Peltier effect in strongly driven quantum wires

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We study a microscopic model of a thermocouple device with two connected correlated quantum wires driven by a constant electric field. In such isolated system we follow the time– and position–dependence of the entropy density using the concept of the reduced density matrix. At weak driving, the initial changes of the entropy at the junctions can be described by the linear Peltier response. At longer times the quasiequilibrium situation is reached with well defined local temperatures which increase due to an overall Joule heating. On the other hand, strong electric field induces nontrivial nonlinear thermoelectric response, e.g. the Bloch oscillations of the energy current. Moreover, we show for the doped Mott insulators that strong driving can reverse the Peltier effect.

PACS numbers: 71.27.+a,72.10.Bg,05.70.Ln

Significant progress has recently been achieved in understanding the properties of strongly driven quantum many–body systems. The physics beyond the linear response (LR) regime is interesting for basic research and important for future applications. The underlying phenomena have become accessible to novel experimental techniques like ultrafast time–resolved spectroscopy of solids or measurements of relaxation processes in ultracold atoms driven far from equilibrium. Most of theoretical studies on transport beyond LR focus on charge currents driven by strong electromagnetic fields or heat/spin transport in electric insulators subject to a large temperature gradient. The thermoelectric phenomena beyond LR while important for power generation or cooling applications remain mainly unexplored, except phenomena beyond LR which may include several free parameters. With our choice of reasonable can be introduced also for moderate drivings far beyond the LR. We find that LoE persist up to much stronger fields, when the energy current starts to undergo the Bloch oscillations.

We choose as the simple model for TEC the one-dimensional (1D) ring with L sites and spinless but interacting fermions where different materials are modeled by site-dependent local potentials \( \varepsilon_i \). Steadily increasing magnetic flux \( \phi(t) \) induces an electric field \( F = -\dot{\phi}(t)/L \), as described by the time–dependent Hamiltonian

\[
H(t) = -t_0 \sum_i \left\{ e^{i\phi(t)/L} \hat{c}_i \hat{c}_{i+1} + \text{h.c.} \right\} + \sum_i \varepsilon_i n_i + V \sum_i \hat{n}_i \hat{n}_{i+1} + W \sum_i \hat{n}_i \hat{n}_{i+2},
\]

where \( n_i = \hat{c}_i \hat{c}_{i}^\dagger \) and \( \hat{n}_i = n_i - 1/2 \), \( t_0 \) is the hopping integral and periodic boundary conditions are used. V and W are repulsive interactions on nearest neighbors and next to nearest neighbors, respectively. The reason behind introducing W is to stay away from the integrable case (W = 0, \( \varepsilon_i = \text{const} \)), which shows anomalous relaxation and charge transport. We model different wires assuming a symmetric situation and next to nearest neighbors, respectively. In a closed circuit the either weak or strong electric field can we introduce via induction. We follow the real–time evolution of the TEC by solving the time–dependent Schrödinger equation. Since the system is isolated (decoupled from any thermal bath) the essential tool to investigate the local thermal properties is the concept of reduced density matrix (DM) of small subsystems. The latter allows to study how the entropy density increases/decreases in different parts of the TEC. It allows also to specify the limits of the local equilibrium (LoE) regime. Although the Joule heating is the dominating non–linear effect it does not immediately break the LoE. On the contrary, the time– and position–dependent temperature consistent with a canonical en...
The source term on the rhs. of Eq. (3). However, the heating is of the order of at least $F^2$ while $\nabla j_i^E \propto F$.

Since the initial state is a pure state with the corresponding DM $\rho(t=0) = |\Psi(0)\rangle\langle\Psi(0)|$ and the TEC is isolated from the surroundings, it stays in a pure state $|\Psi(t)\rangle\langle\Psi(t)|$ and the von Neumann entropy is identically zero. However, employing the concept of local reduced DM [37] the entropy density can be obtained from DM of small subsystems of the TEC. For subsystems of $M$ consecutive lattice sites we calculate $\rho = \text{Tr}_{L-M}[|\Psi(t)\rangle\langle\Psi(t)|]$ where the partial trace is taken over the remaining $L-M$ sites. Then, $S_i(t) = -\text{Tr}_M(\rho \log \rho)$ is the local entropy and $s_i(t) = S_i(t)/M$ corresponding entropy density where $i$ labels the position of the subsystem within TEC. $s$ is thermodynamically relevant intensive quantity [37, 38] except for the low–energy regime where typically $s \propto M^{-1}$ according to the area laws [39]. Hence, we choose in this study the initial microcanonical states corresponding to high temperatures, i.e. initial $\beta(0) \simeq 0.3$. Furtheron we also set the size to largest available within our numerical approach, $L = 26$.

In order to identify the hallmarks of LoE we focus on the weak–field regime. We consider metallic regime $V = 1.4, W = 1$ where the linear response functions are featureless [41]. Figs. [4] and [5] show $s_i(t)$ for the TEC driven by $F = \text{const}$. Major changes of $s_i(t)$ are clearly visible at the junctions, i.e. at $i = 13$ and 26. For short times $t < 10$, $s_{13}(t)$ strongly decreases (we dub it the cold junction) while $s_{26}(t)$ strongly increases (hot junction). Due to particle–hole symmetry, driving does not affect the average concentration of fermions in subsystems covering the junctions. Therefore, the change of the entropy at the junctions must be due to genuine heating/cooling. Further support for this interpretation follows from Fig. [5], which shows the difference of the total entropies of subsystems which cover the hot and the cold junctions. Initially, the results are independent of $M$, indicating that entropy is gained/lost mostly at the junctions consistently with Peltier heating $Q = T\dot{S} = 2\Pi j_i^N$. At high $T$ we can employ the Heikes formula for each wire $\Pi \simeq -\mu \sim \pm \varepsilon_0$. The estimate is then

$$\Delta S^{hc} \equiv S^{bot}(t) - S^{cold}(t) \simeq 4\beta(0) \int_0^t dt' \varepsilon_0 j_i^N(t'),$$  \hspace{1cm} (4)$$

In the investigated regime the particle currents are determined by LR [14, 15]. Hence, the rate of the entropy gain/loss at the junctions is roughly proportional to $F$ as it is shown in Fig. [2a], well consistent with Eq. (4).

Next we discuss the long–time regime shown in Fig. [2b]. Here $\Delta S^{hc}(t) = \Delta S^{hc}(0)/M$ decays approximately as $\exp(-aF^2t)$, where $a$ is independent of $F$. The same time–dependence has been found for particle current (see Fig. [2] and Refs. [14, 15]) and explained as a result of the Joule heating. It has also been recognized as a hallmark of the quasiequilibrium (QE) evolution when $\rho$ is
FIG. 2. (Color online) Results for $M = 4$ and $\varepsilon_0 = 1.2$. Difference of the entropy-densities $\Delta s^{hc}$ is shown vs. a) $Ft$ and b) $F^2t$. c) shows $j^N$ and $j^E$ in the middle of the left wire for $F = 0.2$; d) the same but for $F$ switched off at $t = 15$.

determined only by the instantaneous energy [37]. Contrary to the case of homogeneous systems [14, 15, 37], the QE regime of TEC cannot be characterized by a single time–dependent $\beta(t)$.

An important property of the long time regime can be inferred from Fig. 2 that shows $j^N$ and $j^E$ in the middle of the left part of TEC (far from the junctions). Initially, both currents show similar time–dependence, however $j^E$ vanishes for $t > 10$ while $j^N$ remains large. In order to explain this result we recall that the in LoE regime both currents are driven by two independent forces: $F$ and $\nabla \beta$. A particular combination of these forces may cause vanishing of $j^N$ (Seebeck effect) or $j^E$ (present case). In order to explicitly show that vanishing of $j^E$ originates from compensation of two forces we instantaneously switch off one of them: the electric field. As shown in Fig. 2d, the remaining force drives $j^E$ in the opposite direction. The magnitude of the resulting energy current is comparable with its values during the initial evolution under $F \neq 0$. Below we demonstrate that $\nabla \beta_i(t)$ is indeed the second driving force.

It has been shown for a driven homogeneous wire that $\rho$ is block–diagonal with respect to the number of particles in the subsystem. In the QE regime $\rho \propto \exp[-\beta(t)H_{eff}]$ within each block [37] and the spectrum $\{E_m\}$ of the effective Hamiltonian $H_{eff}$ is independent of $\beta$. Although for small subsystems $H_{eff}$ may significantly differ from $H$, one may still estimate $\beta(t)$ without specifying explicit form of $H_{eff}$. For the initial microcanonical state with known inverse temperature $\beta(0)$ we determine the eigenvalues $\lambda_m$ of the largest block of $\rho$. Then a similar spectrum $\lambda_m$ is determined for a driven system in a QE. Assuming the same $\{E_m\}$ one can then estimate $\beta_i(t)/\beta(0) = \log(\lambda_m/\lambda_i)/\log(\lambda_m/\lambda_1)$. Fig. 3a shows the resulting $\beta_i(t)$ (averaged over $m \neq 1$) for the subsystem in the middle between hot and cold junctions. Being almost independent of $M$, $\beta$ is a well defined intensive quantity. Finally, we demonstrate that $\beta$ is consistent with the 2nd law of thermodynamics. In Fig. 3b we compare $s_i(t) - s_i(0)$ determined directly from $\rho$ with the integral $\int_0^t d\epsilon_i(t')\beta_i(t')$ where $\epsilon_i(t) = \langle h_i(t) \rangle$ is the energy density in the subsystem. Both quantities are very close to each other. Therefore, we conclude that in the QE regime one may introduce $\beta_i(t)$ consistent with the canonical ensemble as well as with equilibrium thermodynamics. This consistency breaks down only for subsystem covering one of the junctions. In Fig. 3c we show snapshots of the temperature profiles $T_i$ for various $t$ in the QE regime. The temperature gradient is clearly visible, however there exists also an asymmetry between the change of $T_i$ at hot and cold junctions due to the heating effects.

In an inhomogeneous system $j^N \neq 0$ causes a redistribution of particles within the TEC. This in turn may be another (in addition to $F$) driving force for the transport of particles. In the investigated TEC this effect should be insignificant at least within the QE regime because of the particle–hole symmetry. In order to confirm this expectation we plot in Fig. 3d the spatial distribution of particles $\langle n_i(t) \rangle$ and compare it with the equilibrium high–
temperature expansion (HTE), $n_i^{HTE}(t) = \epsilon_i \beta_i(t) / 4$, where $\epsilon_i$ are averaged over all sites of the subsystem. Indeed, the changes of $(n_i(t))$ can be reasonably explained as originating only from the time–dependence of $\beta_i(t)$.

Next we concentrate on nonequilibrium phenomena related with the operation of the TEC under strong $F$. The first one concerns the magnitude of $F$ which destroys the LoE. Since the TEC is spatially inhomogeneous LoE can be destroyed in certain parts of TEC while persisting in the other parts. In the LoE regime, intensive quantities including $s_i(t)$ and $\epsilon_i(t)$, are uniquely determined by $\beta_i(t)$. Such a universal relation is confirmed for $F \leq 0.4$ in Figs. 4a (cold junction) and 4b (hot junction). In the former case the curves for weak $F$ merge during the entire evolutions, while in the latter case it happens only in the long–time regime after the nonequilibrium transient. Results for $s_i(t)$ within the wires (not shown) are intermediate to the cases shown in Figs. 4a, and 4b. Hence, one can observe that the LoE regime is broken first at the hot junction. For large $F$, $\epsilon_i(t)$ starts to oscillate, while oscillations of $s_i(t)$ are rather limited. Therefore, the equilibrium relation between $\epsilon_i$ and $s_i$ is broken when the energy current $j_i^E(t)$ starts to undergo the Bloch oscillations. It is indicative to compare this result with recent finding for the driven homogeneous systems [13, 19] when the Bloch oscillations of the particle current $j_i^s(t)$ mark the onset of the nonequilibrium evolution.

Finally we test the nonequilibrium response of TEC build out of two doped Mott insulators. Fig. 4c shows the operation of TEC when the interaction $V$ is tuned from small (metallic) $V < 2$ to large values $V \gg 2$ correspond-ing, close to half–filling, to lightly doped Mott insulators. Such tuning reverses the dc flow of entropy (at longer $t$) and effectively interchanges the role of junctions (hot and cold, respectively). This effect is not unexpected being the result of changing the charge carriers close to half–filling from electrons in metallic regime to holes in the Mott-insulating regime. In contrast, results in Fig. 4d are even more surprising. One can see that under strong driving $F > 0.5$, the Mott-insulating TEC operates in the same way as expected for generic metals, i.e. the current is again carried by electrons. Breaking of the Mott insulator ground state by strong $F$ has intensively been investigated during the last decade [9, 11–13, 40–43] and explained mostly as a kind the Landau–Zener transitions from the dispersionless ground state to a dispersionful excited state. However in the present case, the breakdown concerns a doped Mott insulator and involves only excited states with rather high energy, so a proper explanation remains a challenge.

In conclusion, we have studied a simple model of driven isolated TEC that can offer a useful and novel insight into several aspects of thermoelectric and nonequilibrium phenomena. Here, the concept of reduced (subsystem) DM is crucial for the discussion of increasing/decreasing entropy density, local temperature and local equilibrium. Starting with an equilibrium state, we have shown that the onset of driving field $F$ first leads to local Peltier heating/cooling at junctions according to LR theory. Concerning the long–time regime of weakly/moderately driven TEC the behavior can be dubbed as “local quasiequilibrium”. Similarly to the standard LoE one may introduce well defined $\beta_i(t)$. However, the changes of $\beta_i(t)$ originate not only from the energy and particle currents flowing within TEC, but also from the Joule heating due to external driving in analogy to QE in homogeneous systems [14] with homogeneous $\beta(t)$.

The presented method also allows to find the regions of evident departures from LoE. In the metallic regime of the model, strong $F$ leads to the breakdown of the relation between local temperature $T_i(t)$ and local energy $\epsilon_i(t)$ which is incompatible with the notion of LoE. Even more dramatic are the effects in the regime of doped Mott insulator where the charge carriers (within the equilibrium LR response) change the electron/hole character. Such systems are promising for the thermoelectric applications [14]. Here we find that large $F$ can even reverse the thermoelectric response.

Authors acknowledge stimulating discussions with Veljko Zlatič. This work has been carried out within the NCN project "Nonequilibrium dynamics of correlated quantum systems". P.P. acknowledges the support by the Program P1-0044 and project J1-4244 of the Slovenian Research Agency.
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