

# ' $\pi$ State' Induced by Impurities with a Repulsive Interaction

Grzegorz Litak\*<sup>1,2</sup> and Mariusz Krawiec<sup>3</sup>

<sup>1</sup> Department of Mechanics, Technical University of Lublin, Nadbystrzycka 36, PL-20-618 Lublin, Poland

<sup>2</sup> Max Planck Institute for the Physics of Complex Systems Nöthnitzer Str. 38, D-01187 Dresden, Germany

<sup>3</sup> Institute of Physics and Nanotechnology Center, M. Curie-Skłodowska University, pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

Received 2 September 2004

**Key words** superconductivity, fluctuations, impurities,  $\pi$  state.

**PACS** 74.20.-z, 74.25.-q, 74.40.-k, 74.50.+r

We study the properties of a quantum impurity embedded in a superconducting host. The superconductor is described by the negative  $U$  Hubbard model while the impurity introduces a repulsive interaction to the system. We discuss the influence of this 'on-impurity' Coulomb repulsion on the local properties (density of states, electron pairing) of the superconductor. We show the condition of  $\pi$  - like behaviour, defined as two subsystems having a phase difference of  $\pi$ , in the system by using a proper combination of attractive pairing interaction and repulsive one located at impurity site.

Copyright line will be provided by the publisher

## 1 Introduction

The role of impurities in superconducting hosts has been a subject of intensive theoretical and experimental studies [1, 2, 3, 4, 5] recently. Mainly, the bulk properties, like transition temperature or density of states have been investigated [6]. However in a conventional (as discussed in this paper)  $s$ -wave superconductors ( $SC$ ), non-magnetic impurities have only little effect on the transition temperature according the Anderson theorem [7, 8, 9]. On the other hand very little attention has been payed to the understanding the properties of the local environment of a single impurity, like local density of states ( $DOS$ ) or spatial variation of the order parameter (see however [10]). The effect of non-magnetic impurities on the local properties of superconductors with exotic pairing has been studied more extensively in [11, 12] and references therein. The large interest in the subject of impurities in exotic  $SC$  comes from the fact that the Anderson theorem does not work in the later case and impurities have more drastic influence on the properties of the high- $T_c$  and other non- $s$ -wave superconductors. In particular, it is widely accepted that high- $T_c$  materials have  $d$ -wave pairing state [13], which means that  $SC$  order parameter changes its sign under  $\pi/2$  rotation. This leads to the so called  $\pi$ -phase behaviour and can be seen in nonuniform systems, like those with surfaces, vortices, cracks, twin boundaries or impurities [14, 15].

A system is regarded as in the  $\pi$ -phase if there is a sign change of the order parameter between two subsystems. The simplest example is the junction made from two superconductors with the phase of the order parameter equal to  $\pi$  [14, 15]. In this case Josephson current becomes negative in contrast to the usual 0-phase junction. An other example are granular high- $T_c$  materials which can likely form network of microscopic  $\pi$ -junctions [16] between small regions with different phases of the order parameter. In such systems the zero-energy Andreev bound states, zero-bias conductance peaks, paramagnetic Meisner effect and spontaneously generated currents take place [14, 15].

The situation is very similar to those in which paramagnetic impurities with strong on-site Coulomb repulsion are placed in classical  $s$ -wave superconductor. Due to the proximity effect [17] the  $SC$  order

\* Corresponding author: e-mail: g.litak@pollub.pl, Phone: +48 81 5381573, Fax: +48 81 5250808

parameter is created on the impurity site. Moreover, because of the fact that the impurity coupling constant has opposite sign to  $SC$  one, there is a sign change of the order parameter between impurity and surrounded  $SC$ . Therefore, we regard the system as in  $\pi$ -phase. It is the purpose of the present work to clarify if such system has all necessary ingredients to regard its as a  $\pi$ -phase state.

## 2 The model

The system is described by negative  $U$  Hubbard model [18] with the Hamiltonian:

$$H = \sum_{ij\sigma} (t_{ij} - \mu\delta_{ij}) c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma}, \quad (1)$$

where  $i, j$  label sites of a square lattice,  $t_{ij} = -t$  is the hopping integral between nearest neighbour sites and  $\mu$  is the chemical potential.  $U_i < 0$  describes attraction between electrons with opposite spins occupying the same site  $i$ . The effect of impurity is introduced in one of the lattice sites  $i_A$  via repulsive interaction  $U_A > 0$ .

In the following we shall work in the Hartree-Fock approximation. To simplify the set equations we dropped the Hartree terms ( $U_i \langle n_{i\sigma} \rangle$ ), which means that we have only off-diagonal impurity induced disorder in the system. So the corresponding Gorkov equation has the form:

$$\sum_{j'} \begin{pmatrix} (\omega + \mu)\delta_{ij'} - t_{ij'} & \Delta_i \delta_{ij'} \\ \Delta_i^* \delta_{ij'} & (\omega - \mu)\delta_{ij'} + t_{ij'} \end{pmatrix} \hat{G}(j', j; \omega) = \delta_{ij}. \quad (2)$$

In the zero temperature the  $SC$  order parameter  $\Delta_i$  and the total local charge  $n_i$  are given by self-consistent relations:

$$\Delta_i \equiv U_i \chi_i = -U_i \frac{1}{\pi} \int_{-\infty}^{E_f} d\omega \text{Im} G^{12}(i, i; \omega + i\epsilon), \quad (3)$$

$$n_i = -\frac{2}{\pi} \int_{-\infty}^{E_f} d\omega \text{Im} G^{11}(i, i; \omega + i\epsilon), \quad (4)$$

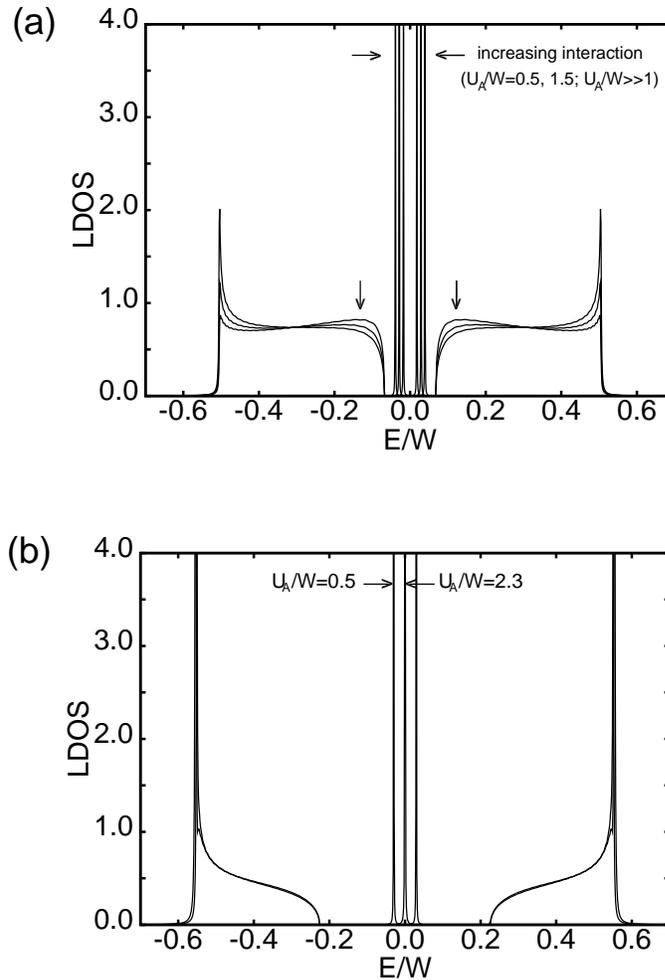
where  $E_f$  denotes Fermi energy, and  $\epsilon$  is a small positive number. The local quasiparticle density of states ( $LDOS$ ) can be written as follows

$$D_i(\omega) = -\frac{1}{\pi} \text{Im} G^{11}(i, i; \omega + i\epsilon). \quad (5)$$

Eqs. (2)-(4) have been solved self-consistently using one site approximation at two dimensional lattice. The pairing amplitude  $\Delta_A$  has been found at the impurity site. The surrounding sites were treated homogeneously as in a bulk (clean) superconductor.

## 3 Results and discussion

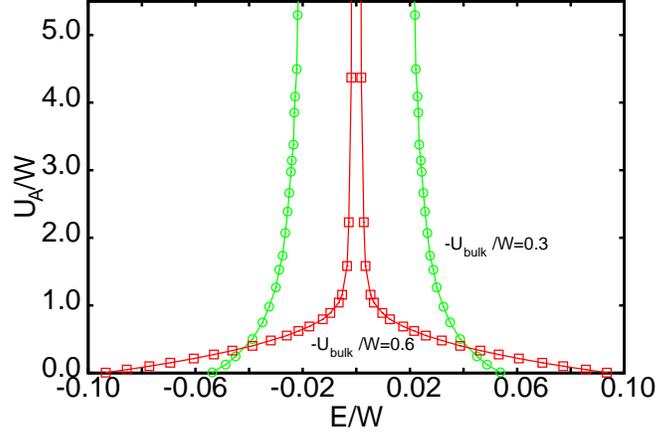
It is well known that the local density of states at an impurity embedded in  $SC$  host has bound states within energy gap  $\Delta_{bulk}$  which are symmetrically located with respect to the Fermi energy. Especially this is true if the on-impurity Coulomb interaction has the same sign as  $SC$  one or if it is equal to zero. In this case bound states always have non-zero energies. However situation is quite different if the interaction has opposite sign to the  $SC$  one. One can show that under special conditions it is possible to get bound states which are exactly at the Fermi energy.



**Fig. 1** Local density of states for  $U_{bulk}/W = -0.3$  (a) and  $U_{bulk}/W = -0.6$  (b). In Fig. 1a vertical and horizontal arrows show the change of  $LDOS$  with increasing interaction  $U_A$ .

The example of the impurity local density of states ( $LDOS$ ) is shown in the Fig. 1 where two situations are depicted. In Fig. 1a  $LDOS$  is plotted for  $U_{bulk} = -0.3 W$ , where  $W = 8t$  is a bandwidth, and for a number of on-impurity interactions  $U_A > 0$ . One can see that to get zero energy states it is not enough to have  $U_A$  of opposite sign to  $U_{bulk}$ . In this case bound states have non-zero energies for all  $U_A$ . If we increase  $U_{bulk}$  (see Fig. 1b) and calculate  $LDOS$  one can find that those bound states do approach zero energy. It can be read from Fig. 2 where the positions of the bound states are plotted as a function of  $U_A$  for different values of the  $U_{bulk}$ .

However it is very difficult to judge numerically if those states are really zero energy states. Therefore we supplemented our study by simple analytical calculations with constant bulk bare  $DOS$ . (Note that in numerical calculations we have chosen  $2D$  tight binding  $DOS$  with Van Hove singularity in the middle of the band.) It turns out that the zero energy solution occurs for only one value of  $U_A$  which can be calculated



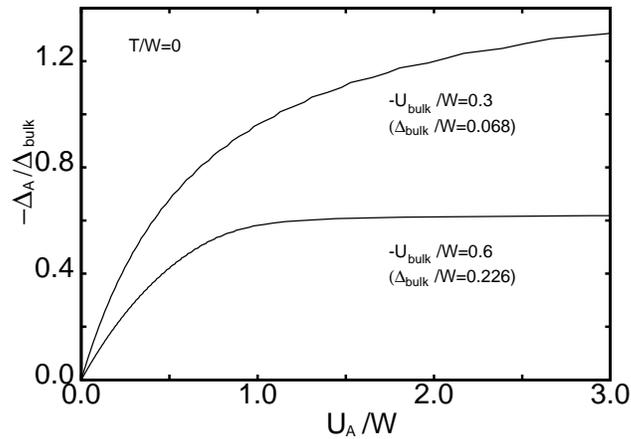
**Fig. 2** Position of the bound states as a function of  $U_A$  for  $U_{bulk} = -0.3 W$  (a) and  $U_{bulk} = -0.6 W$  (b).

from

$$\Delta_A \equiv U_A \chi_A = -2\pi t^2 \rho(0), \quad (6)$$

where  $\rho(0)$  is the bulk bare density of states at the Fermi energy.

To get such a large value of  $\Delta_A$  we have to take large  $U_A$  as well as large value of  $\Delta_{bulk}$  because  $\chi_A$  in Eq. 6 depends on it via proximity effect. Physically we can imagine that there could be a strong on-impurity Coulomb repulsion. However as we can see in the Fig. 3 we cannot take large values of  $U_A$  because  $\Delta_A$  tends to a constant value as we increase  $U_A$ . The other possibility is to have large values of



**Fig. 3**  $\Delta_A/\Delta_{bulk}$  plotted as a function of  $U_A$ .

$\Delta_{bulk}$  which in fact is impossible to achieve in real materials. We need large values of the bulk pairing potential, much larger than the bandwidth.

## 4 Conclusions

From the present calculations we conclude that it is in general not possible to get states at exactly zero energy in the system consisting of a single impurity embedded in *BCS* superconductor described by the negative  $U$  Hubbard model. However we were able to find one condition at which such situation can take place, which seems to be physically impossible to meet it in reality. Note the present calculations were performed assuming a rather small scattering rate  $\epsilon = 10^{-3}t$  (Eq. 5, Fig. 2). Of course taking a large enough  $\epsilon$  will be sufficient to broad and eventually connect the two neighbour bound states into one at zero energy.

In this paper we have shown results for a half-filled band but we have also checked the situation for other fillings and as far as the bound states are concerned we got no qualitative differences. On the other hand present calculations are not fully self-consistent ones. We hope that proper treatment of the problem taking into account the Hartree term in Eq. 2 and calculating  $\Delta_{bulk}$  at each surrounding site we will be able to give more precise conditions for  $\pi$ -like state appearance in such systems.

Note also that relatively large values of the impurity potential  $U_A$  (Fig. 1b) make Hartree-Fock approximation questionable so the results obtained here should be treated as qualitative. Our initial calculations show that fluctuations of the pairing parameter  $\Delta_i$  around the central site would also influence the critical value of  $U_A$  making it even higher. Such an analysis will be performed systematically for various band fillings  $n$ .

**Acknowledgements** This work has been partially supported by the Polish State Committee for Scientific Research (KBN), Project No. 2 P03B 06225.

## References

- [1] D. Belitz and T.R. Kirkpatrick *Rev. Mod. Phys.* **66** (1994) 261.
- [2] G. Harań and A.D.S. Nagi, *Phys. Rev.* **B 58** (2001) 012503.
- [3] G. Litak, *Phys. Stat. Sol.* **B 229** (2002) 1427.
- [4] J.L. Tallon *et al.*, *Phys. Rev. Lett.* **79** (1997) 5294.
- [5] K. Karpińska *et al.*, *Phys. Rev. Lett.* **84** (2000) 610.
- [6] N. E. Bickers and G. E. Zwicknagl, *Phys. Rev.* **B 36** (1987) 6746.
- [7] P. W. Anderson, *Phys. Rev. Lett.* **3**, (1959) 325.
- [8] R. Moradian *et al.*, *Phys. Rev.* **B 63** (2001) 024501.
- [9] B. L. Györfy *et al.*, in *Fluctuation Phenomena in High Critical Temperature Superconducting Ceramics*, eds. M. Ausloos and A.A. Varlamov (Kluwer Academic Publishers NATO ASI Series, Dordrecht 1997) 385.
- [10] H. Kim and P. Muzikar, *Phys. Rev.* **B 48** (1993) 3933.
- [11] H. Tsuchiura *et al.*, *Journal of the Phys. Soc. of Japan* **68** (1999) 2510.
- [12] M. Vojta, R. Bulla, *Phys. Rev.* **65**, 014511 (2001).
- [13] J. F. Annett *et al.*, in *Physical Properties of High Temperature Superconductors* ed. D. M. Ginsberg, World Scientific, Singapore (1996).
- [14] S. Kashiwaya and Y. Tanaka, *Rep. Prog. Phys.* **63** (2000) 1641.
- [15] T. Löfwander *et al.*, *Superconduct. Sci. Technol.* **14**, (2001) R53.
- [16] M. Sigrist and T. M. Rice, *Rev. Mod. Phys.* **67** (1995) 503.
- [17] C. J. Lambert and R. Raimondi, *J. Phys. Condens. Matter* **10** (1998) 901.
- [18] R. Micnas *et al.*, *Rev. Mod. Phys.* **62** (1991) 113.
- [19] G. Litak *et al.*, *Physica C* **251** (1995) 263.
- [20] W. Belzig, PhD. thesis, Univ. of Karlsruhe (1999).
- [21] P. G. de Gennes and D. Saint-James, *Phys. Lett.* **4** (1963) 151.
- [22] C. R. Hu, *Phys. Rev. Lett.* **72**, (1994) 1526.
- [23] A. L. Fauchère *et al.*, *Phys. Rev. Lett.* **82** (1999) 3336.

