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Metastable and spin-polarized states in electron systems with localized electron–electron interaction

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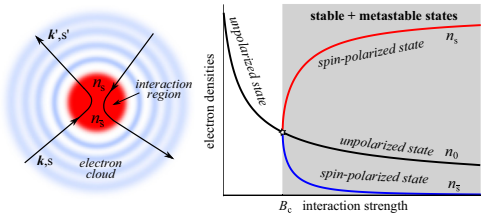
HIGHLIGHTS

- A metastable state arises in the electron system when pair interaction is localized.
- In the metastable state, the system can be both spin polarized and unpolarized.
- Critical conditions for the metastable state to appear are studied.
- Electron cloud around the interaction region affects the metastable state energy.

GRAPHICAL ABSTRACT



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ABSTRACT

We study the formation of spontaneous spin polarization in inhomogeneous electron systems with pair interaction localized in a small region that is not separated by a barrier from surrounding gas of non-interacting electrons. Such a system is interesting as a minimal model of a quantum point contact in which the electron–electron interaction is strong in a small constriction coupled to electron reservoirs without barriers. Based on the analysis of the grand potential within the self-consistent field approximation, we find that the formation of the polarized state strongly differs from the Bloch or Stoner transition in homogeneous interacting systems. The main difference is that a metastable state appears in the critical point in addition to the globally stable state, so that when the interaction parameter exceeds a critical value, two states coexist. One state has spin polarization and the other is unpolarized. Another feature is that the spin polarization increases continuously with the interaction parameter and has a square-root singularity in the critical point. We study the critical conditions and the grand potentials of the polarized and unpolarized states for one-dimensional and two-dimensional models in the case of extremely small size of the interaction region.

1. Introduction

Spin-related phenomena due to electron–electron (e–e) interaction in mesoscopic systems attract great interest, since they exhibit non-trivial physics of many-body systems and open new possibilities to manipulate the spin degrees of freedom. One of the most intriguing is the question of spontaneous breaking of the spin symmetry in quantum point contacts [1]. These structures have attracted attention also because they allow one to manipulate the spin and generate spin currents [2,3]. However, currently there are fundamental physical problems in understanding their electronic structure and transport properties. Numerous experiments reveal transport features, such as puzzling $0.7 \times 2e^2/h$ conductance anomaly observed at finite temperature, and other nonuniversal plateaus of the conductance arising at a finite voltage bias [1,4]. Their nature remains a mystery whose solution lies in unclarified so far physics of interacting electrons in these systems [5]. Nevertheless, it is clear that the origin of the anomalies is closely related to the spin-charge structure of the quantum contact.

In the present paper we have found an unusual feature of the interacting electron behavior that could be a reason of the above anomalies. This feature arises when the phase transition with

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spontaneous breaking the spin symmetry occurs in the case where the e–e interaction is highly nonuniform, namely the interaction is concentrated in a small region of space that is not separated by any barrier from the surrounded gas of non-interacting electrons.

The problem is the following. The electrons in the quantum point contact are often considered as a one-dimensional (1D) system. However a rigorous theorem due to Lieb and Mattis [6] shows that the ground state of a 1D system is unmagnetized. In reality, the 1D part of the quantum point contact is continuously transformed at its ends into surrounding system of higher dimensionality. Therefore this theorem is not applicable and the 1D segment can have a magnetic momentum. We draw attention to two facts. First, the e–e interaction in the narrow constriction is effectively much more strong than in the surrounding electron gas. Second, there is no physical reason to divide the system under consideration into a two coupled systems: a small system in which the e–e interaction is present, and a large system where electrons do not interact. The interaction region and the surrounding gas should be considered non-perturbatively as a single system. It is also important that under the equilibrium the charge and spin densities are formed in the constriction and the surrounding electron gas. Therefore, following questions arise: what spin and charge textures are formed in the equilibrium, whether the system can be spontaneously magnetized and under what conditions a magnetic momentum arises in the interaction region, what effective potential landscape is ultimately formed.

In this paper we consider a minimal model that allows one to answer qualitatively these questions and to reveal non-trivial features of the spin-polarized state formation. The problem is solved within the self-consistent field approach by the way of minimizing the grand potential of the whole system. We come to an unexpected conclusion that the formation of a spin-polarized state strongly differs from Bloch or Stoner transition in homogeneous systems [7,8]. It turns out that a metastable state appears in the critical point in addition to the globally stable state, and only one of these states is polarized.

The outline of the paper is the following. In Section 2 we present the model and the approaches used in the calculations of the grand potential and the electron densities. Section 3 contains the analysis of a 1D model including the effect of an additional scatterer on the metastable state. In Section 4, a 2D system with the localized e–e interaction is considered. In Section 5 we discuss main results and possible applications. In Appendices we prove the existence of the branching in the critical point and analyze the stability of solutions.

2. The model

Consider 2D or 1D electron system in which the pair interaction potential $V_{ee}(\mathbf{r},\mathbf{r}=\mathbf{r}')$ is nonzero only in a finite region and vanishes outside it. Inhomogeneous interaction of this kind can actually be realized because of two reasons: (i) due to the screening of the Coulomb interaction by nearby conductors and (ii) as a result of the confinement of electrons by lateral gates in 2D systems. The latter is realized in quantum point contacts, where the e–e interaction is effectively the strongest in the most narrow part of the constriction which is effectively one-dimensional. The effective interaction potential is estimated as [9]

$$[V_{ee}(x,x')]_{nn'}=\frac{e^2}{\varepsilon}\iint dy\,dy'\frac{\chi_{n,x}(y)|^2|\chi_{n',x'}(y')|^2}{\sqrt{|\mathbf{r}-\mathbf{r}'|^2+d_z^2}}, \tag{1}$$

where $\chi_{n,x}(y)$ is the transverse wave function of n-th subband, d_z is the thickness of 2D layer, ε is the dielectric constant. The effective 1D pair interaction potential as a function of the longitudinal coordinates x and x' of interacting electrons is illustrated in Fig. 1.

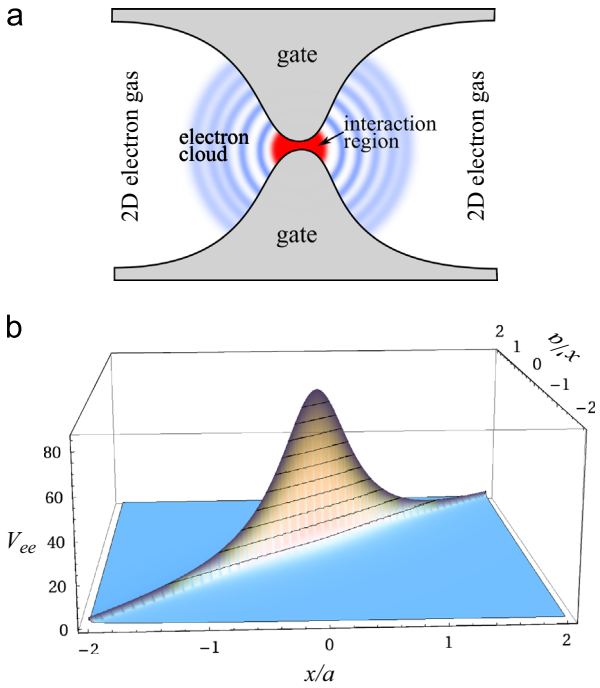

Fig. 1. (a) Schematics of quantum point contact. (b) The effective 1D interaction potential $V_{ee}(x,x')$ in the parabolic constriction $d(x)=d_0+x^2/a$, for $d_0/a=0.2$ and $n=n'=1$.

Since the inhomogeneous interaction is caused by nearby gates, we include for generality into the model also a single-particle potential $U(\mathbf{r})$ created in the interaction region by external charges, such as a background charge and charges on the gates.

The problem is to find the equilibrium densities of electrons with spin up and spin down in the interaction region and around it. To this end we will calculate the grand potential of the system and find the wave functions which minimize it. In this way there is a difficulty associated with taking into account the electron correlations which are strongest in the interaction region. The problem is simplified if one suppose that the size of the interaction region is small compared to the average distance between electrons. In this case we use the self-consistent field approximation without restrictions imposed by spin and spatial symmetry of the wave functions. Using this approximation for inhomogeneous systems has a decisive advantage since it is non-perturbative and goes far beyond the first-order expansion in the interaction [10]. Ultimately, this approach allows us to solve a highly nonlinear problem of self-consistent finding the wave functions with account of the charge and spin densities in the interaction region.

Our study is based on the analysis of the grand potential using the method developed by Memrin [11]. Calculations are carried out as follows. First, the self-consistent equations for the wave functions are obtained by minimizing the grand potential Ω over a restricted class of trial density matrices, which are chosen in the form of the equilibrium density matrix for non-interacting particles in an effective field. Stationary points of the grand potential yield self-consistent equations for the single-particle wave functions. Next, we show that these equations have several solutions and investigate their stability by analyzing the second variation of the grand potential. Finally, we compare the grand potentials of the stable solutions and study their dependence on the interaction strength and other parameters of the system.

The self-consistent equations for single-particle wave functions $\Psi_{\mathbf{k}s}(\mathbf{r})$ have form of the Hartree–Fock equations in which the electron density matrix contains the Fermi distribution function. In what follows we consider a simplified case of short-range e–e