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Superfluidity, superconductivity and magnetism in mesoscopics

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Contents

Abstract. The nature of superfluid, superconducting, and magnetic ordering is elucidated for mesoscopic systems in which the single-particle level spacing is much larger than both the temperature and the critical temperature of ordering. Ordering is defined as a spontaneous violation of symmetry, the gauge invariance and time reversal being by definition symmetries violated in superfluidity (superconductivity) and magnetism contexts, respectively. Superfluidity and superconductivity are realized in thermodynamic equilibrium states with a non-integral average number of particles and are accompanied by the spontaneous violation of time homogeneity. In Fermi systems two types of superfluidity and superconductivity are possible which are characterized by the presence of pair or single-particle 'condensates'. The latter is remarkable in that spontaneous violation of fundamental symmetries such as spatial 2π rotation and double time reversal takes place. Possible experiments on metallic nanoparticles and ultracold atomic gases in magnetic traps are discussed.

1. Introduction

Devoting this paper to the 90th anniversary of the great physicist Lev Davidovich Landau, it is pertinent to emphasize that superfluidity, superconductivity and magnetism are phenomena which determine, to a large extent, the face of modern physics and that it is precisely these phenomena which are most closely associated with his name.

Superfluidity, superconductivity and magnetism are typical macroscopic quantum effects caused by the availability of a relevant long-range order in a system. The most fundamental property of one or other type of order is, according to Landau [1], a change in the symmetry of a system or, to put it in modern terms, spontaneous symmetry breaking. The transition of a system from the normal state to a superfluid or superconducting one occurs with spontaneous symmetry breaking with respect to gauge transformations. Magnetic ordering is followed by spontaneous symmetry breaking with respect to the sign of time. The fact that just a change in the symmetry was a fundamental property of matter in an ordered state was clearly demonstrated by V L Ginzburg and L D Landau [2] who showed, long before the development of the Bardeen – Cooper – Schrieffer (BCS) theory, that all the main properties of superconductors could be deduced from reasoning of symmetry alone.

The main aim of this paper, which is a further development of the results of Refs [3, 4] is to bring out the rather peculiar nature of superfluidity, superconductivity and magnetism in mesoscopic systems where these phenomena manifest themselves in the simplest, primitive form. Of special interest is that spontaneous breaking can take place in such fundamental symmetries as homogeneity of time, spatial 2π rotations and double time reversal.

2. Main definitions

First, it is necessary to define a mesoscopic system. Restricting ourselves to thermodynamic equilibrium phenomena, we will use the following definition.

A mesoscopic system (as well as a macroscopic one) results from a finite system tending to the limit $N \to \infty$ (and $V \to \infty$) where N is the number of particles and V is the volume. However, at the same time, the temperature should decrease indefinitely, i.e. $T \to 0$, and the sensitivity of measurements should be indefinitely improved. The decrease in the temperature provides quantum coherence over an arbitrary large system. In combination with enhanced sensitivity of measurements this results in a property typical for a mesoscopic system, i.e. a change in the number of particles in a system by one, $\Delta N = 1$, yields a finite (measurable) effect despite the fact that $N \to \infty$. 'Improve-

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ment of the sensitivity of measurements' can arbitrarily be treated as a change in the scale for ΔN without changing the scale for N, so that as a result of a limit transition to a mesoscopic system one variable N changes into two essentially different variables ΔN and $N \to \infty$.

A mesoscopic system, as distinct from a finite one, shows phase transitions and, on the whole, some other peculiarities of thermodynamic quantities typical for a macroscopic system. However, the modified character of the limit transition leads to a qualitative difference in the behavior of macroscopic and mesoscopic systems.

As an example of feasible mesoscopic systems we refer to systems of a great number of neutral ultracold atoms in magnetic traps [5 – 7] and metal nanoparticles at ultralow temperatures [8 – 10].

There are two different limiting cases of a mesoscopic system. In the first case, the limit transition $N \to \infty$ takes place under the condition $T, T_c \gg \delta\varepsilon$, where T_c is the critical temperature of the transition to an ordered state, $\delta\varepsilon$ is the characteristic difference between the energies of two neighboring quantum levels of the system. The type of ordering is essentially the same as in a macroscopic system. According to Anderson's theorem [11], superconducting particles can be described within the BCS theory, as was done for the mesoscopic systems in Refs [8, 9]. The transition of Bose atoms in magnetic traps into a superfluid state can be treated as the appearance of the Bose condensate. (To produce it in experiments, the number of particles should be rather large $N > 10^3$ [5 – 7].) In this case, ordering, including magnetic, can generally be described as the occurrence of long-range order.

The other case, which is the subject of this paper, corresponds to the inverse inequality $T, T_c \ll \delta\varepsilon$. The systems to be studied can be called mesoscopic quantum dots, since despite their large dimensions, the degrees of freedom in them, associated with spatial motion of the particles, can be considered as completely frozen. Actually we will deal with metal particles of the type of those realized by D C Ralph et al. [10] or with atoms in magnetic traps at $N < 10^3$ [5 – 7].

The key problem is concerned with the criterion of ordering in mesoscopic quantum dots. Use was made of various definitions of superconductivity and superfluidity based on the effect of parity (the difference between the functions $E_o(N)$ and $E_e(N)$ obtained by analytical continuation of the energy of a system containing integral odd $E_o(N)$ and integral even $E_e(N)$ numbers of fermions N with respect to N, see, for example, Ref. [10]), a strong pairwise correlation of fermions, a large number of bosons in the same quantum state, etc. Criteria of this type are not unambiguous for mesoscopic quantum dots, since the properties indicated above are always inherent in a system whether it is in a superconducting, superfluid or normal state. In keeping with what was said in Introduction we will use a criterion based on the symmetry of a system. A mesoscopic system is, by definition, superfluid (when the constituent particles are neutral) or superconducting (when the particles are charged) if its state is not invariant with respect to the gauge transformations $\Psi \to \Psi \exp(i\phi)$, where Ψ are the particle operators and ϕ is a constant. The system is normal if its state is invariant with respect to gauge transformations. Similarly, a system is magnetically ordered if its symmetry breaks spontaneously with respect to time reversal.

Since a mesoscopic system does not reveal purely spatial symmetry, the symmetry of the Hamiltonian is only presented by gauge transformations and change in sign of time. Thus, superfluidity, superconductivity and magnetism are the only possible types of ordering in a mesoscopic system. We are leaving aside spin nematic type ordering [12] related to the approximate exchange symmetry [13].

A mesoscopic system, unlike a macroscopic one, does not show superfluid and superconducting properties such as persistent currents, the Meissner effect, and long-range order. However, according to our definition, a system in an ordered state is characterized by a certain phase non-invariant with respect to gauge transformations. Therefore, given a set of systems ordered in the way discussed above and linked by tunneling leads, persistent currents can arise in the whole system.

3. Superfluidity in Bose systems

Turning our attention to the elucidation of the origin of superfluidity and superconductivity in mesoscopic dots, i.e. the origin of spontaneous breaking of gauge transformations, assume for simplicity, that they are unique symmetry transformations and that time reversal is broken by exposure to rather a strong magnetic field. In this case the only degree of freedom, which, in general, is not frozen in the systems under consideration as $T \to 0$, is the total number of particles.

Suppose, $|N\rangle$ and $E(N)$ are, respectively, the ground state of the system with a certain (integer) number of particles N and the energy of this state. The set of states $|N\rangle$ for all N is a complete quantum mechanical set of states. They are all invariant with respect to gauge transformations, since the generator of the transformations is the operator $\hat{N}$ of the number of particles:

$$|N\rangle \to \exp(i\hat{N}\phi)|N\rangle = \exp(iN\phi)|N\rangle \propto |N\rangle \,. \quad (1)$$

Let us apply a unitary transformation $U = \exp\left[(i/\hbar)\mu\hat{N}t\right]$ and use a frame of reference 'rotating' at an angular rate $\mu/\hbar$, where μ is the chemical potential. We mean rotation not in the coordinate system, but in the space of the 'order parameter', where the parameter ϕ of gauge transformations plays the role of the rotation angle, so in the rotating system $\phi = (\mu/\hbar)t$. According to the fundamental principles of statistics, a uniform rotation does not break thermodynamic equilibrium and at $T = 0$ the system is in the ground state corresponding to the energy minimum $E'(N,\mu) = E(N) - \mu N$ in the rotating system at a given μ (the grand canonical distribution, see Ref. [14]). Under changes of μ, the minimum of E' will correspond to various integer N. Figure 1 shows the dependencies (straight lines) $E' = E'(N,\mu)$ at various N (Fig. 1a) and the dependence of the averaged equilibrium number of particles $\langle N\rangle = -\partial E'/\partial\mu$ on μ (Fig. 1b) corresponding to the solid line $E' = E'(\mu)$ in Fig. 1a. The straight lines corresponding to N and $N+1$ intersect at the point $\mu = \mu_c(N)$ resulting in $\langle N\rangle = N_c$ over the interval $\mu_c(N_c - 1) < \mu < \mu_c(N_c)$, where N_c is a certain large integer.

The curves in Fig. 1 demonstrate that the peculiarity of the thermodynamic behavior of mesoscopic quantum dots is the fact that any change in the averaged number of particles $\langle N\rangle$ under changes of their chemical potential results from peculiar phase transitions of the first type. The diagram (E',μ) in Fig. 1a depicts the points $A, B, \ldots$ of phase transitions between the phases $N = N_c - 1,\ N_c,\ N_c + 1, \ldots$. These points correspond to finite regions (vertical segments CD and EF) of 'phase coexistence' on the diagram $(\langle N\rangle,\mu)$ in Fig. 1b. In a mesoscopic system the 'phase coexistence' should

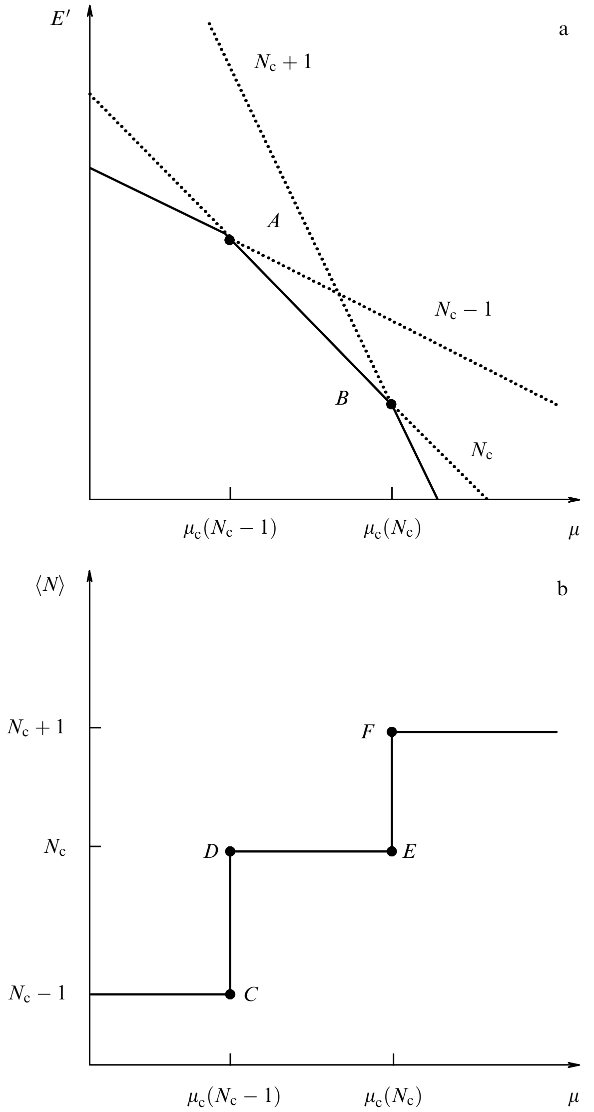

Figure 1. Dependencies of the energy (a) and the averaged number (b) of Bose particles on the chemical potential in the rotating reference frame.

be described by a certain wave function. The points on the curve EF correspond to the ground states $|\bar{N}\rangle$ with a non-integral averaged number of particles $\langle N\rangle = \bar{N}$ of the form

$$|\bar{N}\rangle = u|N_c\rangle + v\exp(i\varphi)|N_c+1\rangle\,, \qquad (2)$$

where $u>0$, $v>0$, $u^2+v^2=1$, and φ is the phase; the arbitrary common phase multiplier is chosen so that the coefficient at $|N_c\rangle$ is positive. The averaged number of particles $\langle N\rangle = \bar{N}$ in state (2) is equal to N_c+v^2.

The fact that the phase coexistence is described by a wave function, rather than, for example, a density matrix with zero non-diagonal elements is associated with the large dimensions ($N\to\infty$, $V\to\infty$) of mesoscopic systems. In any case we can say that the relative rate of the three limit transitions determining a mesoscopic system (see Section 2) should be chosen so that in the limit the phase coexistence takes place in a pure state. We will discuss this problem in Sections 5 and 6 and now make the following remark.

As μ changes in the vicinity of the critical point $\mu=\mu_c\equiv\mu_c(N_c)$ (Fig. 1a) there are two states having close $E'(\mu)$. One of them corresponds to the ground state (solid broken line)

$$E'_1(\mu) = \begin{cases} E'(N_c,\mu) & \text{for } \mu<\mu_c\,,\\ E'(N_c+1,\mu) & \text{for } \mu>\mu_c\,. \end{cases}$$

The other one (the dotted broken line) is

$$E'_2(\mu) = \begin{cases} E'(N_c+1,\mu) & \text{for } \mu<\mu_c\,,\\ E'(N_c,\mu) & \text{for } \mu>\mu_c\,. \end{cases}$$

At $\mu\neq\mu_c$ only the former state corresponds to thermodynamic equilibrium, since $E'_1(\mu)<E'_2(\mu)$. At the critical point the energies of both the states coincide, but there again only $E'_1(\mu)$ satisfies the thermodynamic inequality:

$$\frac{\partial\langle N\rangle}{\partial\mu} = -\frac{\partial^2 E'}{\partial\mu^2} > 0\,.$$

Thus, at $\mu=\mu_c$ there is only one stable state for mesoscopic systems, whose phase φ is not determined. This is state (2).

The gauge transformation $\exp(i\hat{N}\phi)$ transforms state (2) into a state of the same form, but with modified phase φ: $\varphi\to\varphi+\phi$. Therefore, according to our definition, states (2) are superfluid. Thus, there are two types of ground states of mesoscopic systems:

(1) normal ones of the form (1) characterized by a certain (integral) number of particles (horizontal segments in Fig. 1b);

(2) the superfluid ones of the form (2) with non-integral averaged numbers of particles (vertical segments in Fig. 1b).

Superfluid states are characterized by a nonzero average $\langle\Psi\rangle$ which can be considered as an order parameter describing the spontaneous breaking of the gauge invariance. In this sense mesoscopic superfluidity is similar to macroscopic. However, in a macroscopic system $\langle\Psi\rangle\neq 0$ means the presence of the one-particle Bose condensate, i.e. the availability of a c-number part in the Ψ-operator. The latter is related to the equivalence of states with the numbers of particles N and $N+1$, which holds for a macroscopic system, but not for a mesoscopic one.

The peculiarity of this case is in the fact that the degeneracy of the ground state typical for systems with spontaneously broken symmetry takes place in a rotating reference frame. State (2) is a linear superposition of the states $|N_c\rangle$ and $|N_c+1\rangle$ with the same energy in a rotating reference frame. In a laboratory reference frame state (2) is a superposition of two states with different energies. Thus, the superfluid ground states are not steady. But, as we have seen, they are in thermodynamic equilibrium. We arrive at an interesting conclusion that in a mesoscopic system superfluidity occurs with spontaneous breaking of time homogeneity. Since in states (2), two (not more) eigenvalues of energy mix, the superfluid states turn out to be periodic in time with period $2\pi\hbar/\Delta E = 2\pi\hbar/\mu_c$, where ΔE is the difference of the eigenvalues.

It might be well to point out an analogy with rotation in an ordinary coordinate system, where the rotation angle plays the role of ϕ, while N is the momentum M, and the angular rate $\hbar\omega$ corresponds to the chemical potential μ. Let us consider a mesoscopic body of irregular shape, which can rotate around a fixed axis. In thermodynamic equilibrium, at a given constant non-integral averaged value of $M/\hbar$ and $T\to 0$ the body will rotate at an angular rate ω_c determined by that the energies of the two ground states with the momenta $\left[\langle M\rangle/\hbar\right]$ and $\left[\langle M\rangle/\hbar\right]+1$ (where $[x]$ is the integer part of x) should be equal in the rotating reference frame. The equilibrium state is not steady, but periodic in time with period $2\pi/\omega_c$.

4. Superfluidity and superconductivity in Fermi systems

The above considerations, as applied to systems of Fermi particles, should be modified. In Fermi systems, the ground state energy $E(N)$ calculated with an accuracy appropriate for a mesoscopic system contains in an explicit form the number of particles in the combination $(-1)^N$. In order to deal only with quasicontinuous functions at large N, we should introduce two different functions $E_o(N)$ and $E_e(N)$ individually for odd and even values of the number of particles (the parity effect). The behavior of crossing of the energy levels in Fig. 1 is changed. Straight lines corresponding to odd N should be shifted upwards or downwards (depending on the character of the interaction) in parallel with respect to the straight lines with even N. As a result, the segments with even N on the solid line representing the ground state will increase with increasing shift, while those with odd N will decrease (or vice versa) until they disappear altogether.

Therefore, besides states (2) corresponding to the coexistence of $|N\rangle$ and $|N+1\rangle$ (if the parity effect is small), Fermi systems can also contain (at substantial parity effect) the states

$$|\bar{N}\rangle = u|N_c\rangle + v\exp(i\varphi)|N_c+2\rangle\,, \qquad (3)$$

describing the coexistence of states with neighboring numbers of particles of the same parity.

In state (3) spontaneous breaking of gauge invariance corresponds to the order parameter $\langle\Psi\Psi\rangle \neq 0$, while the transformation of the phase $\varphi \to \varphi + 2\phi$ corresponds to the pairwise 'condensate'. State (3) is what becomes of the superconducting BCS state when a macroscopic system changes into a mesoscopic one, though we do not mean coupled states of the type of Cooper pairs, and the integer N_c in formula (3) can, in principle, be either odd or even.

Superfluid states (2) in Fermi systems are remarkable not only for spontaneous breaking of gauge invariance and time homogeneity. First and foremost, the transformation of the phase $\varphi \to \varphi + \phi$ and the order parameter $\langle\Psi\rangle \neq 0$ correspond to the one-fermion 'condensate' (a one-electron superconductor!). But an even more striking property of such states is that invariances break spontaneously with respect to rotations through 2π around any axis in an ordinary coordinate system and with respect to double time inversion. Under either of the transformations the wave functions with an odd number of fermions change sign, while those with even number of fermions remain unchanged. In both the transformations the phase φ in formula (2) becomes $\varphi + \pi$ (so the invariance with respect to the product of these transformations holds).

5. Occurrence of superfluid and superconducting states

Let us consider a problem of actual occurrence of superfluid and superconducting states in quasi-closed systems of the type of the magnetic traps and metal nanoparticles discussed in Section 2. Systems of these two types differ in that in magnetic traps the number of particles is given, while nanoparticles are connected with macroscopic leads which are endless reservoirs of electrons, so the chemical potential is given there.

Let a mesoscopic quantum dot, i.e. a system of a large number of Bose or Fermi particles, be localized in a trap from which particles can tunnel into an outside state. Assume that in the absence of tunneling $E(N)$ is the ground state energy of the dot with N particles, and ε is the energy of the outside state. Suppose that at a certain integer $N = N_c$, the difference $E(N_c+1) - E(N_c)$ is close to ε, so that for a given integral number of particles $N_c + 1$, in the absence of tunneling the total system has two states with close energies. In one of them, all the $N_c + 1$ particles are localized in the mesoscopic dot. In the other, the number of particles in the mesoscopic dot is N_c and one particle resides in the outside state. Considering the number of particles N in a mesoscopic dot as a quantum number characterizing the total system, we can express the Hamiltonian of the total system (with due regard for tunneling) as

$$H = E(N_c) + \varepsilon + 2\xi|N_c+1\rangle\langle N_c+1| - \Delta|N_c+1\rangle\langle N_c| - \Delta^*|N_c\rangle\langle N_c+1|\,, \qquad (4)$$

where Δ is the complex tunneling amplitude, and $2\xi \equiv E(N_c+1) - E(N_c) - \varepsilon$ is a small value.

The ground state of the Hamiltonian (4) of the total system characterized by the averaged number of particles in the mesoscopic dot $\bar{N} = N_c + v^2$ is written as

$$|\bar{N}\rangle = u|N_c\rangle + v\,\frac{\Delta}{|\Delta|}\,|N_c+1\rangle\,, \qquad (5)$$

where

$$u^2 = \frac{1}{2}\left(1 + \frac{\xi}{\sqrt{|\Delta|^2+\xi^2}}\right), \qquad v^2 = \frac{1}{2}\left(1 - \frac{\xi}{\sqrt{|\Delta|^2+\xi^2}}\right). \qquad (6)$$

The ground state energy is equal to

$$E_g = E(N_c) + \varepsilon + \xi - \sqrt{|\Delta|^2+\xi^2}\,. \qquad (7)$$

As a part of the closed system in the state (5) the mesoscopic dot should be described by a density matrix (see Ref. [15], § 14). However in our conditions the density matrix corresponds to the pure state determined by formula (2) with $u = (N_c + 1 - \bar{N})^{1/2}$ and $v = (\bar{N} - N_c)^{1/2}$.

6. Superconducting phase transitions

Suppose, $\mu_c^{(1)}$ is a critical value of the electron chemical potential at which the mesoscopic dot of metal nanoparticle type transforms from the state $N = N_c$ to the state $N = N_c + 1$ and which corresponds to the superconducting states (2) with one-particle phase. We have $E(N_c+1) - E(N_c) = \mu_c^{(1)}$, where $E(N)$ is the ground state energy of the dot with N electrons. Let us introduce the energy $E' = E - \mu N$ in a reference frame 'rotating' at an angular rate $\mu/\hbar$, where μ is the chemical potential of the electrons in the leads (reservoir). As is customary [9], suppose that the mesoscopic dot resides in an external field induced by the gate, which leads to a shift of its chemical potential by $\mu_{ext} = \alpha V_G$, where α is a constant, and V_G is the gate potential [9]. As a result, we have

$$E'(N_c+1) - E'(N_c) = \mu_c^{(1)} + \mu_{ext} - \mu \equiv 2\xi\,. \qquad (8)$$

Let the gate potential be close to the value given by the condition $\xi = 0$. In this case there are two states, $|N_c\rangle$ and

$|N_c+1\rangle$, with close energies (in the rotating reference frame); the other states can be neglected. Ignoring the tunneling into the leads, the Hamiltonian of the dot H_0 is diagonal with respect to N. Choosing the reference point of the energy such that $E(N_c)=0$, we have

$$H_0 = 2\xi |N_c+1\rangle\langle N_c+1| \,. \tag{9}$$

A similar formula

$$H_0 = 2\xi |N_c+2\rangle\langle N_c+2| \tag{10}$$

can be written near the point $\mu_{ext}=\mu-\mu_c^{(2)}$ of the transition between the states of the same parity $|N_c\rangle$ and $|N_c+2\rangle$, corresponding to superconducting states (3) with the pairwise phase.

6.1 The ND_1N system

The interaction between the mesoscopic dot D_1 occurring near the transition $N_c\to N_c+1$ and the leads is described by the tunneling Hamiltonian

$$H_T = \int K(\mathbf{R},\mathbf{r})\Psi^+(\mathbf{R})\Psi(\mathbf{r})\,d^3R\,d^3r + \text{h.c.}\,, \tag{11}$$

where the integration with respect to $\mathbf{r}$ is performed over the quantum dot volume, the integration with respect to $\mathbf{R}$ — over the volume of the leads, and K is a core.

Let us consider a possibility for the occurrence of superconducting states (2) with the one-electron phase in the quantum dot D_1 in the ND_1N system where the leads are in the normal state. Due to the proximity effect the one-electron anomalous value $\langle\Psi(\mathbf{r})\rangle$ averaged over the dot volume leads to a nonzero average $\langle\Psi(\mathbf{R})\rangle$ in the lead region immediately adjacent to the dot. In the mean field approximation we replace the operator $\Psi^+(\mathbf{R})$ in Eqn (11) by its averaged value $\eta^*(\mathbf{R})=\langle\Psi^+(\mathbf{R})\rangle$:

$$\bar H_T = \int K(\mathbf{R},\mathbf{r})\eta^*(\mathbf{R})\Psi(\mathbf{r})\,d^3R\,d^3r + \text{h.c.} \tag{12}$$

Operator (12) has nonzero matrix elements

$$\Delta = -\langle N_c+1|\bar H_T|N_c\rangle\,, \qquad \Delta^* = -\langle N_c|\bar H_T|N_c+1\rangle \tag{13}$$

for transitions as N changes, where

$$\Delta = -\int K^*(\mathbf{R},\mathbf{r})\eta(\mathbf{R})\Phi^*(\mathbf{r})\,d^3R\,d^3r\,,$$

$$\Phi(\mathbf{r}) = \langle N_c|\Psi(\mathbf{r})|N_c+1\rangle\,. \tag{14}$$

The nonzero parameter Δ and its associated field $\eta(\mathbf{R})$ cause a change in the energy of the leads. Since in the equilibrium state of the leads not interacting with the mesoscopic dot the field $\eta(\mathbf{R})$ is zero, this change in the energy is positive and at small Δ can be written as $|\Delta|^2/2\xi_0$, where ξ_0 is a positive constant energy. Thus in view of Eqns (9) and (13), the total Hamiltonian of the system consisting of the dot D_1 and leads is equal to

$$H = \frac{1}{2\xi_0}|\Delta|^2 + 2\xi|N_c+1\rangle\langle N_c+1| - \Delta^*|N_c\rangle\langle N_c+1| - \Delta|N_c+1\rangle\langle N_c|\,. \tag{15}$$

The ground state $|g\rangle$ of the Hamiltonian (15) and the ground state energy E_g are

$$|g\rangle = u|N_c\rangle + v\,\frac{\Delta}{|\Delta|}\,|N_c+1\rangle\,, \tag{16}$$

$$E_g = \frac{1}{2\xi_0}|\Delta|^2 - \left(|\Delta|^2+\xi^2\right)^{1/2} + \xi\,, \tag{17}$$

where the amplitudes u and v are expressed in terms of ξ and Δ using relations (6). Requiring E_g to be minimum, the equilibrium value of $|\Delta|$ is found as the function of the gate potential:

$$|\Delta| = \begin{cases} (\xi_0^2-\xi^2)^{1/2} & \text{for} \quad |\xi|<\xi_0\,, \\ 0 & \text{for} \quad |\xi|>\xi_0\,. \end{cases} \tag{18}$$

At $|\xi|<\xi_0$ the phase of Δ remains indeterminate, and the ground state is degenerate with respect to its values. The equilibrium energy E_g and the averaged number of electrons $\langle N\rangle$ in the dot D_1 are

$$E_g = -\frac{(\xi_0-\xi)^2}{2\xi_0}\,, \qquad \langle N\rangle = N_c + \frac{\xi_0-\xi}{2\xi_0}\,. \tag{19}$$

At $\xi=\pm\xi_0$, the second order phase transitions from the normal states $|N_c\rangle$ and $|N_c+1\rangle$ into a superconducting state with the one-electron phase take place. Since the anomalous averaged value $\langle\Psi(\mathbf{r})\rangle$, which, according to Eqns (16) and (14) is equal to

$$\langle\Psi(\mathbf{r})\rangle = uv\,\frac{\Delta}{|\Delta|}\,\Phi(\mathbf{r}) = \frac{\Phi(\mathbf{r})}{2\xi_0}\,\Delta\,, \tag{20}$$

is proportional to Δ, this parameter can be treated as the order parameter of these transitions.

6.2 The ND_2N system

In ND_2N systems the conditions for the occurrence of superconducting states (3) with pairwise phase at mesoscopic dots D_2 in the vicinity of the transition $N_c\to N_c+2$ can be considered in a similar way using the Hamiltonian

$$H_T^{(2)} = \int K_2(\mathbf{R},\mathbf{R}';\mathbf{r},\mathbf{r}')\Psi^+(\mathbf{R})\Psi^+(\mathbf{R}') \times \Psi(\mathbf{r})\Psi(\mathbf{r}')\,d^3R\,d^3R'\,d^3r\,d^3r' + \text{h.c.}\,, \tag{21}$$

corresponding to the second approximation of the perturbation theory for the tunnel Hamiltonian. Introducing the mean field $F^*(\mathbf{R},\mathbf{R}')=\langle\Psi^+(\mathbf{R})\Psi^+(\mathbf{R}')\rangle$ instead of $\eta^*(\mathbf{R})$, we find the matrix elements of the total Hamiltonian, which are non-diagonal with respect to N, similar to Eqns (13):

$$\langle N_c|\bar H_T^{(2)}|N_c+2\rangle = -\Delta^* \equiv \int K_2(\mathbf{R},\mathbf{R}';\mathbf{r},\mathbf{r}')F^*(\mathbf{R},\mathbf{R}')\Phi(\mathbf{r},\mathbf{r}')\,d^3R\,d^3R'\,d^3r\,d^3r'\,, \tag{22}$$

where

$$\Phi(\mathbf{r},\mathbf{r}') = \langle N_c|\Psi(\mathbf{r})\Psi(\mathbf{r}')|N_c+2\rangle\,. \tag{23}$$

The total Hamiltonian

$$H = \frac{1}{2\xi_0}|\Delta|^2 + 2\xi|N_c+2\rangle\langle N_c+2| - \Delta^*|N_c\rangle\langle N_c+2| - \Delta|N_c+2\rangle\langle N_c| \tag{24}$$

differs from Eqn (15) only in that the term $|N_c + 1\rangle$ is replaced by $|N_c + 2\rangle$ and the phase of the parameter Δ is pairwise. With regard to this replacement all the formulae retain their form, except the expression for the averaged number of electrons at the dot, $\langle N\rangle = N_c + (\xi_0 - \xi)/\xi_0$.

6.3 The SD_2S system

Let us consider the superconducting states with pairwise phase at the dot D_2 when the leads are bulky superconductors. In this case the function $F(\mathbf{R}, \mathbf{R}')$ is nonzero due to the superconducting leads. The total Hamiltonian is determined by formula (24) with $\xi_0 \to \infty$, so that the second order phase transitions disappear at $\xi = \pm\xi_0$. Formally, superconducting states can occur at any ξ. In view of Eqn (22) the modulus of the parameter Δ is determined by the tunneling transparency, and the pairwise phase of the parameter Δ coincides with the phase of the order parameter in a bulky superconductor.

Let us consider a SD_2S system consisting of a mesoscopic dot D_2 between two bulky superconductors (we denote the left one L and the right one R). In this case $\Delta = \Delta_L + \Delta_R$, where $\Delta_{L,R} = |\Delta_{L,R}|\exp(i\varphi_{L,R})$, $|\Delta_{L,R}|$ are determined by the transparencies of the barriers separating respectively the left and the right superconductor and the dot; $\varphi_{L,R}$ are the respective phases of the left and the right superconductors.

The ground state energy E_g and the averaged number of electrons at D_2 are

$$E_g = -\left(|\Delta|^2 + \xi^2\right)^{1/2} + \xi\,,$$
$$\langle N\rangle = N_c + 1 - \frac{\xi}{\left(|\Delta|^2 + \xi^2\right)^{1/2}}\,, \tag{25}$$

and

$$|\Delta|^2 = |\Delta_L|^2 + |\Delta_R|^2 + 2|\Delta_L||\Delta_R|\cos\theta\,, \qquad \theta = \varphi_R - \varphi_L\,.$$

The superconducting Josephson's current flowing through the system is

$$J(\theta) = \frac{2e}{\hbar}\frac{\partial E_g}{\partial\theta} = \frac{2e}{\hbar}\frac{|\Delta_L||\Delta_R|\sin\theta}{\sqrt{\xi^2 + |\Delta_L|^2 + |\Delta_R|^2 + 2|\Delta_L||\Delta_R|\cos\theta}}\,. \tag{26}$$

Notice that this formula is coincident with the result of Ref. [15] obtained by K A Matveev et al. for the current in an *SSS* system, where the intermediate superconductor is described by the BCS theory under a considerable Coulomb blockade.

6.4 The SD_1S system

Finally, let us consider the most interesting case of the SD_1S system when the mesoscopic dot occurs in the vicinity of the transition $N_c \to N_c + 1$ corresponding to superconducting states with the one-electron phase.

The Hamiltonian of the system differs from Eqn (15) for normal leads by the first term. Expanding the energy of superconducting leads in powers of the small parameter Δ characterized by the one-electron phase φ, we should bear in mind that besides $|\Delta|^2$, there are some other terms which satisfy the condition of gauge invariance, i.e. the expressions $\exp(-i\varphi_{L,R})\Delta^2$ and their complex conjugates ($\varphi_{L,R}$ are, as above, the superconducting phases of leads). Such terms remove the degeneracy with respect to φ. For an appropriate choice of the origin of coordinates the φ-dependent part of the total energy can be written as

$$H_\varphi = -\frac{b}{4}|\Delta|^2\left[\cos(2\varphi - \varphi_L) + \cos(2\varphi - \varphi_R)\right]$$
$$= -\frac{b}{2}|\Delta|^2\cos(2\varphi - \bar\varphi)\cos\frac{\theta}{2}\,, \tag{27}$$

where b is a constant, $\bar\varphi = (\varphi_L + \varphi_R)/2$, $\theta = \varphi_R - \varphi_L$. For simplicity we assume the system to be geometrically symmetric with respect to the replacement $L \leftrightarrow R$.

The energy (27) does not change under the transformation $\varphi \to \varphi + \pi$ for a given $\varphi_{L,R}$, so the degeneracy with respect to φ is not completely removed, and a two-fold degeneracy having a simple physical meaning still remains. The superconducting states with the one-electron phase correspond to spontaneous breaking of the invariance with respect to spatial rotations through 2π and double time reversal. Under these transformations the state with the phase φ changes to the state with the phase $\varphi + \pi$, so the two-fold degeneracy is a direct consequence of the spontaneously broken symmetry.

Depending on the sign of the expression $b\cos(\theta/2)$, the minimum of the energy (27) is achieved for two different pairs of φ: $\bar\varphi/2$, $\bar\varphi/2 + \pi$ and $(\bar\varphi + \pi)/2$, $(\bar\varphi + \pi)/2 + \pi$. In both cases the minimum is equal to

$$H_\varphi = -\frac{1}{2}|\Delta|^2\left|b\cos\frac{\theta}{2}\right|\,. \tag{28}$$

The total Hamiltonian of the system is determined by Eqn (15) if we treat the parameter ξ_0 involved in Eqn (15) as a function of the phase difference θ:

$$\xi_0(\theta) = \left(a - \left|b\cos\frac{\theta}{2}\right|\right)^{-1}\,, \tag{29}$$

where a is a constant such that $a > |b|$. All the results of Eqns (16) – (20) hold true.

The derivative of the energy E_g with respect to θ given by the first formula from (19) determines the superconducting Josephson's current $J(\theta)$. The current $J(\theta)$ is periodic with respect to θ with period 2π and over the interval $-\pi < \theta < \pi$ is equal to

$$J(\theta) = \frac{2e}{\hbar}\frac{\partial E_g}{\partial\theta} = \frac{e|b|}{2\hbar}(\xi_0^2 - \xi^2)\sin\frac{\theta}{2}\,. \tag{30}$$

A characteristic feature of function (30) is that its analytical continuation from the interval $(-\pi, \pi)$ to the whole real axis of θ is a function with period not 2π, but 4π. The 2π value of the period is due to breaks in the current

$$\Delta J \equiv J(\pi) - J(-\pi) = \frac{e|b|}{\hbar}\left[\xi_0^2(\pi) - \xi^2\right] \tag{31}$$

at $\theta = \pi k$, $k = \pm1, \pm2, \ldots$ This peculiarity is a result of the unusual physical nature of $J(\theta)$, which is a superconducting current of Cooper pairs only in the regions far away from the dot D_1. In the regions adjacent to D_1, this current is transformed into one of single electrons and flows through D_1 as a superconducting current of single electrons.

7. Magnetism

Recall that starting with Section 3 we have assumed gauge transformations to be the only elements of symmetry of mesoscopic systems, which actually arise under the conditions of a strong external magnetic field. Suppose now that the external magnetic field is zero and the Hamiltonian of the system is invariant with respect to time reversal. Then all the states corresponding to an odd number of fermions are characterized by the Kramers degeneracy. In the simplest and most commonly encountered case, when the properties of the system are mainly determined by exchange interaction and relativistic interactions are negligible, the Kramers doublet corresponds to the two-dimensional presentation of the purely spin rotation group characterized by the total spin of the system, equal to 1/2. The mechanism of spontaneous breaking of time reversal (and spin rotations), or, according to our definition, the mechanism of magnetic ordering is absolutely similar to the superconducting ordering discussed in the previous section.

Let us consider the exchange Hamiltonian

$$H_{\rm T} = -\int J(\mathbf{R},\mathbf{r})\,\mathbf{s}(\mathbf{R})\mathbf{s}(\mathbf{r})\,\mathrm{d}^3R\,\mathrm{d}^3r \tag{32}$$

for the interaction between the mesoscopic dot and the leads. Here $\mathbf{s}(\mathbf{R}), \mathbf{s}(\mathbf{r})$ are the operators of the electron spin density of the leads and the dot, respectively, and $J(\mathbf{R},\mathbf{r})$ is a core. Due to the proximity effect the spin polarization $\langle\mathbf{s}(\mathbf{r})\rangle$ to be expected in the mesoscopic dot generates a nonzero average $\langle\mathbf{s}(\mathbf{R})\rangle$ in the region of the leads immediately adjacent to the dot. In the mean field approximation, we can replace the operator $\mathbf{s}(\mathbf{R})$ in Eqn (32) by its mean value $\langle\mathbf{s}(\mathbf{r})\rangle$:

$$\bar{H}_{\rm T} = -\int \mathbf{s}(\mathbf{r})\mathbf{b}(\mathbf{r})\,\mathrm{d}^3r\,, \tag{33}$$

where $\mathbf{b}(\mathbf{r}) = \int J(\mathbf{R},\mathbf{r})\langle\mathbf{s}(\mathbf{R})\rangle\,\mathrm{d}^3R$.

Let the indices $n, m = 1, 2$ number the states of the Kramers doublet corresponding to the projections of the total spin of the system equal to $\pm 1/2$. According to well-known selection rules [15] the spin density operator $\mathbf{s}(\mathbf{r})$ has the following matrix elements between the degenerate states:

$$\langle n|\,\mathbf{s}(\mathbf{r})|m\rangle = \boldsymbol{\sigma}_{nm}F(\mathbf{r})\,, \tag{34}$$

where $\boldsymbol{\sigma}_{nm}$ are the elements of the Pauli matrices

$$F(\mathbf{r}) = \frac{1}{6}\,\boldsymbol{\sigma}_{nm}\langle m|\,\mathbf{s}(\mathbf{r})|n\rangle\,. \tag{35}$$

The Hamiltonian (33) has the same matrix elements of transitions between degenerate states $n = 1, 2$ as the matrix operator

$$H_{\rm eff} = -\mu\boldsymbol{\sigma}\mathbf{B}_{\rm i}\,, \tag{36}$$

where μ is the Bohr magneton, and

$$\mathbf{B}_{\rm i} = \frac{1}{\mu}\int \mathbf{b}(\mathbf{r})F(\mathbf{r})\,\mathrm{d}^3r = \frac{1}{6\mu}\int J(\mathbf{R},\mathbf{r})\langle\mathbf{s}(\mathbf{R})\rangle\Big(\boldsymbol{\sigma}_{nm}\langle m|\,\mathbf{s}(\mathbf{r})|n\rangle\Big)\,\mathrm{d}^3R\,\mathrm{d}^3r$$

is an effective internal field acting on the spin of the system. Since the leads uncoupled with the mesoscopic dot are not magnetic, the polarization $\langle\mathbf{s}(\mathbf{R})\rangle$ and its associated field $\mathbf{B}_{\rm i}$ increase the energy of leads by a value which at small $\mathbf{B}_{\rm i}$ can be written as $(\mu/2B_0)\mathbf{B}_{\rm i}^2$, where B_0 is a positive constant. So the total effective Hamiltonian is

$$H_{\rm eff} = -\mu\boldsymbol{\sigma}\mathbf{B}_{\rm i} + \left(\frac{\mu}{2B_0}\right)\mathbf{B}_{\rm i}^2\,. \tag{37}$$

Expression (37) is absolutely similar to Eqn (15) at $\xi = 0$. The effective field $\mathbf{B}_{\rm i}$ plays the role of the parameter Δ; the parameter B_0 plays the role of ξ_0.

The ground state of Hamiltonian (37) is completely polarized (pure):

$$\langle\boldsymbol{\sigma}\rangle = \mathbf{n}\,, \tag{38}$$

where $\mathbf{n}$ is the unit vector directed along the effective field $\mathbf{B}_{\rm i}$. The ground state energy

$$E_{\rm g} = -\mu|\mathbf{B}_{\rm i}| + \frac{\mu}{2B_0}\,\mathbf{B}_{\rm i}^2 \tag{39}$$

is independent of $\mathbf{n}$. The minimum energy condition (39) yields $|\mathbf{B}_{\rm i}| = B_0$. The effective field direction $\mathbf{n}$ remains arbitrary. The equilibrium energy of the system is equal to $E_{\rm g} = -(\mu/2)B_0$.

The degeneracy of the ground states with respect to the directions of the effective field and spin polarization is removed under the conditions of relativistic interactions and an external magnetic field. If the external field $B \ll |\mathbf{B}_{\rm i}| = B_0$, the $\mathbf{n}$-dependent part of the energy can be written as

$$E_{\rm g} = -\mu\mathbf{n}\mathbf{B} + \frac{1}{2}\,a_{ik}n_in_k\,, \tag{40}$$

where the first term means the energy of magnetic moment $\mu\mathbf{n}$ in the external field $\mathbf{B}$ and the second term stands for the anisotropy relativistic energy depending on the anisotropy tensor a_{ik}. The anisotropy energy is determined with the accuracy of the additive constant. Let us choose it putting $a_{zz} = 0$, where the z-axis is aligned with the major axis of the symmetric tensor a_{ik}, corresponding to the smallest eigenvalue of a_{zz}. We also have $a_{z\alpha} = 0$, $\alpha = x, y$.

In the range of weak magnetic fields $\mu B \ll a$, the direction of $\mathbf{n}$ is close to $\mathbf{n}_0 = (0, 0, 1)$, corresponding to the minimum of the anisotropy energy. Considering the first term in Eqn (40) as a small correction, we find the correction to the vector $\mathbf{n}$ from the condition of the minimum of this expression, such that $n_\alpha = \mu\left(a^{-1}\right)_{\alpha\beta}B_\beta$, where a^{-1} is a matrix 2×2 inverse of a. The minimum energy will be

$$E_{\rm g} = -\mu\,\mathbf{n}\mathbf{B} - \frac{\mu^2}{2}\,(a^{-1})_{\alpha\beta}B_\alpha B_\beta\,. \tag{41}$$

Differentiating expression (41) with respect to the magnetic field, we find the equilibrium value of the total magnetic moment of the system:

$$\mathbf{M} = -\frac{\partial E_{\rm g}}{\partial\mathbf{B}} = \mu\,\mathbf{n}_0 + \mu^2(a^{-1})_{\alpha\beta}B_\beta\,. \tag{42}$$

In the range of strong magnetic fields $\mu B \gg a$ (but $B \ll B_0$), we may believe the directions of the vectors $\mathbf{n}$ and $\mathbf{B}$ in Eqn (40) to coincide, so that

$$E_{\rm g} = -\mu B + \frac{1}{2}\,a_{ik}h_ih_k\,, \tag{43}$$

where $\mathbf{h} = \mathbf{B}/|\mathbf{B}|$. The magnetic moment is equal to

$$\mathbf{M} = -\frac{\partial E_{\rm g}}{\partial\mathbf{B}} = \mu\mathbf{h} - \frac{a_{ik}h_k - h_ih_la_{lk}h_k}{B}\,. \tag{44}$$

In the range of fields $\mu B \sim a$, which are small relative to the exchange field B_0, the magnetic moment varies from $\mu\,\mathbf{n}_0$ to $\mu\,\mathbf{h}$.

Thus, the normal states $|N\rangle$ of mesoscopic dots with an odd number of fermions N are (ferro)magnetic. Therefore, following the reasoning of Section 4, we conclude that the states of the Fermi systems (2) at any N_c are magnetic and superconducting (superfluid) for a time. States (3) possess this property at odd N_c.

8. Experiments

Let us discuss possible experiments which could provide support for the above suggested treatment.

For systems of neutral atoms in magnetic traps it would be interesting to observe phenomena associated with spontaneous breaking of time homogeneity, i.e. with nonstationary nature of the ground state of the system. Suppose $\varepsilon(N)$ is the energy of excitation of the system for a given integral number of particles N. These quantities can be measured in spectroscopic experiments, for example, on inelastic light scattering. Transitions from superfluid states (2) or (3) give rise to doublets of closely spaced lines in the scattered light spectrum, which correspond to pairs of excitation energies $\varepsilon(N_c)$, $\varepsilon(N_c+1)$ or, respectively, $\varepsilon(N_c)$, $\varepsilon(N_c+2)$. In fact, the presence of doublets and the associated beating of the scattered light amplitude is a direct result of the nonstationary nature of the ground state. To observe the doublets one should cool the system after each scattering event in such a way that the change of the number of particles in the system is negligible (if dealing with 'evaporation' type cooling). It is required that the change in $\bar{N}$ during cooling compensating one scattering event, be much less than one.

The most interesting property of superfluid Fermi systems (2) which can be followed experimentally, is that they change their state upon rotation through 2π around any axis in an ordinary coordinate system. To observe such a change in systems with spontaneously broken symmetry, one should have at least two similar systems. Schematically, the experiment is as follows. Suppose two identical magnetic traps are connected for a long time by a weak link (a Josephson's junction). In this case the systems have the same phase φ. Then the traps are disconnected and one of them slowly rotates around a certain axis. After the rotation the link is set up anew. Since the phase of the rotated trap has changed by π, while that of the immobile one remained the same, the phases should be equalized by relaxation, which can be registered. A similar process should take place upon rotation through $2\pi n$ with odd n, but it should not be observed upon rotation through an angle multiple of 4π.

This experiment resembles in many ways† a remarkable experiment [17] on the interference of two neutron beams, one of which passes through a region with nonzero magnetic field with the resulting turning of the spins of neutrons through 2π. This experiment straightforwardly demonstrates that the phase of a neutron wave function changes by π as the spin turns through 2π. However, there is a point to be made. According to conventional quantum mechanics, any state of any system does not physically change as the system turns through 2π. The experiment with neutron beams is consistent with this statement. The change in the phase of the wave function is not a physical change of state. In our case the state of the superfluid system of type (2) physically changes upon rotation through 2π, so a positive result for the suggested experiment may signify that the traditional views on the physical properties of space and time should be revised. An alternative standpoint implying the introduction of superselection rules [18] to forbid linear combinations of states with odd and even numbers of fermions does not seem adequate, in view of what was said in Sections 5 and 6.

The one-electron character of the phase of superconducting states of mesoscopic dots D_1 should be observed experimentally as a peculiar dependence of the Josephson's current on the phase difference of superconductors described by Eqns (30) and (31). Evidence of breaks in the current would provide support for the conclusion that linear combinations of states with even and odd numbers of fermions could take place. In this connection, it is interesting, however, to note that such a dependence of the Josephson's current on the phase difference was predicted [19, 20] for point leads in ordinary superconductors.

Finally, a specific ferromagnetism for mesoscopic dots with odd numbers of fermions considered in Section 7 would be confirmed experimentally if we could observe a typical nonlinear behavior of the magnetic moment of the system at weak magnetic fields, of the order of anisotropy field. As the field changes, the direction of the magnetic moment substantially changes, with no virtual change in the absolute value of the magnetic moment.

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