Rectification in Luttinger liquids

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We investigate the rectification of an ac bias in Luttinger liquids in the presence of an asymmetric potential (the ratchet effect). We show that strong repulsive electron interaction enhances the ratchet current in comparison with Fermi liquid systems, and the dc $I - V$ curve is strongly asymmetric in the low-voltage regime even for a weak asymmetric potential. At higher voltages the ratchet current exhibits an oscillatory voltage dependence.

Asymmetric conductors have asymmetric $I - V$ curves. This phenomenon is known as the diode or ratchet effect and plays a major role in electronics. Recently much interest has been attracted by transport asymmetries in single-molecule devices and other mesoscopic systems \textsuperscript{1}. The idea that asymmetric molecules can be used as rectifiers is rather old \textsuperscript{2}, however, it was implemented experimentally \textsuperscript{3} only recently. Another experimental realization of a mesoscopic rectifier is an asymmetric electron waveguide constructed within the inversion layer of a semiconductor heterostructure \textsuperscript{4}. The ratchet effect was observed in carbon nanotubes \textsuperscript{5} and strongly asymmetric $I - V$ curves were recently reported for the tunneling in the quantum Hall edge states \textsuperscript{6}. These experimental advances have stimulated much theoretical activity \textsuperscript{7, 8, 9, 10, 11} with the main focus on the simplest Fermi-liquid systems \textsuperscript{12}.

Transport in one-channel quantum wires, where electrons form a Luttinger liquid, differs significantly from the Fermi liquid case. In particular, impurity effects are stronger in Luttinger liquids, and even a weak impurity potential may render the linear conductance zero at low temperatures \textsuperscript{13}. In this Letter we investigate the ratchet effect in Luttinger liquids. We show that strong repulsive electron interaction enhances the ratchet current, and the low-voltage part of the $I - V$ curve is strongly asymmetric even in quantum wires with weak asymmetric potentials.

We consider the ratchet effect in the presence of a weak asymmetric potential $U(x) \ll E_F$, where $E_F$ is the band width. We calculate the ratchet current $I_r(V) = [I(V) + I(−V)]/2$ for a one-channel quantum wire with spin-polarized electrons. The ratchet current vanishes for systems with symmetric $I - V$ curves. It can be measured as the dc response to a low-frequency square voltage wave of amplitude $V$. First, we consider voltages $V < V_0 = hv_F/(ea)$, where $v_F$ is the Fermi velocity, $e$ the electron charge, and $a$ the size of the region containing the asymmetric potential. We find a weak ratchet effect in the interval $eV_0 > eV > \sqrt{UE_F}$ for both Fermi and Luttinger liquids, $I_r \sim (e/h)U^2(eV)^{2g}/E_F^{2g+1}$, where $g = 1$ for Fermi liquids and $g < 1$ for Luttinger liquids with repulsive interaction. However, at strong repulsive interaction (the Luttinger liquid parameter $g \ll 1$) and sufficiently low voltages, the ratchet current $I_r(V)$ grows as the voltage decreases until $I_r(V)$ becomes comparable with the total current $I(V)$ at $eV = eV^* \sim (UE_F^{-g})^{1/(1-g)}$. At $E_F \gg eV > eV_0$ the ratchet current oscillates as a function of the voltage and can become comparable with the total current $I(V)$ for any repulsive interaction strength. We also briefly discuss the ratchet effect in the presence of a strong asymmetric potential $U > E_F$. The complicated ratchet-current behavior is caused by the energy dependence of the effective impurity strength in Luttinger liquids \textsuperscript{14}. This introduces an additional energy scale $V^*$ absent in Fermi-liquid systems.

One-channel quantum wires can be described by the Tomonaga-Luttinger model with the Hamiltonian

$$H = \int dx \left\{ -\hbar v_F[\psi_R^\dagger(x)i\partial_x \psi_R(x) - \psi_L^\dagger(x)i\partial_x \psi_L(x)] + U(x)\rho(x) + \int dy K(x-y)\rho(x)\rho(y) \right\},$$  \hfill (1)

where $\psi_R^\dagger$ and $\psi_L^\dagger$ are the creation operators for right- and left-moving electrons, $\psi^\dagger = \psi_R^\dagger + \psi_L^\dagger$ gives the conventional electron creation operator, $\rho = \psi^\dagger \psi$ is the electron density, $U(x)$ is the asymmetric potential, and $K(x-y)$ the interaction strength. Our aim is to calculate the current $I_r$ as a function of the applied voltage $V$. We assume that the long-range Coulomb interaction is screened by the gates so that $K(x-y)$ decreases rapidly for large $(x-y)$. Electric fields of external charges are also assumed to be screened. Thus, the applied voltage reveals itself only as the difference of the electrochemical potentials $E_L$ and $E_R$ of the particles injected from the left and right reservoirs.

We assume that one lead is connected to the ground so that its electrochemical potential $E_{\text{L}} = E_F$ is fixed. The electrochemical potential of the second lead $E_{\text{R}} = E_F + eV$ is controlled by the voltage source. In such situation a symmetric potential $U(x)$ is sufficient for rectification. For example, in a non-interacting system $I(V) \sim \int_{E_F}^{E_F+U} [1 - R(E)]dE$, where $R(E)$ is the reflection coefficient. If the only relevant scale for the energy dependence of the reflection probability is the band width $\sim E_F$ then the ratchet current $I_r \sim \int_0^V dE[R(E_F-E) - R(E_F+E)] \approx -2 \int_0^V dE R'(E_F)E \sim R(E_F)(eV)^2/E_F \sim U^2(eV)^2/E_F^3$ for small $U$ and $V$, and any coordinate dependence $U(x)$. 

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A ‘not-trivial’ ratchet effect can be observed when the injected charge density is voltage-independent, $E_{L/R} = E_F \pm eV/2$. Symmetry considerations require an asymmetric $U(x)$ for a non-vanishing ratchet current in this case. Also an electron interaction must be present. Indeed, for free particles the reflection coefficient $R(E)$ is independent of the electron propagation direction \[1\] and hence $I(V) = -I(-V)$.

The ‘non-trivial’ ratchet effect is absent in the first two orders in $U(x)$. Indeed, in the lowest two orders the ratchet current \[I_r^{(1,2)} = \int dx C(x)U(x) + \int dx dy D(x,y)U(x)U(y).\] $I_r^{(1,2)}$ must be zero for any symmetric potential. Substituting $U(x) = U\delta(x-x_0)$ we find that $C(x_0), D(x_0, x_0) = 0$. Substituting $U(x) = U\delta(x-x_1) + U\delta(x-x_2)$ we see that $D(x_1, x_2) + D(x_2, x_1) = 0$. Hence, $I_r^{(1,2)} = 0$ for any $U(x)$.

We first consider the ‘non-trivial’ ratchet effect and then check what changes after the voltage dependence of the injected charge density is taken into account. Let us begin with a qualitative explanation before we make a rigorous calculation. The origin of the ratchet current can be understood from a simplified Hartree-Fock picture. In this approximation, electrons are backscattered off a combined potential $U(x) = U + W(x)$, where $W(x)$ is a self-consistent electrostatic potential created by the average local charge density. To obtain $W(x)$ we use the following approximation in the last term of Eq. (1): \[\rho(x)\rho(y) \approx (\psi_R^+(x)\psi_R(x) + \psi_L^+(x)\psi_L(x))(\psi_R^+(y)\psi_R(y) + \psi_L^+(y)\psi_L(y)) + (\rho(x))\psi_R^+(y)\psi_L(y) + (\rho(y))\psi_L^+(x)\psi_R(x) + h.c.\] Hence, the relation between $W$ and $\rho$ is linear. The combined potential $\tilde{U}$ is different for the opposite voltage signs.

In the model \[1\] the electron interaction is short-ranged due to the screening gates, and hence, the relation between the potential $W(x)$ and the electron density $\rho(x)$ is local, $W(x) \sim \rho(x)$. The simplest choice of $U(x)$ is a two-impurity asymmetric potential $\tilde{U}(x) = U_1\delta(x + a/2) + U_2\delta(x - a/2)$. The charge density profile \[14\] in the presence of a two-impurity potential and the voltage drop $V$ is sketched in Fig. 1. Depending on the voltage sign, the charge density decreases or grows as a function of the coordinate $x$. Do the electrostatic potential $W(x)$. Hence, $\tilde{U}(x)$ is different for the opposite voltage signs. The density is essentially independent of the coordinate between the impurities \[14\], as well as on the left and on the right of the impurities, since no backscattering occurs in those regions. The charge density and the electrostatic potential drop at the positions of the impurities. The magnitude of a drop is proportional to the electric charge backscattered off the impurity. Indeed, if the incident charge densities of the electrons approaching the impurity from the left and from the right are $\rho_L^+ + \rho_L^-$ and $\rho_R^+ + \rho_R^-$, and the backscattered charge densities are $\rho_L^+$ and $\rho_L^-$, then the density drop across the impurity $\Delta \rho = (\rho_L^+ + \rho_L^- - \rho_R^+ - \rho_R^-) = \frac{1}{2}(\rho_L^+ - \rho_R^-)^2 \sim I_{bs}$, where $I_{bs}$ is the current backscattered off the impurity. Thus $W(x) = U - U \sim I_{bs}$. From Ref. \[15\] we know that for a weak potential $U$

\[I_{bs} \sim |U_{2k_F}|^2[V^{2g-1} \text{sign}(V/E_F^g)],\]

where $U_{2k_F} \sim k_F \int dx \exp(2ik_Fx)U(x)$, $k_F$ is proportional to the mean electron density, and the dimensionless constant $g$ characterizes the interaction strength, $g = 1$ for non-interacting electrons (in which case $W(x) = 0$).

Now we can substitute the renormalized potential $\tilde{U} = U + W$ for $U$ in Eq. (2). The Fourier component $W_{2k_F}$ is different for the opposite voltage signs. Hence, we obtain the asymmetric part of the $I - V$ characteristics $I_r \sim eU^3|V|^{4g-2}/(hE_F^g)$. The ratchet effect is strongest for $g \to 0$ when the ratchet current grows as the voltage decreases.

The above Hartree-Fock argument provides a qualitatively correct picture at small $g$ but underestimates fluctuations in Luttinger liquids. As shown below, the ratchet current growth at small voltages differs from our estimate: $I_r \sim U^3|V|^{4g-2}$. $E_F \gg V > V^* \sim (UE_F^g)^{3/(1-g)}$, $g \ll 1$. We will see that the growth terminates at $V = V^*$. At such voltage $I_r(V^*)/I(V^*) \sim [(V^*)^{3g+1}/E_F^{3g}]/[V^*] \sim (V^*/E_F)^{3g} \sim 1$ as $g \ll 1$. Fluctuations are less important in many-channel systems and the Hartree-Fock picture gives exact results for some two-channel systems and for Fermi liquids \[15\].

We use the bosonization technique \[17\] to calculate the ratchet current. After an appropriate rescaling of the time system, the variable can be described by the action \[13\]

\[S = \int dt dx \left\{ \frac{1}{8\pi}((\partial_t \Phi)^2 - (\partial_x \Phi)^2) - \delta(x) \sum_{n \geq 1} 2\tilde{U}_{2nk_F} \cos(n\sqrt{g}\Phi + \alpha_n) \right\},\]

where the bosonic field $\Phi$ is related to the charge density as $\rho = \epsilon(\sqrt{g}\partial_t \Phi + 2k_F)/(2\pi)$, and $\tilde{U}_{2nk_F} \exp(\alpha_n)$ are of the order of the Fourier components of the asymmetric potential, $k_F \int \exp(2ink_Fx)\tilde{U}(x)dx$. We assume that the charge density $\sim k_F$ is independent of the voltage. The operator $\cos(n\sqrt{g}\Phi + \alpha_n)$ describes scattering events involving $n$ electrons. We assume that $\alpha_1 = 0$. Indeed, we can always set $\alpha_1 = 0$ by a constant shift of the bosonic field $\Phi$. For a general asymmetric potential, $\alpha_n$ with $n > 1$ remain non-zero after this shift. On the other hand, for a symmetric potential $U(x) = U(-x)$ all $\alpha_n = 0$. In most problems it is sufficient to keep only the $n = 1$ term. The $n = 2$
As a result, \( t \) is an infinitesimal positive constant. This transformation induces time dependence in the electron creation and annihilation operators. Expanding Eq. (5) to the order \( \tau_0 \) the action (3) is invariant under the transformation \( \Phi \rightarrow -\Phi, V \rightarrow -V \) while the current operator (1) changes its sign. As discussed above, for an asymmetric potential we expect \( \alpha_2 \neq 0 \). Then a ratchet current \( I_r \) emerges in the order \( \tilde{U}_{2kF}^2 \tilde{U}_{4kF} \). Before the calculation of \( I_r \) let us determine its voltage dependence with a heuristic argument similar to Ref. [13]. As one changes the energy scale \( E \), the backscattering amplitudes \( \tilde{U}_{2kF} \) in the action (3) scale as \( \tilde{U}_{2kF}(E) \sim \tilde{U}_{2kF}(E^{n_2g-1}) \) [13]. This renormalization stops at the energy scale \( V \). Assuming that a scattering matrix approach could be applied for an estimation of the current, we write \( I_{bs}(V) \sim V R_{\text{eff}}(V) \), where \( R_{\text{eff}}(E) = \sum \text{const} \tilde{U}_{2kF}^2 + \sum \text{const} \tilde{U}_{2kF}(E)\tilde{U}_{2kF}(E) + \ldots \) is an effective reflection coefficient. Quadratic terms do not contribute to the ratchet current. The leading contribution emerges in the order \( \tilde{U}_{2kF}^2 \tilde{U}_{4kF} \). One gets \( I_r \sim V \tilde{U}_{2kF}^2(\tilde{U}_{2kF}(V) \sim V^{6g-2} \). Below we obtain the same result rigorously from Eqs. (15).

Expanding Eq. (5) to the order \( \tilde{U}_{2kF}^2 \tilde{U}_{4kF} \) gives

\[
I_r = 2 \sin \alpha_2 \tilde{U}_{2kF}^2 \tilde{U}_{4kF} \left\{ \int_0^F dt_1 \int_{-\infty}^{t_1} dt_2 \cos(Vt_1 - 2Vt_2)P(t_1, t_2, t_2 - t_1) \\
+ \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2 \cos(Vt_1 - 2Vt_2)P(t_1, t_2, t_1 - t_2) - \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2 \cos(Vt_1 - 2Vt_2)P(-t_1, t_2, t_1 - t_2) \\
- \frac{1}{2} \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2 \cos(Vt_1 + Vt_2)P(t_2 - t_1, t_2, t_1 - t_2) + \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2 \cos(Vt_1 + Vt_2)P(t_2 - t_1, -t_1, t_2) \right\} + c(6)
\]

where \( P(t, s, q) = (\delta - it)^2(\delta - is)^{-1}q(\delta - iq)^{-4g} \). Dimensional analysis shows that \( I_r \sim V^{6g-2} \) in agreement with our previous estimate. It is convenient to change variables in the integrals with \( \cos(Vt_1 - 2Vt_2) \) as \( \tau_1 = t_2 - t_1, \tau_2 = t_2 \). Then after tedious but straightforward manipulations Eq. (6) can be represented as

\[
I_r = 2 \sin \alpha_2 \tilde{U}_{2kF}^2 \tilde{U}_{4kF} \left\{ \int_{-\infty}^{\infty} d\tau d\tau \cos(V(\tau - t))P(-t + \tau, -\tau, -t) - \int_{-\infty}^{\infty} d\tau d\tau \cos(V(\tau + t))P(t - \tau, \tau, t) \right\} . \quad (7)
\]
The first integral in \(7\) is zero as seen from the location of the branching points of the function \(P\). The second integral yields

\[
I_r = -\sin \alpha_2 \tilde{U}_{2k_F}^2 \tilde{U}_{4k_F} \cos(\pi g) \frac{2^{2+2g} \pi^{3/2} \Gamma(g + 1/2)}{\Gamma(4g) \Gamma(3g)} |V|^{6g - 2}.
\]

(8)

This expression becomes 0 at \(g = 1/2\). We also get a zero ratchet current for non-interacting electrons, \(g = 1\), because the Hamiltonian \(11\) is quadratic in Fermi-operators in the non-interacting case and hence no operators which backscatter more than one electron can appear, \(\tilde{U}_{2k_F} = 0\).

At small \(g\) the ratchet current \(3\) is proportional to a negative power of the voltage. This means an unusual behavior: the dc response to an ac voltage grows as the ac voltage decreases.

So far we ignored the voltage dependence of the injected charge density. At \(g \ll 1\), Eq. \(8\) gives the main contribution to the ratchet current only for \(eV < \sqrt{U} E_F\). For \(g\) close to 1 the result \(8\) is always exceeded by another contribution. This contribution emerges in the second order in \(U\) and is related to the voltage dependence of the injected charge density. The density is proportional to \(k_F\) which enters the expression for \(U_{2k_F}\) in Eq. \(2\). At small \(V \ll E_F\) the correction \(22\) to \(U_{2k_F}\) is a linear function of \(V\). The substitution of this correction into Eq. \(2\) gives an additional ratchet current

\[
I_r^{(\text{density})} \sim \frac{e U_{2k_F}^2 (eV)^{2g}}{\hbar E_F^{g + 1}}.
\]

(9)

For \(g > 1/3\) and \(V > V^*\) the contribution \(9\) always exceeds \(8\). At \(g < 1/3\) the current \(9\) is greater than \(8\) above a threshold voltage that depends on \(U\) and \(g\). As we already discussed, \(I_r\) \(8\) is comparable with the total current \(I(V) \sim e^2 V/h\) at small \(g\) near the border of the perturbatively accessible region \(UV^{g-1}/E_F^g < 1\). On the other hand, Eq. \(8\) provides only a small correction to the total current for any \(g\). Still a repulsive interaction of any strength enhances the ratchet effect as seen from the comparison of the current \(9\) for \(g < 1\) and for the non-interacting case \(g = 1\).

What happens beyond the perturbative region when \(V < V^* \sim U^{1/(1-g)}\)? As the energy scale decreases the effective impurity strength grows. Hence, we need to consider a strong \(U > E_F\) limit. In this limit we have a weak tunneling between the left and right halves of the wire. The current \(I(V) \sim t^2 V^{(2/g) - 1}/E_F^{2/g}\), where \(t\) is the tunneling amplitude \[15\]. Inserting the voltage dependence of the tunneling amplitude in the expression above we estimate \(I_r(V) \sim V^{2/g}\).

A single impurity model \(3\) can be used only when the potential \(U(x)\) is confined in a small space region of size \(a < a_V \sim hV_F/(eV)\). If the potential changes slowly at the scales \(x > a_V \gg 1/k_F\) it cannot backscatter electrons since backscattering involves high momentum transfers, \(\Delta k \geq k_F\). Interesting interference effects are possible for a two-impurity potential \(U_1 \delta(x) + U_2 \delta(x-a)\) and other \(U(x)\) which significantly change at the scale \(1/k_F\) but are non-zero in a region of size \(a \approx a_V\). In the two-impurity case the current oscillates as a function of the voltage bias \[22\]. For \(U_1, U_2 \ll E_F, I - e^2 V/h \sim |U_1^2 + U_2^2 + 2U_1 U_2 \cos(2k_F a) H(geVa/[hV_F])|V|^{2g-1} \text{sign}V\), where \(H(x) = \sqrt{\pi} \Gamma(2g) J_{g-1/2}(x)/[\Gamma(g)(2x)^{g-1/2}]\) and \(J_{g-1/2}(x)\) is the Bessel function of the first kind \[22\]. The main contribution to the ratchet current at \(a \approx a_V\) comes from the shift of \(k_F\) due to the change of the electrochemical potential of the left reservoir by \(eV\). From the minimum of the quadratic part of the bosonized Hamiltonian one finds the charge density shift \[24\]. This gives \(k_F = k_F^{(0)} + g^2 eV/(2hV_F)\). After the substitution to the expression for the total current \(I\) we find

\[
I_r(V) \sim U_1 U_2 \sin(2k_F^{(0)} a)|V|^{2g-1} \sin(g^2 eV|a/[hV_F])|H(geV a/[hV_F])|
\]

(10)

Thus, \(I_r(V)\) oscillates. Notice that for \(V \sim V^* \ll E_F, a \sim a_V\) the ratchet current \(10\) is of the order of the total current \(\sim e^2 V/h\).

In conclusion, we have found the ratchet current for strong and weak asymmetric potentials. It exhibits a set of universal power dependencies on the voltage and can grow as the voltage decreases. This work was supported by the US DOE Office of Science under contract No. W31-109-ENG-38.

[1] Special issue on “Ratchets and Brownian motors: Basics, Experiments, and Applications”, Appl. Phys. A 75 (2002).
[2] A. Aviram and M. A. Ratner, Chem. Phys. Lett. 29, 277 (1974).
[3] C. Joachim, J. K. Gimzewski, and A. Aviram, Nature 408, 541-548 (2000).
[4] H. Linke, T. E. Humphrey, A. Löfgren, A. O. Sushkov, R. Newbury, R. P. Taylor, and P. Omling, Science 286, 2314 (1999); A. Löfgren, I. Shorubalko, P. Omling, and A. M. Song, Phys. Rev. B 67, 195309 (2003).
[5] H. W. C. Postma, T. Teepen, Z. Yao, M. Grifoni, and C. Dekker, Science 293, 76 (2001).
[6] S. Roddaro, V. Pellegrini, F. Beltram, G. Biasiol, L. Sorba, R. Raimondi, and G. Vignale, Phys. Rev. Lett. 90, 046805 (2003).
[7] P. Reimann, M. Grifoni, and P. Hänggi, Phys. Rev. Lett. 79, 10 (1997).
[8] J. Lehmann, S. Kohler, P. Hänggi, and A. Nitzan, Phys. Rev. Lett. 88, 228305 (2002).
[9] S. Scheidl and V. M. Vinokur, Phys. Rev. B 65, 195305 (2002).
[10] A. Konnik and A. O. Gogolin, Phys. Rev. B 68, 235323 (2003).
[11] B. Spivak and A. Zyuzin, cond-mat/0404408; D. Sanchez and M. Buttiker, Phys. Rev. Lett. 93, 106802 (2004).
[12] V. I. Belinicher and B. I. Sturman, Sov. Phys. Usp. 23, 199 (1980).
[13] C. L. Kane and M. P. A. Fisher, Phys. Rev. B 46, 15233 (1992).
[14] L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Addison-Wesley, Reading, Massachusetts, 1965).
[15] D. E. Feldman, S. Scheidl, and V. M. Vinokur, unpublished.
[16] We do not take Friedel oscillations into account since they do not change our estimate qualitatively (Ref. 15).
[17] A. O. Gogolin, A. A. Nersesyan, A. M. Tsvelik, Bosonization and Strongly Correlated Systems (Cambridge University Press, Cambridge, 1998)
[18] D. L. Maskov and M. Stone, Phys. Rev. B 52, R5539 (1995); V. V. Ponomarenko, ibid. 52, R8666 (1995); I. Safi and H. J. Schultz, ibid. 52, R17040 (1995).
[19] D. E. Feldman and Y. Gefen, Phys. Rev. B 67, 115337 (2003).
[20] B. Trauzettel, I. Safi, F. Dolcini, and H. Grabert, Phys. Rev. Lett. 92, 226405 (2004); e-print cond-mat/0409320.
[21] J. Rammer and H. Smith, Rev. Mod. Phys. 58, 323 (1986).
[22] The applied voltage renormalizes other terms in the action too (for example, the Luttinger parameter $g$). Power counting shows that some of them could also give rise to ratchet current contributions of the order of $U^2 V^2 \ln^s V$, $s = \text{const}$.
[23] C. de C. Chamon, D. E. Freed, S. A. Kivelson, S. L. Sondhi, and X. G. Wen, Phys. Rev. B 55, 2331 (1997).
[24] H. Grabert, cond-mat/0107175.
FIG. 1: Density profiles averaged over the period of Friedel oscillations for a potential with $U_1 < U_2$. The averaged densities show drops at the impurity positions.