

Aharonov-Bohm-Type Oscillations of Thermopower in a Quantum Dot Ring Geometry

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We investigate Aharonov-Bohm-type oscillations of the thermopower of a quantum dot embedded in a ring for the case when the interaction between electrons can be neglected. The thermopower is shown to be strongly flux dependent, and typically the amplitude of oscillations exceeds the background value. It is also shown to be essentially dependent on the phase of the scattering matrix which is determined by the experimental geometry and is not known in the given experiment. Two procedures to compare theory and experiment are proposed.

The interest in phase-sensitive measurements has increased recently due to a series of beautiful experiments by Yacoby *et al.* [1] and Schuster *et al.* [2] in which the electron phase shift due to transmission through a quantum dot has been directly measured. These experiments led to a number of theoretical papers [3–6] in which the phase dependence of the conductance in the presence of a quantum dot was investigated.

Below we present a theoretical investigation of phase-sensitive effects in the thermopower. The thermopower of a system of electrons is extremely sensitive to the energy dependence of the density of states [7]. As examples, we mention the behavior of the thermopower in Kondo systems [8] and the sensitivity to the band structure [9]. In both cases the thermopower exhibits singularities and can be experimentally used to detect the corresponding effects. Shubnikov-de-Haas-type oscillations of the thermopower are a similar phenomenon [10]: the amplitude of oscillations exceeds the mean value of the thermopower, and, as a consequence, the thermoelectric effect changes sign as a function of the applied magnetic field.

In the present paper we investigate the thermopower of a particular mesoscopic system, corresponding to the experiment [1] – a quantum dot embedded in an Aharonov-Bohm (AB) ring. While the flux dependence of the conductance was studied, e.g. in Ref. [5], in both the linear and nonlinear regime, for interacting and non-interacting electrons, we concentrate below on the case of linear transport and consider non-interacting electrons only. We find that the thermopower exhibits AB-type oscillations; in contrast to the conductivity, typically the amplitude of these oscillations exceeds the mean value

of the thermopower, causing a sign change of the thermoelectric effect vs. magnetic field. Moreover, we show that the shape of these oscillations essentially depends on the phase of the scattering matrix. This phase is an individual characteristic of a given system, and is determined by its microscopic details. It remains unknown in the given experiment, complicating direct comparison with the theory. We suggest two ways of overcoming this difficulty. The first one is to vary this phase in the experiment in the spirit of Refs. [1,2]; another way is to consider it as a random variable. Statistical fluctuations of the thermopower with respect to this variable exceed the mean value. Our calculations can be easily generalized to arbitrary scattering geometries, for which we expect similar results.

Recent progress in the investigation of the thermopower of mesoscopic systems both on the experimental [11–16] as well as on the theoretical [17–21] side allows us to hope that experimental studies of the thermopower in this system will soon be available.

We consider the two-terminal configuration shown in Fig. 1.

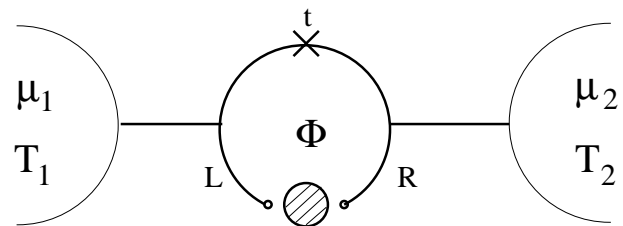


FIG. 1. Geometry of the ring connected to reservoirs 1 and 2. The ring is connected to a quantum dot via high tunneling barriers. Φ is the flux penetrating the ring.

In the absence of a magnetic field, the upper arm is characterized by the scattering matrix

$$\hat{T}_{up} = \exp(i\theta) \begin{pmatrix} r_1 & t_1 \\ t'_1 & r'_1 \end{pmatrix}. \quad (1)$$

We now specialize to the case of good transmission through the upper arm, and consequently choose $t_1 = t'_1 = 1$ and $r_1 = r'_1 = 0$. The quantum dot with one single-electron level [22] is described by the scattering matrix

$$\hat{T}_{dot} = \frac{\exp(i\theta')}{E - \epsilon + i,} \begin{pmatrix} i, & -E - \epsilon \\ -E - \epsilon & i, \end{pmatrix}. \quad (2)$$

Here, ϵ , E and ϵ are the tunneling rate through the dot, the electron energy, and the position of the level (both measured from the Fermi energy). The level position is controlled by an external gate voltage. Only the difference between the phases θ and θ' matters, and therefore we put $\theta' = 0$. Then the phase θ is acquired by motion along the ring: $\theta = kL + \delta\theta$, with k , L , and $\delta\theta$ being the wavenumber, the ring circumference, and the phase shift in the quantum dot, respectively, i.e. this phase is a geometrical characteristic of the system. Furthermore, we assume that the ring is penetrated by the magnetic flux Φ .

The transmission coefficient $t(E)$ of the whole structure has been obtained in the literature [23,24]; for our particular scattering matrices (1), (2) we obtain:

$$t(E) = 4 \frac{(\Delta E)^2 + 4\Delta E, \cos\theta \cos\phi + \epsilon^2 \cos\theta}{\lambda_1(\Delta E)^2 + \lambda_2\Delta E, + \lambda_3, \epsilon^2}. \quad (3)$$

Here, $\Delta E = E - \epsilon$, $\phi = 2\pi\Phi/\Phi_0$, $\Phi_0 = hc/e$ is the flux quantum, and the quantities λ_i are given by

$$\begin{aligned} \lambda_1 &= 16 + 9\cos^2\theta; \\ \lambda_2 &= \cos\theta(10\cos\phi - 6\sin\theta); \\ \lambda_3 &= 1 + \cos^2\phi + 3\cos^2\theta. \end{aligned}$$

The ring is connected to two reservoirs, and the current is given by the usual expression

$$I = (e/2\pi) \int t(E)(f_L - f_R)dE, \quad (4)$$

where f_L is the Fermi distribution function of the left reservoir (temperature $T_1 = T - \Delta T/2$ and chemical potential $\mu_1 = eV/2$), and f_R is the Fermi distribution function of the right reservoir (temperature $T_2 = T + \Delta T/2$ and chemical potential $\mu_2 = -eV/2$). In the linear regime we obtain

$$\left[\frac{G}{B} \right] = \frac{e}{2\pi T} \int \left[\frac{-e}{E} \right] t(E) \frac{\partial f}{\partial E} dE. \quad (5)$$

Here, G and B are the conductance and the thermoelectric coefficient, respectively. The thermopower is expressed as $S = -B/G$. The sequel of the paper is devoted to the analysis of this expression. We restrict ourselves to the case $T \ll \epsilon$, since in the opposite case all structure in the function $t(E)$ is washed out by temperature.

Not too close to the points $\theta = (2n+1)\pi/2$, $n \in \mathbb{Z}$ we obtain the following asymptotic expressions:

$$S = \begin{cases} \frac{\pi^2 T}{3e} \left(\frac{4\cos\phi}{\cos\theta} - \frac{\lambda_2}{\lambda_3} \right) & \epsilon \ll \epsilon, \\ -\frac{\pi^2 T}{3e^2} (\cos\phi \cos\theta - \frac{\lambda_2}{\lambda_1}) & |\epsilon| \gg \epsilon, \end{cases} \quad (6)$$

The thermopower shows Φ_0 -periodic AB-type oscillations as a function of magnetic flux. The oscillations are strong in the sense that the thermoelectric effect changes sign as a function of AB flux. Generally, the shape of these oscillations is anharmonic. In Fig. 2 we show the thermopower as a function of the AB phase ϕ in the intermediate regime $\epsilon = \epsilon$, for different values of θ .

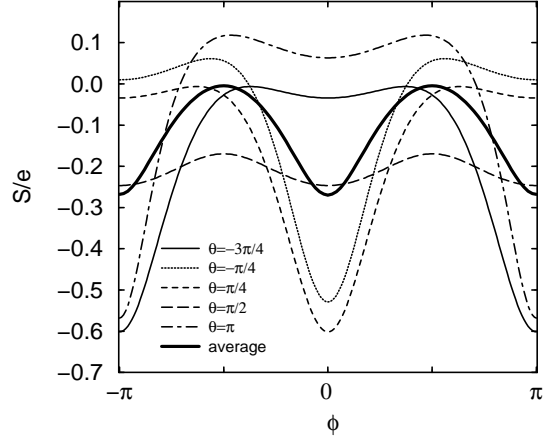


FIG. 2. Dependence of the thermopower on the AB flux for $\epsilon = \epsilon$, $\epsilon = 5T$ for different values of the phase θ .

The gate-voltage dependence of the thermopower is shown in Fig. 3. The thermopower shows a characteristic shape with two maxima around the resonance (see e.g. [20]) as a function of the level position ϵ (or, equivalently, of the gate voltage). This shape can be easily explained using the Mott formula [7] $S \propto dG/d\epsilon$: since the conductance exhibits a peak as a function of the gate voltage, its derivative shows a two-peak structure.

Another important feature is the strong dependence of the shape of the oscillations and even the sign of the thermopower on the geometric phase θ , which is controlled by the microscopic details of the sample and is not known in the given experiment. In this sense we deal with a typical mesoscopic system: the fluctuations of the thermopower with respect to the parameter θ exceed the mean expectation value. Therefore a direct comparison of the theory with experimental results is impossible. We suggest, however, two ways to overcome this difficulty.

1. The phase θ can be varied by the gate voltage (i.e. the level position ϵ). The experiments [1] show that the phase is changed by π in a narrow window of gate voltages, so that in this window an explicit dependence $S(\epsilon)$ is negligible. Hence, in this window one can expect to observe an unusually strong gate voltage dependence of the thermopower, originating purely from the dependence $S(\theta)$.

2. For multi-channel rings or ring ensembles the phase θ can be considered as a random quantity, and only the averaged expressions make sense (see Ref. [25]). The corresponding disorder is expected to be “strong”, since a

relatively weak variation of the microscopic structure of the system changes the phase θ completely. Hence the random variable θ can be considered as uniformly distributed. The corresponding curves are shown in Fig. 2 and Fig. 3c. Note that the averaged thermopower is again a periodic function of the applied AB flux, but with the period $\Phi_0/2$, i.e. half that of a given θ . As could be expected, the amplitude of these oscillations is less than the typical amplitude for arbitrary θ .

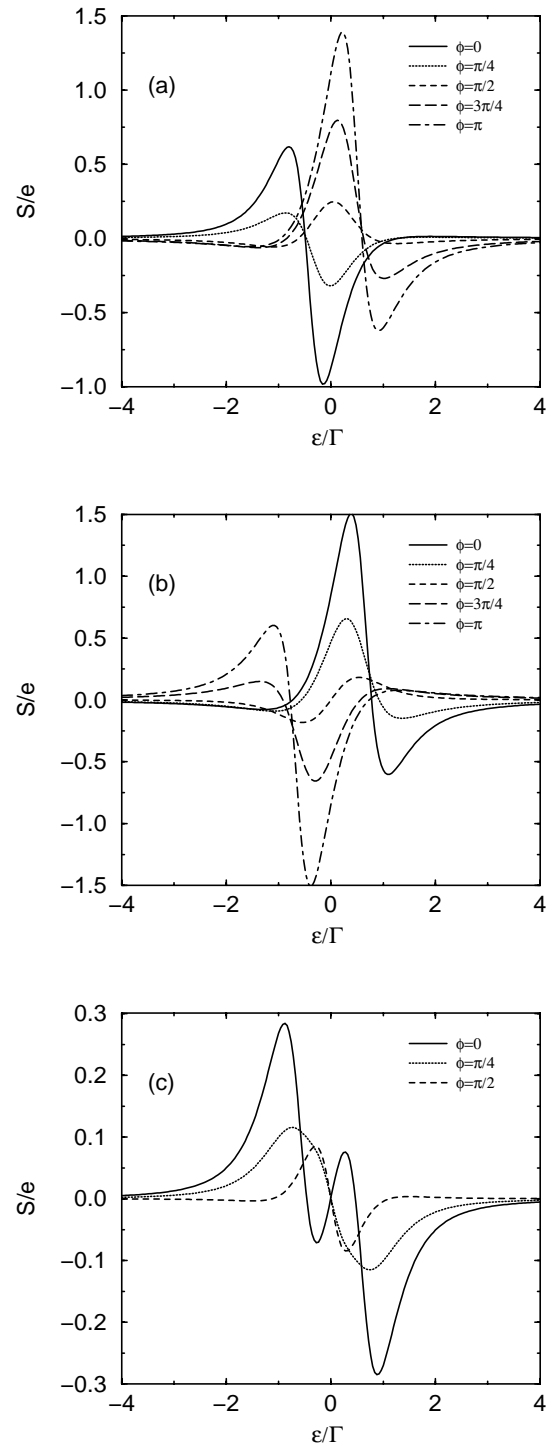


FIG. 3. The gate voltage dependence of the thermopower for $\gamma = 5T$. (a) $\theta = -3\pi/4$; (b) $\theta = 0$; (c) curves averaged over θ .

In conclusion, we have considered AB-type oscillations of the thermopower of a quantum dot embedded in a ring for the case of non-interacting electrons. We have shown that the oscillations are strong, and the thermoelectric effect typically changes sign as a function of AB flux.

All details of the oscillations depend essentially on the microscopic structure of the system. However, ways to compare the theory with experiment are proposed.

The regime considered is the most favorable one for AB-type oscillations; if the transmission t through the upper arm is small, the amplitude of the oscillations is suppressed with t being the corresponding small parameter. As a consequence the thermoelectric effect changes sign only in a very narrow range of parameters, viz. for very low ($\epsilon \ll , /t$) or very high ($\epsilon \gg , t$) gate voltages. We expect a different behavior for interacting electrons, since the interacting quantum dot can be described by an Anderson impurity model [26], and the corresponding physics is equivalent to Kondo systems. Strong singularities in the behavior of the thermopower appear even for an isolated quantum dot [27]. However, these features are expected to show up only in small and clean dots, whereas usually a behavior similar to the one described above will be observed.

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Note added in proof: After submitting this paper, the previously published work by Guttman, Ben-Jacob, and Bergman [28] came to our attention. The AB oscillations of the thermopower are also discussed in this work, however the authors do not see a sign change in the thermoelectric effect as the function of magnetic field and also do not discuss the geometric phase effects.

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