos(\alpha)]/[A\sin(\alpha) + B\cos(\alpha)]\) where \(A\) and \(B\) are of the same order of magnitude. Therefore \(r\) is in principle tuneable through \(\alpha\) to any value. Although its initial value is arbitrary this may provide an advantage if tuning by gates can be achieved.

The efficiency of the heat transport is assessed by comparing \(\dot{Q}_e\) to the total dissipated power \(P = IV\) (Joule heating). Since \(U\) is a perturbation the total current \(I\) is proportional to \(V\) and thus \(\dot{Q}_{eR}/P \sim |V|^{-3}\). For \(1 < \gamma < 2\) the divergence at \(V \rightarrow 0\) tells that heat rectification is most effective when dissipation is generally low. For \(\gamma < 1\) there is a strong suppression at \(V < V^*\) and the benefit of strong rectification near \(V^*\) involves a larger dissipation. Examples are shown in the inset of Fig. 3. We should also notice that since temperature of the reservoirs does not appear in these considerations there is no counterpart of the thermoelectric figure of merit \(ZT\). Instead \(\dot{Q}_{eR}/P\) directly addresses the efficiency.

**Conclusions** — We have shown that the many-body effects governing backscattering on spatially asymmetric potentials in quantum wires lead to a decoupling of
heat and charge current rectification that is very sensitive to the interaction strength and quantum interference from backscattering. In particular for spin polarised electrons we predict a pronounced decoupling at interaction strengths $1/3 < K < 1/2$ which are not untypical for high quality quantum wires. This behaviour is nonuniversal but due to the sensitivity of the quantum interference should be manipulable through local gating.

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