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Thermopower as a tool to investigate many-body effects in quantum systems

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Measuring the thermopower of a confined quantum system reveals important information about its excitation spectrum. Our simulations show how this kind of transport spectroscopy is able to extract a clear signal for the onset of Wigner localization in a nanowire segment. This demonstrates that thermopower measurements provide a tool for investigating complex many-body quantum effects, which is less intrusive than the usual charge-stability diagram as no high source-drain bias is required. While the effect is most pronounced for weak tunnel coupling and low temperatures, the excited states also significantly affect the thermopower spectrum at moderate temperature, adding distinct features to the characteristic thermopower lineshape.
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Temperature differences appear everywhere in our environment. Between two conductors, a temperature gradient may result in electrical power. This idea goes back to Seebeck who discovered the effect in the beginning of the 19th century. Obviously, thermoelectricity has a great potential for applications, and much of the current activity in the field is spurred by the ever-increasing need to find better ways to efficiently recycle waste heat.

Thermoelectric effects in nanostructured quantum systems have recently attracted much interest, in part for the prospect to exploit the quantum properties of a nanosystem to enhance the usually low thermoelectric efficiency, see, e.g., Refs. 1 and 2 and references cited therein. In addition, the measurement of the electric response to a small thermal bias in a nanoscale system is emerging as a very useful complement to traditional conductance measurements in the investigation of novel effects in nanostructures, including their intricate quantum-mechanical properties. Examples are the recent study of the renormalization of energy states in quantum dots,[3] rectification effects,[4,5] quantum-thermoelectric reciprocity relations in quantum thermoelectric transport,[6] and the proposed use of thermovoltage measurements as a novel method to identify Majorana states.[7]

As thermal transport probes a relatively large energy window, excited states may manifest as additional peaks in the thermopower signal.[8–10] Here, we apply this concept to the Wigner localization[11] in a nanowire.[12–17] Wigner localization is a prime example for a pronounced many-body effect, caused by the dominance of the repulsive interaction over the kinetic energy of the electrons in the system.[11,18] Clearly, such spatially correlated quantum states cannot be described by the constant interaction model commonly used for thermal transport simulations,[8] see also Ref. 19 for its extension to exchange effects. Thus, we need to work with a more realistic many-particle picture, fully taking into account the correlations in the system. Our approach follows Ref. 16, where we probed the Wigner localization by the conductance signal of excited states under finite bias. Using the thermopower signal, these features can be extracted already in linear response as demonstrated in this letter. This is of great benefit, as high source-drain biases are often problematic due to stray fields and sample heating.

The nanowire system that we investigate here is depicted in Fig. 1. We consider a segment of a nanowire, which is connected to leads on either side via a tunneling barrier. Possible realizations are, e.g., semiconductor nanowires with metal stripes acting as leads and simultaneously providing a Schottky barrier,[16] nanowires with embedded heterostructures,[20] or nanowires defined by cleaved edge overgrowth.[21]

The nanowire segment is modeled as a hard-wall cylinder of radius 35 nm. We use the single-mode approximation, i.e., assume that the electrons are in the ground state in the transverse directions. In contrast, the length of the wire (160 nm), set by a finite well potential of depth $V_0 = 0.1$ eV, allows for a multitude of spin-degenerate states. (Standard parameters for InSb are used.) The Hamiltonian including the full Coulomb interaction between the electrons is solved by the configuration interaction method (exact diagonalization)

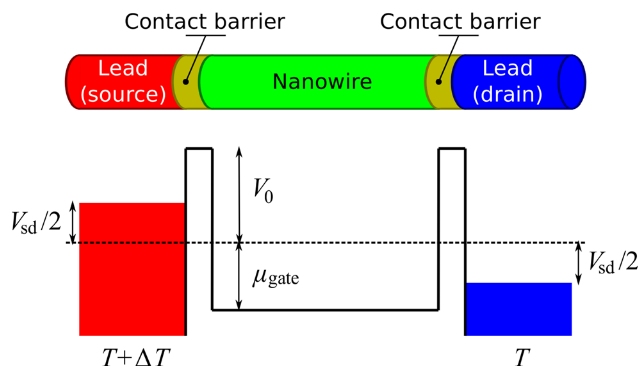

FIG. 1. Schematic figure of the system. A finite segment of a nanowire is embedded between metallic leads. One lead is kept at a higher temperature by ΔT. A bias V_{sd} is applied between source and drain. The energy levels of the nanowire segment are shifted by a gate potential μ_{gate}. The contacts provide barriers of height V_0.

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to find the energies and many-particle eigenstates of the electrons in the nanowire segment, see Ref. 16 for further details. The entire system can be shifted downwards in energy by μ_{gate} by applying an appropriate gate contact. The leads are represented by Fermi seas of non-interacting electrons with temperatures $T + \Delta T$ and T, and chemical potentials $\mp eV_{\text{sd}}/2$, respectively, where ΔT is the temperature difference and V_{sd} is the source-drain bias applied.

Electron transitions between the leads and the many-particle states are treated within the master equation model[22–24] with tunneling matrix elements calculated as in Ref. 14. In the stationary state, we find the current I between source and drain as a function of V_{sd} and ΔT. The thermopower $S = -(V_{\text{th}}/\Delta T)|_{I=0}$ is easily accessible to quantify thermal transport. It is defined via the thermo-voltage V_{th}, the bias point of vanishing I for a finite ΔT.

The ground and low-lying excited states of confined systems provide knowledge of fundamental properties of the system. Let us, for example, consider the lowest excitation energies $\Delta\varepsilon$ and ΔE_2 for a one- and a two-particle system, respectively. If the Coulomb interaction is relatively weak, the independent-particle shell model applies. In that case, we find $\Delta E_2 \approx \Delta\epsilon$, as the lowest single particle level is spin-degenerate. In contrast, for strong Coulomb repulsion, the two-particle ground state is better described by the two electrons being localized at either end of the wire segment, which is the Wigner localization addressed above. Here, we have four different spin configurations with a ground state singlet, which is almost degenerate with the excited triplet. (The energy difference results from residual coupling between the localized states.) Consequently, one can detect the onset of Wigner localization by observing that ΔE_2 becomes significantly smaller than $\Delta\varepsilon$.

Commonly, the energy levels in a confined quantum system are measured by transport spectroscopy.[18,25] Here, the conductance is measured as a function of source-drain bias and gate potential, see our calculated results in Fig. 2. The borders of the Coulomb blockade regions, where tunneling is energetically forbidden, are given by transitions between the ground states with different particle numbers, e.g., the lines 1 and 3 in the inset. Similarly, lines for tunneling to excited states (such as lines 2 and 4) can be identified. In this way, the onset of Wigner localization could be experimentally proven in Ref. 16 via the criterion $\Delta E_2 \ll \Delta\varepsilon$. However, these lines are not visible in the Coulomb blockade region. Thus, a significant source–drain bias is required for their observation. Such biases provide electric fields inside the sample, which may disturb the electronic structure. Detection of these lines far from equilibrium does therefore not always provide reliable information.

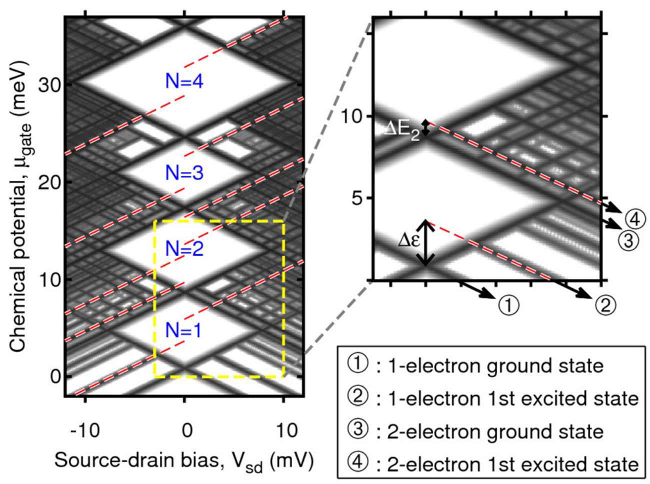

FIG. 2. Charge stability diagram showing the differential conductance dI/dV_{sd} in grey-scale. The number N of electrons is denoted in the Coulomb blockade regions. The inset shows the main lines to determine the excitation energies $\Delta\varepsilon$ and ΔE_2 of the one-particle and two-particle states, respectively. The red dashed lines highlight tunneling through those excited states that appear in the thermopower, see Fig. 3.

At low enough temperatures,[26] low lying excitations become discernible in the Seebeck coefficient (thermopower), as fine-structure in the otherwise saw–tooth shaped thermopower[8] for the case of weak contact couplings. This may sound surprising; since the thermopower is measured at vanishing source-drain bias in the Coulomb blockade regime, where there is no visible effect of excited states in the conductance (see Fig. 2). In fact, the conductance due to excited states is exponentially suppressed in the Coulomb blockade area.[8] Although this makes tunneling via excited states invisible in the conductance, the small effect of the excited states on the current is still large enough to make a visible shift of its zero and, hence, the thermopower $S = -(V_{\text{th}}/\Delta T)|_{I=0}$. This opens up the possibility of detecting the low lying excitation energies. In fact, Fig. 3 shows that for the nanowire system considered here, the energy differences $\Delta\varepsilon$ and ΔE_2 can be directly extracted from the μ_{gate}-dependence of the thermopower. Even if the lever arm factor, relating the measured gate potential to μ_{gate}, is not precisely known, the relative size of $\Delta\varepsilon$ and ΔE_2 remains accessible. This provides a clear indication of the onset of Wigner localization, as it also becomes (gradually) visible in the spatial structure of the ground state shown in the inset of Fig. 3.

Thus, we propose to use thermopower measurements to identify the excited states in complex many particle systems. This approach provides two important benefits compared to standard tunneling spectroscopy: (i) One only needs to sweep the gate bias, and not also the source-drain bias, which reduces measurement times. (ii) The system is less affected by the measurements, as the source-drain bias remains small. It is proportional to the energy scale of the applied thermal bias (less than 1 K, or tens of μeV), as compared to the measurement of Coulomb diamonds that typically require a bias of order several mV.

Regarding the technical realization, thermal biasing of short segments of nanowires has been demonstrated,[27,28] which, however, was somewhat cumbersome and required careful tuning to avoid disturbances in the measurement circuit. A recent improvement in biasing technique[29] allows for highly local (avoiding overall heating), continuously tunable, and electrically non-intrusive thermal biasing, which strongly facilitates the proposed thermopower measurements.

At higher temperatures $(3k_BT > \Delta E)$, the excitations are no longer discernible in the Seebeck coefficient (Fig. 4). However, they add distinct features to the thermopower lineshape (which at finite temperature evolves away from a sawtooth pattern[8,28]), and even shift the zeroes off their usual positions (at the Coulomb peak positions and in the middle

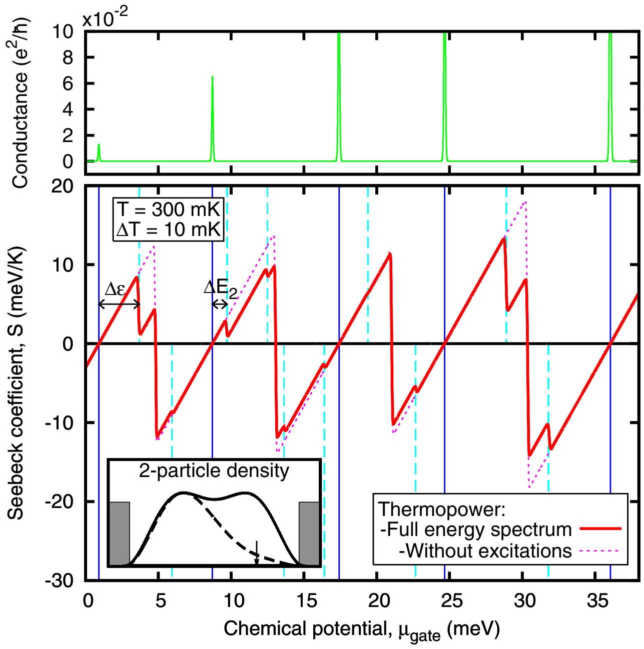

FIG. 3. *Upper panel*: Coulomb peaks (the highest shown three peaks reach up to 0.24, 0.285, and 0.465 $e^2/\hbar$, respectively). Note that conductance peaks due to tunneling through excited states are exponentially suppressed and hence invisible.[8] *Lower panel*: Thermopower at $T = 300$ mK, $\Delta T = 10$ mK. If only the ground states for each particle number are taken into account, one obtains the common sawtooth-like dotted curve, where the conductance peaks (vertical blue lines) correspond to zero thermopower. Adding the excited states (vertical cyan dashed lines) to the calculations, the thermopower (full line) shows distinct dips at the corresponding energies. The one-particle and two-particle excitation energies, $\Delta\varepsilon$ and ΔE_2, respectively, are marked by arrows. The inset shows the two-particle density (solid) along the wire and the two-electron pair-correlated density (dashed), where the arrow shows the position of the reference electron.

between those, see the magenta dotted line). It is an important message from this work that such shifts and distortions, which are commonly seen in experiment, are not experimental artifacts but carry important information.

Finally, we want to point out that our calculations only include sequential tunneling, in which case the thermopower has the well-known sawtooth shape. If higher-order processes are present, the sawteeth shrink and plateaus will appear between them.[28,30,31] This provides a limit for the observation of excited states for systems with a high conductance, as discussed in Ref. 19.

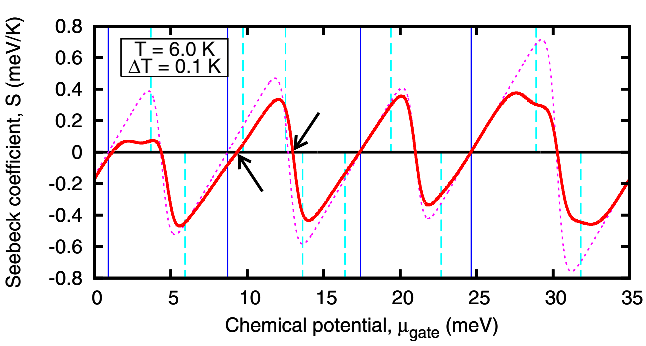

FIG. 4. Thermopower at $T = 6.0$ K, $\Delta T = 0.1$ K. The effect of excited states (vertical cyan dashed) on the thermopower lineshape (red thick solid) is smeared out due to temperature broadening. Still, the thermopower appears skewed and its zeroes are even shifted (arrows) off their usual positions, i.e., at the Coulomb peak positions (vertical blue solid) and in the middle of those. Shown as a reference, by excluding the excitations, the thermopower has the well known saw-tooth shape (magenta dotted).

While we focused on electrons in semiconductor nanowires here, we emphasize that our findings apply to a much broader range of physical systems. The thermal properties of mesoscopic devices have been studied extensively, see, for example, the review by Giazotto *et al*.[32] Thermopower measurements on molecular junctions have already provided insight into how the chemical structure effects the electronic structure and the charge transport, see, e.g., Refs. 33 and 34. A very recent and highly interesting new research direction has opened up in the field of ultra-cold atomic quantum gases:[35] Brantut *et al*.[36] reported the measurement of thermoelectric transport properties of a cold-atom channel, where a temperature difference between two atom reservoirs was realized by a laser pulse directed towards one of them. The setup is completely analogous to that of a semiconductor nanowire. However, the advantage here is that the system is very clean, and free from other effects such as phonon scattering or impurities that in the solid-state case may complicate the picture significantly. Moreover, the atom-optical confinement as well as the form and strength of the particle interactions are highly controllable, providing entirely new experimental opportunities for studying many-body effects on quantum transport.

Our findings demonstrate that a finer structure in the thermopower line shape of a nanowire segment appears due to the low-lying excitations at low temperatures. We have demonstrated how this can be used to identify the onset of Wigner localization of electrons in the nanowire segment. At higher temperatures, where the finer structure is smeared out due to thermal broadening, the saw-tooth shape of the thermopower is skewed due to the excitations. The saw-tooth shape of the thermopower is generally known and expected. Therefore, in an experiment, the finer structure in the thermopower or the skewing of its line shape can easily be misinterpreted as noisy and/or faulty data, while these are, quite on the contrary, signatures of low-lying excitations and the fascinating physics they convey.

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