Leggett's conjecture for a mesoscopic ring

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We show that the generic feature of topological defects in a ring, which acts as an energy-dependent one-body potential, is that they can produce a discontinuous phase change of the electron wave function and then Leggett's conjecture breaks down. [S0163-1829(96)03423-6]

A normal metal ring pierced by a magnetic field carries a persistent current.[1] Persistent current has been observed experimentally[2] but some aspects of it are still not fully explained.[3] The ring shows a strong parity effect in the sense that for spinless electrons, a clean one-dimensional ring with an odd number of electrons has a diamagnetic response and a ring with an even number of electrons has a paramagnetic response.[4] It was conjectured by Leggett that this fact follows just from the symmetry property of the wave function (the electrons being fermions, the wave function must be antisymmetric) and is independent of electron-electron interaction as well as defect scatterings.[5] See Ref. 6 for a discussion of earlier works.

In the multichannel situation[7] parity exists. In a multichannel ring, the slope of the states changes within an energy scale Ec, the Thouless energy of the system. In open systems,[8] we can define the parity effect with the phase of the persistent current or with the phase of the conductance.[9] However, the parity of the phase of the conductance in such open systems is related to the parity of the eigenenergies of closed systems.[9]

It has been shown[6] that in a loop of length u, to which a single stub of length v is attached (Fig. 1), the parity effect is completely destroyed when $v/u>1$ and the slopes of the states change after each v/u state (on the average and not exactly). However, Ref. 6 studies the effect of a single stub and says that for $v/u<1$ the parity effect is not violated in the ring. In this paper we show that topological defects of the type $v/u<1$ can also violate the parity effect under some special situations and in general the parity effect is destroyed if we have many such geometric scatterers. In Ref. 6 it has also been argued that the length of the stub provides an additional energy scale that creates some additional states. But why these additional states do not obey the parity effect was left as an open question. In this paper we try to analyze the physical reasons behind the breakdown of the parity effect.

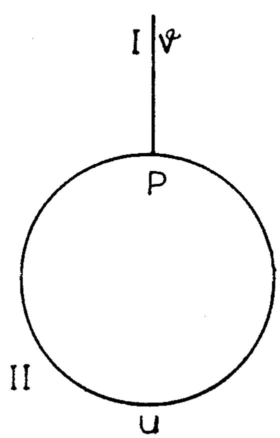

FIG. 1. A stub of length v attached to a ring of length u.

If there are some sharp variations in thickness then some resonant cavities may be formed at certain places in the ring. Resonant cavities can be taken as stubs[10] and the width of the resonant cavities only lowers the energy.[11] Recently the parity effect of such geometries has gained a lot of importance because of a recent experiment[12] and subsequent theories.[9] The relevant situation in that experiment was $v/u<1$.

If k is the allowed wave vector and $\alpha=2\pi\phi/\phi_0$ is the Aharonov-Bohm phase, ϕ being the flux through the ring and ϕ_0 the flux quantum then, following Ref. 6,

$$\cos(\alpha)=\mathrm{Re}[1/T(k)], \tag{1}$$

where $T(k)$ is the transmission amplitude across the ring when the ring is cut open. For a clean ring the bound state condition is $e^{i(ku-\alpha)}=1$. Whereas Eq. (1) is just the condition

$$e^{i\{\cos^{-1}[\mathrm{Re}(1/T)]-\alpha\}}=1. \tag{2}$$

This simple analogy has far reaching consequences.[13] $\cos^{-1}(\mathrm{Re}1/T)$ is the Bloch phase Ku (where K is the Bloch momentum) acquired by the electron in traversing a unit cell of an infinite periodic system where T is the transmission amplitude across a unit cell of the periodic system.[6] Hence Eq. (2) is just $e^{i(Ku-\alpha)}=1$. This suggests that inside the ring the electron moves clockwise or anticlockwise with momentum K and not with the free particle momentum k. One of them is a diamagnetic (anticlockwise moving) state and the other is a paramagnetic (clockwise moving) state. Without a magnetic field $\alpha=0$. If the magnetic field is increased continuously then α also increases continuously to give rise to an E versus α dispersion.[1] Hence α is called a pseudo Bloch momentum. Initially as the magnetic field is increased the two states move away from each other. However, the diamagnetic and paramagnetic states are not degenerate for any value of α for reasons explained later. Equation (2) is due to the single valuedness of the wave function. Hence if the Bloch phase of an electron, in traversing a unit cell of an infinite periodic system, Ku equals α, then the single val-

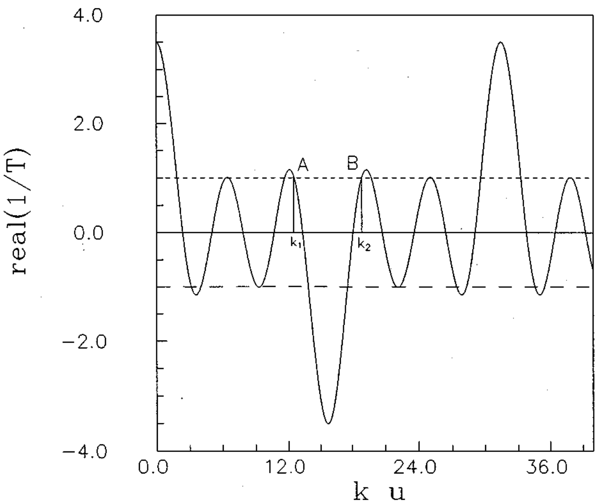

FIG. 2. Graphical solutions for the allowed modes for $v/u=0.2$.

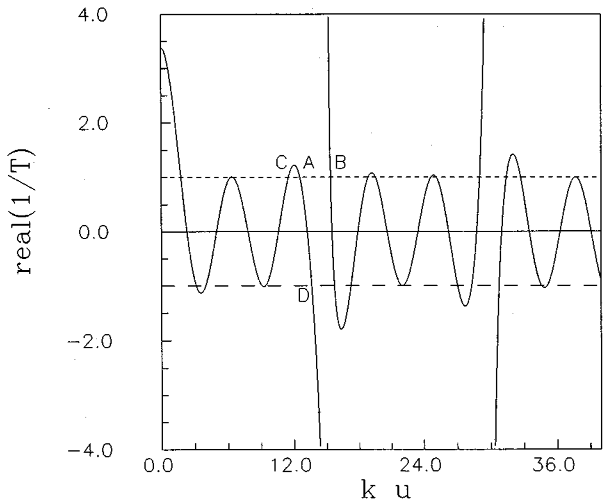

FIG. 3. Graphical solutions for the allowed modes for $v/u=0.21$.

uedness of the wave function is obtained in the ring made of the unit cell and we get a bound state. So the bound states can be determined by graphically solving $\mathrm{Re}(1/T)=\cos(\alpha)$. This equation is satisfied at certain k values and then k^2 is the energy of the electron in that particular state K. This is in analogy with a scattering problem where k is the momentum outside the potential where it vanishes, and K is the momentum inside the potential. K can be quite different from k. However, the energy throughout the space under consideration is k^2 (we have set $\hbar=1$ and $2m=1$).

In Fig. 2 we show a simple plot of $y=\mathrm{Re}(1/T)$ (solid curve) with ku for $v/u=0.2$. Wherever this curve intersects the straight line $y=\cos(\alpha)$, the corresponding k gives a bound state of the system. Let us start with $\alpha=0$, and the $y=\cos(0)$ curve is shown in Fig. 2 by the dotted line. Two consecutive points where the curve $y=\mathrm{Re}(1/T)$ intersects the straight line $y=\cos(0)$ are denoted by A and B in the figure. The corresponding k values are denoted by k_1 and k_2 in the figure. If α is increased gradually then the straight curve $y=\cos(\alpha)$ shifts gradually downwards towards the dashed curve. As the curve $y=\cos(\alpha)$ goes gradually downwards, with α, the allowed wave vectors k_1 and k_2 slowly drift rightwards and leftwards, respectively, along the k axis. Since k_1 drifts towards higher energy with α, k_1 is a diamagnetic state. Similarly, k_2 is a paramagnetic state. That k_1, k_2, etc. gradually increase or decrease with α gives rise to a dispersion with α (E versus α) with close by consecutive states going further away from each other with α up to $\alpha=\pi$. $y=\cos(\pi)$ is also shown in Fig. 2 with dashed lines. If we increase α further then the straight curve $y=\cos(\alpha)$ starts moving upwards and comes back to its original position at $\alpha=2\pi$. This ensures the ϕ_0 periodicity of the dispersion curves. Since $\cos(\alpha)$ can vary from -1 to $+1$ (dotted lines to dashed lines) the dispersion curve for any two consecutive states can never cross (see Fig. 2). So the dispersion curve is exactly similar to that of a ring with a random potential (see Fig. 6 in Ref. 4). In our case the rotational symmetry is destroyed by the topological defect (i.e., the stub) and so levels do not cross. Hence from Fig. 2 it is evident that consecutive states carry persistent currents with opposite signs and have opposite magnetic properties up to infinite energy. So the parity effect is maintained.

But this effect is not observed when we plot the same curves for different values of $v/u=0.21$ (Fig. 3) (in fact $v/u=0.2\pm\epsilon$ is sufficient to destroy the effect where ϵ is an infinitesimal quantity). Consider the intersections between the graphs $y=\mathrm{Re}(1/T)$ and $y=\cos(0)$. The first few consecutive states have opposite magnetic properties but the fifth and the sixth states (two consecutive states marked A and B) are both diamagnetic, disobeying the parity effect. This can be seen by slowly increasing α from zero to see that the straight line $y=\cos(\alpha)$, i.e., the dotted line in Fig. 3, shifts downwards and hence the intersections A and B both shift rightwards, i.e., towards higher energy. This means both the consecutive states at A and B are diamagnetic, violating the parity effect. The parity effect is again violated for the 11th and the 12th states, both of which are paramagnetic. After a spacing of five levels we always find two consecutive levels that violate the parity effect. We shall soon see why it does not happen for specific values of v/u. It should be noted that the parity-violating states like A carry an amount of persistent current that is comparable to that of neighboring states like C. Also note that for $kv=n\pi$, the transmission across a stub is zero[14] due to the formation of a node at the junction between the ring and the stub. This mode always lies deep inside a gap of the dispersion curve and is never an allowed mode.

A special feature of the δ function potential is that $|T|^2=\mathrm{Re}(T)$. This feature is also observed in the case of a stub. This makes it possible to map a single stub onto an effective δ function potential $V(x)=k\cot(kv)\delta(x)$. So the strength of the δ potentials depends on the Fermi energy and hence it is a special type of one-body potential. Now let us start with $k=0$ and then slowly and continuously increase k. For $k=0$, $V(x)=(1/v)\delta(x)$, which means it starts with a small positive value. Then it decreases and soon goes to zero. After this the strength of the potential increases monotonously on the negative side and finally becomes $-\infty$ at $kv=\pi$. After this $V(x)$ undergoes a discontinuous jump from $-\infty$ to $+\infty$. If the strengths of the δ potential at

$kv=\pi$ and $kv=\pi+\epsilon$ are discontinuous the scattering phase shifts and hence the Bloch phase (which is the phase of the electron wave function in the ring) will also undergo a discontinuous jump. Re$(1/T)$ also make a discontinuous jump from $-\infty$ to ∞ and hence the Bloch phase jumps by π (see Fig. 3) [the Bloch phase of the infinite periodic system has to be defined modulo 2π i.e., $-1<\text{Re}(1/T)<1$]. The next allowed Bloch phase of the infinite periodic system of stubs after that at D is that at B and they differ by π. This is markedly different from the next allowed Bloch phase at any other gap; e.g., the Bloch phase at C is the same as that at A. From Eq. (1) we see that if the Bloch phase of the periodic system of stubs equals the AB phase α (for the time being we have taken $\alpha=0$) then the single valuedness of the wave function gets satisfied in the ring and we get a bound state. This additional phase due to a discontinuous phase jump results in satisfying this condition and creates a state at B around the value $kv=\pi$, which otherwise would be absent (that is, if the phase change across $kv=\pi$ were continuous). If it so happens that this singularity in the Bloch phase (or phase of the electron wave function in the ring), due to a singularity in the effective one-body potential $V(x)$, is canceled by another singularity, then the phase difference between two consecutive Bloch phases would not be different by π and this state at B would not exist. This is because the total phase acquired in this state at B would not be enough to satisfy the single-valuedness condition in the ring. All other states, however, would remain qualitatively the same as that of a ring with a random potential. This is what happens in the case of Fig. 2. For $v/u=0.2$ at $kv=n\pi$, $\cot(kv)=\pm\infty$ but $\sin(ku)=0$. And so there is no discontinuity in Re$(1/T)$. Hence the state at B of Fig. 3 will not exist. It is easy to see from Fig. 3 that the slope of Re$(1/T)$ is such that if it jumps from $-\infty$ to $+\infty$ then the broken-parity state is diamagnetic whereas it is paramagnetic for the other case. Specific values of the parameter v/u at which these two singularities exactly cancel are negligibly few compared to the values where they do not and is hardly a likely real situation. Some other values of v/u where these two singularities exactly cancel are 0.05, 0.1, and 0.25.

Having understood that Re$(1/T)$ is the relevant parameter that determines the parity-violating states it is easy to understand the absence of the parity effect for $v/u \gg 1$. The strength of the effective potential being $k\cot(kv)$, it is the length scale v that determines how many times Re$(1/T)$ will undergo discontinuous jumps from $-\infty$ to ∞ in a certain energy interval. Each such jump will create a parity-violating diamagnetic state. Thus there can be v/u consecutive diamagnetic states in the energy interval of two states determined by the length scale u. The discontinuous jumps in Re$(1/T)$ are separated by $\delta k_1=1/v$ and the zeros that can cancel the discontinuous jumps are separated by $\delta k_2=1/u$. Now for $v/u>1$, $\delta k_2>\delta k_1$ and all the discontinuous jumps can never be canceled. Hence for $v/u>1$ the parity effect is invariably broken and there can be no special situation as in the case of $v/u<1$.

The effect of the topology of the system in Fig. 1 can, therefore, be incorporated into the Hamiltonian by mapping the stub into a one-body potential whose strength depends on the energy of the particle. Now we discuss why the parity effect breaks down for this system in spite of the fact that we have Fermions in a single-channel ring. The general Hamiltonian for the electrons in the system is[5]

$$H(\theta_1,\theta_2,\ldots,\theta_n)=\Sigma_i V(k,v,\theta_i)+\Sigma_{i,j}U(\theta_i-\theta_j)+\Sigma_i[p_i-eA(\theta_i)]^2\frac{1}{2m}. \tag{3}$$

V and U are obviously periodic in θ_i with a periodicity of 2π. Leggett has shown that such a two-body potential U does not change the parity effect of the free-electron system and so we can drop the interaction part and go back to the free-electron description. This is because of Leggett's argument that the two-particle potential energies depend only on $|\psi_N|^2$. It does not matter whether ψ_N obeys a periodic or a twisted periodic boundary condition. That is still true in our case. Here ψ_N is the N-body wave function. Hence the single-particle version of Leggett's arguments goes as follows. The magnetic field tunes the kinetic energy (KE) term in (3) and if the difference in phase acquired by the electrons in two consecutive states depends on their KE difference alone then the current carried by them will be of opposite signs. But in our case the phases acquired by an electron in the fifth and sixth states of Fig. 3 are not determined by the KE alone but also due to the fact that the sixth electron encounters a repulsive δ potential whereas the fifth electron encounters an attractive δ potential that results in an extra phase difference of π between these two states. Hence the argument that the one-body potential also depends on $|\psi_N|^2$ breaks down because the strength of the potential can itself change drastically because of the energy dependence of the strength. Alternately (i.e., if we do not include the information of the topology in the Hamiltonian), it may mean that a topological defect makes it possible to have other types of symmetry-dictated nodal planes energetically more favorable than the symmetry-dictated nodal planes that directly act across the cross section of the ring, thereby leading to the violation of the parity effect. But this approach involves a very nontrivial exercise as commented by Leggett.[5] This simple model tells us that Leggett's conjecture, which is strictly valid for potential scattering, is not strictly valid for scattering by a sharp boundary roughness that can be modeled as a stub. In fact, any type of boundary roughness as well as bends can be mapped into a one-body potential whose strengths depend on the energy of the electron in a complicated way.[15] Our simple model suggests that such energy-dependent potentials may destroy the parity effect. Although for every broken-parity state of one type there is a broken-parity state of the opposite type, these broken-parity states of opposite types are separated by $1/v$. For $v\ll 1$ this separation is so large that it is quite possible that the broken-parity states of only one type are populated.

We then study the spectrum of a ring with four small topological defects or stubs present in it. To find the spectrum we have to solve Eq. (1) numerically using the transfer matrix mechanism to compute T.[16] A portion of the E versus ϕ/ϕ_0 plot is shown in Fig. 4 (solid lines) in one-half of the first Brillouin zone. The dashed horizontal lines are to guide the eye. Within a certain energy range $(3400>Eu^2>150)$ there are many more diamagnetic levels than paramagnetic. Below this range consecutive states have opposite slopes. For higher energy there are, however, more paramagnetic

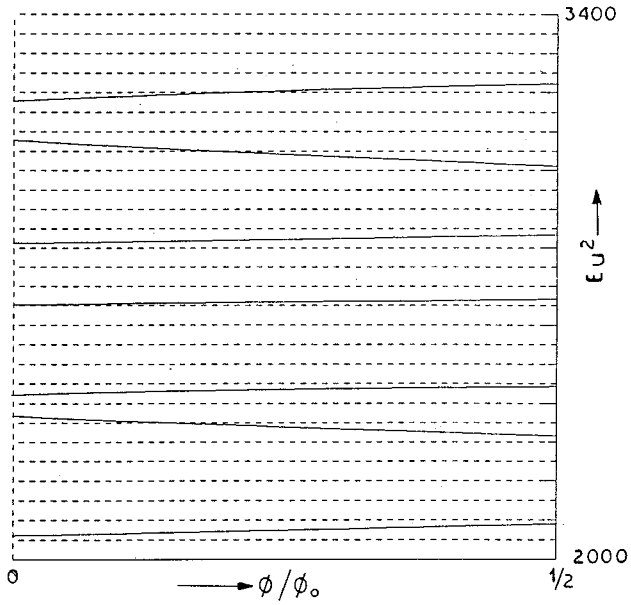

FIG. 4. E vs ϕ dispersion curves in the range $2000<Eu^2<3400$ for a ring with four stubs.

levels than diamagnetic levels. We have plotted for only one configuration i.e., ($v_i/u=0.16,0.21,0.12,0.252$) and ($v_i/u=0.1,0.2,0.3,0.4$) when v_i denotes stub length and u_i denotes separation between stubs. It should be noted that sometimes states over an energy scale that is an order of magnitude larger than the Thouless energy have the same slope. In a multichannel ring there are many subbands and very close by levels. States belonging to a particular subband exhibit the parity effect.[5] Topological defects will destroy the parity effect of each subband with the first one being diamagnetic for each. Even one appropriate topological defect, in that case, can give many broken-parity states of one kind.

It is to be noted that Eq. (1) has been derived[6] from the first principles of quantum mechanics, i.e., Griffith's boundary conditions. The junction is taken to be defect free and in such a situation the Griffith's boundary conditions describe strong coupling of the stub and the loop. As a result the eigenenergies as seen in Fig. 4 are all very smooth functions of magnetic field and nearby states carry a persistent current of the same order of magnitude. As in a single-channel ring $E_n(\phi/\phi_0=0.5)<E_{n+1}(\phi/\phi_0=0)$. There is no trace of crossing between levels in the first Brillouin zone. Only the slopes of the states, unlike that of a single channel ring, violate the parity effect. The system of stubs attached to a ring was first studied by Büttiker[17] as a model to understand the effect of interactions.

We conclude by saying that boundary roughness that can be mapped into energy-dependent one-body potentials can lead to a violation of Leggett's conjecture.

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