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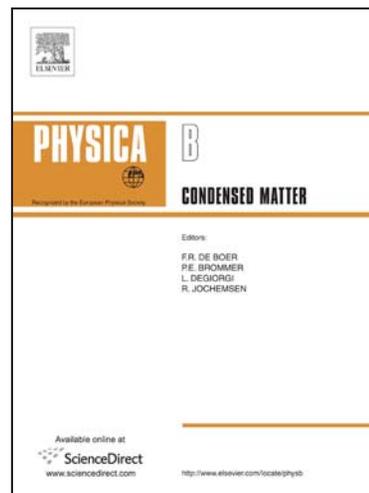
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Thin Spectrum States in Bulk Superconductors and Superconducting Grains

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Abstract

We show how a local pairing model for superconductivity can be used to describe the symmetry breaking mechanism in exact analogy to the case of quantum crystal and antiferromagnets. We find that there are low energy states associated with the symmetry breaking process which are not influenced by the Anderson-Higgs mechanism. The presence of these 'thin spectrum' states in qubits based on superconducting material leads to a maximum time for which such qubits can remain quantum coherent. We also show how the charging energy of superconducting quantum dots may give the thin spectrum states a finite energy gap, impeding the spontaneous breaking of phase symmetry.

Key words:

PACS:

0.1 Introduction

The question whether the superconducting state has a well-defined order parameter lead to a lot of debate over the decades following the discovery of superconductivity. The problem is that it was proved more than thirty years ago by Elitzur that local (gauge) symmetries cannot be spontaneously broken [1]. The (electromagnetic) gauge symmetry of superconducting systems thus forces the expectation values of non gauge invariant operators such as $\langle \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}) \rangle$ or $\langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}') \rangle$ to always remain identically zero [2]. Because of the impossibility to define a local order parameter it has even been suggested that the ordering in superconductors may be topological in nature [3]. However, if one drops the requirement of a *local* orderparameter, and instead looks

at the *global* properties of an isolated piece of superconductor, it turns out to be possible to define symmetry breaking and thus ordering in a way that is exactly analogous to the description of the global properties of for example (quantum) crystals and antiferromagnets.

The resulting measure of order is the same in the case of superconductivity as it is in the cases of crystals or antiferromagnets: a global operator (centre of mass position, sublattice magnetization or total phase) acquires a macroscopic expectation value. Using the Josephson effect, the total phase of an isolated piece of superconductor can be measured relative to that of another piece, just as the position of a crystal can be measured relative to that of the observer. Of course the presence of gauge invariance in superconductors does lead to some unusual effects. Most notably, the superconductor does not have any Goldstone modes, because the gauge invariance enables the Anderson-Higgs mechanism to render those modes massive [4–6]. The defining feature of the symmetry breaking process however, which allows for the occurrence of a global order parameter in crystals and antiferromagnets as well as in superconductors, remains unaffected by the gauge symmetry: all of these systems have a so called *thin spectrum* of low energy states which collapses onto the ground state in the thermodynamic limit and allows a state that is not normally an eigenstate of the Hamiltonian to become stable in that limit [7,8].

In this paper we will develop a description of the superconducting symmetry broken state that naturally brings to the fore the role of the thin spectrum. Using the model description we can then understand such processes as the Anderson-Higgs mechanism and the Josephson effect in terms of the influence of these (in-gap) low energy states. Furthermore, it turns out that the unavoidable presence of thin spectrum states has a direct implication for qubits made of superconducting material: the coherence time of such qubits is fundamentally limited by the properties of the thin spectrum. Finally, we can study the fate of the thin states as a piece of superconducting material crosses over from being a Cooper pair box qubit into the regime of the superconducting quantum dot.

Below we start by explicitly constructing the symmetry broken state of a strong coupling superconductor, a system in which electrons form local pairs. The advantage of the local pairing Hamiltonian is that it provides a manifestly gauge invariant description of a superconductor. It also allows us to solve the resulting symmetry broken Hamiltonian exactly by mapping it onto a modified Lieb-Mattis model. The fact that we consider this particular strong coupling model for a superconductor does not affect the generality of our results on spontaneous symmetry breaking and the associated thin spectrum. The reason is that there is no phase transition between strong and weak coupling superconductivity so that these systems are identical from the point of view of symmetry. Or, in more specific terms: the thin spectrum emerges from a *global*

symmetry breaking and is therefore independent of the microscopic form and range of *local* interactions between electrons.

0.2 Local Pairing Superconductor

We start out with the negative U Hubbard Hamiltonian in presence of an electromagnetic vector potential. This Hubbard Hamiltonian has been studied extensively [9] and it is well known to have a superconducting groundstate. On a hypercubic lattice it reads

$$H = t \sum_{j,\delta,\sigma} \left(e^{i\psi_j^\delta} c_{j+\delta,\sigma}^\dagger c_{j,\sigma} + h.c. \right) - |U| \sum_j n_{j,\uparrow} n_{j,\downarrow} - \mu \sum_{j,\sigma} n_{j,\sigma} + H_{EM}, \quad (1)$$

where c_j^\dagger creates an electron on site j , δ connects neighboring sites and n_j counts the number of electrons. The amplitude of the hopping integral is t , $-|U|$ is the strength of the local attraction between electrons and μ is the chemical potential, which in general breaks particle-hole symmetry. The coupling of the charges to the vector potential comes about via the Peierls construction: while hopping from j to $j + \delta$ an electron picks up a phase ψ_j^δ that is proportional to the electromagnetic vector potential integrated along the bond: $\psi_j^\delta = \frac{e}{\hbar c} \int_j^{j+\delta} A^\delta(l) dl$. A gauge transformation amounts to simultaneously sending $\mathbf{A} \rightarrow \mathbf{A} + \nabla \Lambda$ (equivalently: $\psi_j^\delta \rightarrow \psi_j^\delta + \Lambda_{j+\delta} - \Lambda_j$) and $c_j \rightarrow e^{i\Lambda_j} c_j$. We explicitly include the free electro-magnetic field by the last term in the Hamiltonian. In the next stage of the calculation this term is needed to generate a mass for the Goldstone bosons. The Hamiltonian above is manifestly gauge invariant, in contrast to for instance a BCS mean-field approach in which such invariance is lost.

In the strong coupling limit, where $U \gg t$, the electrons form strongly bound pairs and for the low-energy dynamics of the system we can restrict ourselves to the lowest Hubbard sector. In that sector sites are either empty, or doubly occupied. Sites with single electrons are only virtually allowed and give rise to pair-pair interactions. The effective pair dynamics is computed from a second order perturbation expansion and is given in terms of pseudospin 1/2 operators as

$$H_S = \sum_{j,\delta} \frac{J}{2} \left(e^{-2i\psi_j^\delta} S_j^+ S_{j+\delta}^- + e^{2i\psi_j^\delta} S_j^- S_{j+\delta}^+ \right) + J \sum_{j,\delta} S_j^z S_{j+\delta}^z - h \sum_j S_j^z + H_{EM}, \quad (2)$$

where $J = 2t^2/|U|$, and $S_j^+ \equiv c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger$. The overall pair density is given by the

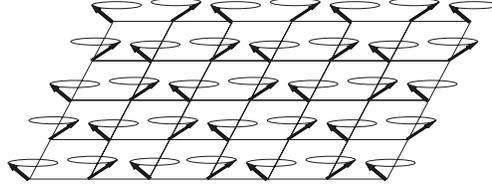


Fig. 1. A schematic representation of the groundstate of the local pairing superconductor on a square lattice. The arrows are semiclassical representations of the pseudospins σ .

z component of the total pseudospin S_{tot}^z , which can be varied by changing the parameter $h \equiv |U| - 2\mu$. Away from half filling, when $h \neq 0$, the global SU(2) symmetry of the Hamiltonian is broken down to a U(1) symmetry that describes the collective rotation of the pseudospins around the z -axis.

Note that the prefactor of both the first and second term in the Hamiltonian above is J . This symmetry is removed when long-range Coulomb interactions between electron pairs are included into the model, having the form $\sum_{j,r} V(\mathbf{r}) S_j^z S_{j+r}^z$. For the discussion that follows, however, this is an inconsequential detail as these interactions preserve the global U(1) symmetry.

The Hamiltonian above can be simplified by introducing another set of pseudospins σ that absorb the vector potential ψ_j^δ . In this procedure one defines the new pseudospins as $\sigma_j^z = S_j^z$ and $\sigma_j^+ = e^{-2i \sum_{j'=0}^j \psi_{j'}^\delta} S_j^+$. The sum over j' that occurs in the definition of σ^+ is a sum over the vector potentials along an arbitrary path that connects site j to an arbitrarily chosen origin at $j = 0$. It is easy to show that due to flux quantization this sum does not depend on the specific path. With this mapping the effective Hamiltonian for the local pairs reduces to an antiferromagnetic Heisenberg model in a uniform magnetic field

$$H_\sigma = J \sum_{j,\delta} \vec{\sigma}_j \cdot \vec{\sigma}_{j+\delta} - h \sum_j \sigma_j^z + H_{EM} \quad (3)$$

Notice that the σ pseudospin operators by themselves are not gauge invariant. They implicitly contain the vector potential and under a general local gauge transformation all σ^+ -operators pick up the same global phase factor $e^{2i \frac{e}{\hbar c} f(0)}$. The Hamiltonian as a whole is, of course, still fully gauge invariant.

Following the study of spontaneous symmetry breaking in magnets and crystals [7] we split up the Hamiltonian into two parts, a finite momentum (\mathbf{k}) sector and a collective, zero momentum sector. In the antiferromagnet the finite \mathbf{k} sector contains the spinwave or Goldstone modes, which for the superconductor become massive. These modes are disjunct from the zero momentum, collective sector which contains the thin spectrum needed for spontaneous symmetry breaking.

0.3 Pseudospinwaves

First we consider the finite momentum (pseudo) spinwave excitations of the Hamiltonian above, for which a semiclassical treatment suffices. Here we only give a brief account as the resulting physics is well known. The main point is that our Hamiltonian properly incorporates the Andersson-Higgs mechanism, generating a gap for the pseudospinwave modes [5,10,6].

The groundstate of H_σ is determined by the competition between the first and second term in the Hamiltonian. The effective magnetic field h tends to align the spins along the z axis, whereas the interaction term in the Hamiltonian favors antiferromagnetic alignment of the pseudospins. The net result is, in terms of semiclassical pseudospins, a canted antiferromagnet in which all spins have equal projections on the z -axis, but are antiferromagnetically ordered in the xy plane (see figure 1). A low energy excitation corresponds to a long wavelength precession of pseudospins around the z -axis, which amounts to a slow variation in the angle ϕ_j^σ of each σ -pseudospin j in the xy plane. According to Hamiltonian (2) the corresponding spinwave energy is proportional to $\sum_{j,\delta} J \cos(2\psi_j^\delta + \phi_j^S - \phi_{j+\delta}^S)$, which in the continuum limit and for small rotations reduces to an excitation energy of $\frac{J}{2}(\mathbf{A} - \nabla\phi)^2$. The important point is that the pseudospinwave excitations in the superconductor are manifestly coupled to the vector potential. This is made explicit by introducing a transformed vector potential $\tilde{\mathbf{A}} = \mathbf{A} - \nabla\phi$ that absorbs the phase rotations. Gauge invariance requires the electro-magnetic part of the Hamiltonian in terms of $\tilde{\mathbf{A}}$ and \mathbf{A} to be identical, so that the total Hamiltonian that governs the elementary excitations becomes $\frac{J}{2}\tilde{\mathbf{A}}^2 + H_{EM}(\tilde{\mathbf{A}})$. For any finite J the elementary excitations of this Hamiltonian (i.e. the transformed photons which combine the excitations of the electromagnetic field and the bare pseudospinwaves) are massive. Via this Andersson-Higgs mechanism a gap is generated for all finite-momentum pseudospinwave excitations in our superconductor. The Meissner effect is a direct physical consequence of this mass generation.

0.4 The Thin Spectrum

The semiclassical approach above considers variations in the relative angles ϕ_j and $\phi_{j+\delta}$ between neighboring pseudospins. The absolute angle of the pseudospins, however, is arbitrary. Consequently no unique classical groundstate exists: if all spins are rotated simultaneously around the z -axis by the same angle a different classical state results, whereas the classical groundstate energy is invariant under such a rotation. In a proper quantummechanical treatment, however, the groundstate will have to be both rotationally invariant and unique. In the following we will show that in the quantum case this global

rotational invariance can be spontaneously broken due to the presence of a thin spectrum.

In exact analogy with the description of spontaneous symmetry breaking in for example crystals and antiferromagnets [7], the collective part of the antiferromagnetic pseudospin Hamiltonian (3) is given by its $k = 0$ and $k = \pi$ part, leading to

$$H_{coll} = \frac{4J}{N} \vec{\sigma}_A \cdot \vec{\sigma}_B - h\sigma_{tot}^z, \quad (4)$$

where we have for convenience defined two sublattices A and B between which the spins have antiparallel projections on the xy -plane. The Hamiltonian above is the Lieb-Mattis Hamiltonian in presence of a uniform external field h and can easily be diagonalized by introducing the total spin $\vec{\sigma}_{tot} = \vec{\sigma}_A + \vec{\sigma}_B$. The groundstate is non-degenerate and characterized by the total spin quantum number σ_{tot} and its z -projection σ_{tot}^z . As in the antiferromagnet, the groundstate does not break the rotational invariance of its governing Hamiltonian. It is easy to see that there is also a set of excited states that have an energy J/N higher than the groundstate. These states form the thin spectrum of the symmetry unbroken Hamiltonian.

To break the symmetry, an external field needs to be added to the Hamiltonian. In order to add this external field in a manifestly gauge invariant way, we are forced to introduce a second, external superconductor. This external superconductor is introduced as a mathematical tool only, and we will take it away again at the end of the calculation. The symmetry broken Hamiltonian in the presence of the external superconductor takes on the form

$$H_{coll}^{SB} = H_{coll} + \left(\Sigma_A^+ \sigma_B^- + \sigma_A^+ \Sigma_B^- + H.c. \right) + H_{ext}. \quad (5)$$

Here $\Sigma_{A,B}$ denotes the pseudospin operators in the external superconductor and H_{ext} describes its dynamics. Notice that this Hamiltonian is still completely invariant under local gauge transformations which acts on the pseudospins $\sigma_{A,B}$ as well as on $\Sigma_{A,B}$. The symmetry that is broken in equation 5 is the global $U(1)$ phase symmetry which rotates all pseudospins σ , but keeps the pseudospins Σ fixed: the phase *difference* between the superconductors acquires a finite expectation value in the symmetry broken state.

The fact that we needed to introduce an external agent to be able to describe spontaneous symmetry breaking is not at all special to the case of superconductivity. In fact, even in the most basic case of the breaking of translational symmetry by a crystal, one also needs to introduce an extra, external crystal to be able to define a coordinate system in which the position of the first crystal can be measured. In the end then also, all that really is well defined is

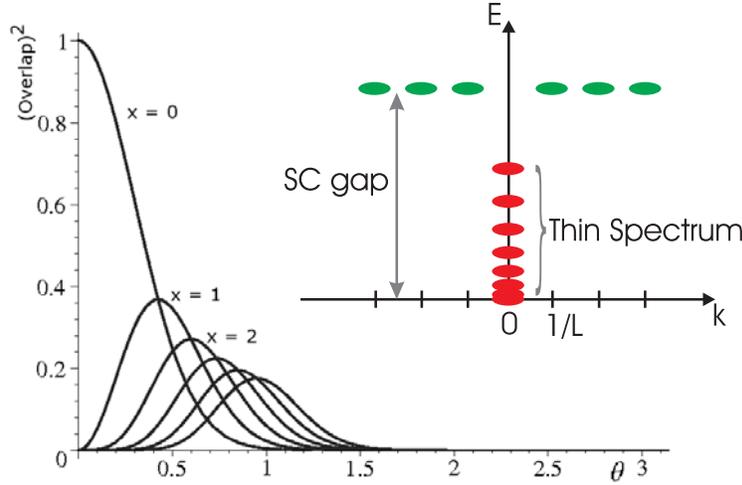


Fig. 2. The overlap between the thin spectrum state $|n\rangle$ and the rotated groundstate $\hat{R}(\theta)|0\rangle$, as a function of the angle of rotation θ , for different values of n . To make this graph we used the values $J = 10$, $B = h = 1$ and $N = 100$. For higher values of N the graph for each n will be scaled horizontally, but the height of the top remains unaffected. The plot is symmetric under mirroring in the $\theta = 0$ axis. The inset shows a schematic dispersion relation of the low-energy, low-momentum states of a finite superconductor: the states at finite k are gapped, while the thin spectrum states at $k = 0$ lie within the gap.

the *difference* in position between the original and the external crystal. In the case of the superconductor it is useful to actually introduce the external agent on the level of the Hamiltonian description so that one can see explicitly that the broken symmetry is a global phase symmetry and not gauge symmetry.

To be able to find a closed form expression for the symmetry broken eigenstates of eq. 5, we are now forced to introduce a gauge-fix: if we assume the phase of the external superconductor to be fixed such that $\langle \Sigma_{A,B}^x \rangle = \pm B$, $\langle \Sigma_{A,B}^y \rangle = 0$, then the symmetry broken Hamiltonian takes on the form $H_{coll}^{SB} = H_{coll} - B(\sigma_A^x - \sigma_B^x)$. This Hamiltonian can be solved exactly. The price to pay for this solvability is the gauge fix which is implicit in the definition of the symmetry breaking field B . Under a gauge transformation, the direction of the symmetry breaking field rotates around the z -axis. States that are related to each other by such a rotation therefore make up a gauge volume of states that in fact all correspond to the same physical state. We will check later that our conclusions about the existence and the form of the thin spectrum are robust under gauge transformations.

The symmetry broken eigenstates of the local pairing superconductor are linear combinations of total spin states. The coefficients of these wavefunctions are given by Hermite polynomials, similar to the case of a regular antiferro-

magnet [7]. The groundstate that is constructed in this manner has a specific absolute total phase determined by the symmetry breaking field. Indeed it corresponds directly to the classically realized superconducting groundstate that we considered before (see figure 1). The states corresponding to the higher order Hermite polynomials are extremely low in energy, and in fact collapse onto the groundstate in the thermodynamic limit. They are thus easily recognized as being the thin spectrum of the symmetry broken local pairing superconductor [13,7,14,12,11].

Let us now address the complication that together with the symmetry breaking field B we introduced an implicit gauge fix. One can wonder whether in this situation the thin spectrum states are still as physical as they are in the symmetry unbroken Hamiltonian (4) – the gauge fixing may have downgraded the thin spectrum states to be just the gauge volume of the superconducting groundstate. We have checked that nothing of this kind happens. With the explicit expressions for the eigenfunctions of H_{coll}^{SB} we can evaluate the overlap between the thin spectrum state $|n\rangle$ and the superconducting groundstate $|0\rangle$ that is rotated over an angle θ . If $|n\rangle$ would be in the gauge volume of $|0\rangle$, the overlap should become unity for a certain rotation angle θ . As shown in figure (2) this overlap is equal to unity if and only if both x and θ are zero. This demonstrates that an excited thin spectrum state is not merely a global rotation of the groundstate. Therefore it is not in the groundstate's gauge volume.

0.5 Decoherence

It is known that the presence of a thin spectrum in mesoscopic spin qubits will lead to quantum decoherence [13,7]. The thin spectrum that we have now identified in superconductors is therefore expected to lead to a finite coherence time of qubits based on superconducting material. One such type of qubit that is experimentally realized is the so called Cooper-pair box qubit [15–17]. In these Cooper-pair boxes a superconducting island can be brought into a superposition of having \bar{N} and $\bar{N} + 1$ Cooper-pairs present. Superpositions of this type can reach coherence times of up to 500 ns [18,19].

In the formalism that is outlined above it is easy to consider the superposition state of the superconductor which corresponds to the experimental one [27]. After computing the exact time evolution of such a qubit, and tracing over the unobservable thin spectrum states, we find that the coherence of the Cooper-pair box qubit decays over time. The resulting maximum coherence time we find to be $t_{spn} = \pi\hbar\bar{N}/k_B T$. The calculation is analogous to the one for decoherence in antiferromagnets [7], but for the superconductor \bar{N} signifies the average number of Cooper pairs on the superconducting island. This coher-

ence time is the maximum coherence time of a superconducting island, which is limited by the existence of a thin spectrum in the superconductor. Just as in the cases of crystals and antiferromagnets, the details of the model (e.g. J or h) do not enter into the expression for the maximum coherence time, which thus appears as a universal timescale [13,7]. Using from experiment the values $\bar{N} \simeq 10^6$ and $T \simeq 40$ mK [17], we find a coherence time for the experimentally realized Cooper-pair boxes of $\simeq 0.5$ ms. Clearly this timescale set by the presence of the thin spectrum states is much larger than the timescale that is the current limit to coherence of the Cooper-pair boxes due to other environmental factors. However, it is well possible that the limit set by the thin states will come within the experimental reach in the near future, either because the isolation from external sources of decoherence will be developed further, or because the size of the Cooper-pair box itself is reduced even more.

0.6 The Superconducting Quantum Dot

It is well known that apart from the superconducting state considered above, characterised by its total phase, there also exists a superconducting state of matter with a well defined total number of Cooper pairs. Because number and phase are conjugate variables, the total number state is qualitatively different from the total phase state. Its lack of a well defined total phase for example does not allow it to participate in the Josephson effect. In terms of the model of equation 4 the total number state corresponds to the exact groundstate of H_{coll} , which has good quantum numbers σ_{tot} and σ_{tot}^z . To stabilize the exact ground state in the thermodynamic limit (i.e. to prevent spontaneous breaking of the total phase symmetry), the thin spectrum states will have to become gapped. The easiest way to realize such a finite energy for all excitations in the thermodynamic limit, is to add a charging term to the Hamiltonian:

$$H_{dot} = \frac{4J}{N} \vec{\sigma}_A \cdot \vec{\sigma}_B + C (\sigma_{tot}^z - \nu)^2. \quad (6)$$

Here C is a charging energy penalizing any departure of the total Cooper-pair density σ_{tot}^z from ν . The uniform field h (and thus the electronic chemical potential μ) have been absorbed into the definition of ν and C . The ground state of this model Hamiltonian has equal values for the total pseudospin quantum number σ_{tot} and its z -projection σ_{tot}^z . If the charging energy C is of at least the same order of magnitude as the interaction energy J , the second term in the Hamiltonian dominates, and the groundstate value of σ_{tot}^z is very close to ν . If ν itself is of the order of N (so that the number of Cooper pairs in the groundstate is of the same order of magnitude as the total number of electrons we started out with), there are no low lying excitations which become degenerate with the groundstate in the thermodynamic limit, and the total

number ground state thus remains stable in that limit.

Although this exact ground state does not have a well defined total phase and is therefore insensitive to the Josephson effect, all of its finite-range correlation functions are in fact indistinguishable from the ones found in the total phase state. It does therefore fall prey to the Anderson-Higgs mechanism (a finite k effect) and the associated Meissner effect, thus allowing for dissipationless electric currents. The relation between the total number and total phase state is analogous to that between the antiferromagnetic Néel state and the total spin singlet: although only the former has a sublattice magnetization, all of its finite-range correlation functions are indistinguishable from those of the latter. A physical realization of the total number state in which all thin spectrum states have been made massive by a large charging energy can be found in isolated superconducting grains or superconducting quantum dots. Their physics is well understood and can also be described by a canonical (rather than grand canonical) variation of the standard BCS theory [20–26].

Upon lowering ν from being of order N to being of order unity (which corresponds to tuning the Cooper pair density into an extremely dilute regime), an alternative set of thin spectrum states becomes available. In this limit, the states which differ from the groundstate in their value for the total pseudospin quantum number σ_{tot} , but not in their value for its z -projection are separated from the groundstate by an energy of order J/N . In the thermodynamic limit these states all collapse onto the groundstates and through the usual mechanism the pseudospin rotation symmetry can be spontaneously broken. The resulting classical state has a finite antiferromagnetic order parameter along the z axis, against a background of uniform magnetization along that same z axis. Electronically, it corresponds to a charge density wave.

Independent of the value of ν , if C is small enough (i.e. of order J/N) the lowest lying excitations consist of simultaneous alteration of σ and σ^z . Using these states to spontaneously break the pseudospin symmetry in the thermodynamic limit we once again find a canted antiferromagnet, corresponding to the superconducting state with a well defined total phase. What kind of classical state may be stabilized in practice in a quantum dot or superconducting grain thus depends on the precise values of the charging energy and the Cooper pair density.

0.7 Conclusions

We have shown that the superconducting state is a state characterised by a well defined total phase, which results from a spontaneously broken global symmetry. Using a strong coupling or local pairing model, we can describe the

symmetry breaking mechanism in exact analogy to that of quantum crystals or antiferromagnets. Because the model is manifestly gauge invariant, it is clear that, in full accordance with Elitzur's theorem, the superconducting state has broken only a global $U(1)$ phase symmetry, and not the local electromagnetic gauge symmetry.

Associated with any spontaneously broken continuous symmetry, in superconductors as well as in crystals or antiferromagnets, is a so called thin spectrum of states which all become degenerate with the exact groundstate in the thermodynamic limit. We have shown that this thin spectrum in superconductors can escape the Anderson-Higgs mechanism because it consists of purely infinite wavelength excitations only. The presence of the low-energy (in gap) thin spectrum states in qubits based on superconducting material, such as the superconducting Cooper-pair box qubits, imposes a finite maximum coherence time on these qubits. In practice that time turns out to be too large to be experimentally relevant at the moment, but it may pose a limit to the lifetime of such qubits in the future. Finally, we have shown that in superconducting quantum dots or isolated superconducting grains the charging energy may be large enough to render the thin spectrum massive. In that case phase symmetry cannot be spontaneously broken, and a total number superconducting state is formed instead.

0.8 Appendix: The BCS superconductor

In weak coupling superconductors the physical picture for symmetry breaking stays the same. A qualitative description of the thin spectrum of a superconductor can be given also within the BCS model, exactly analogous to the description of the strong coupling local pairing model considered here [27]. However, it is more challenging to obtain analytical results and closed expressions in that case. The physical picture of the BCS symmetry breaking comes to the fore most clearly if one follows Anderson by writing the standard BCS Hamiltonian in momentum space in terms of pseudospins [28]. In the superconductor the pseudospins form a domainwall structure around $k = k_F$, which separates two ferromagnetically ordered regions with opposite z -axis projections. Spontaneous symmetry breaking then orients the xy projection of spins in the domain wall along a specific direction in the plane. Again a thin spectrum is associated with this symmetry breaking.

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