HIGH $T_c$ SUPERCONDUCTIVITY IN A SUPERLATTICE OF QUANTUM STRIPES

A. Bianconi, A. Valletta, A. Perali and N.L. Saini

"Università di Roma ‘La Sapienza’, Dipartimento di Fisica, 00185 Roma, Italy

bIstituto Nazionale di Fisica Nucleare, Dipartimento di Fisica, P. A. Moro 2, 00185 Roma, Italy

(Received 5 November 1996; accepted in revised form 3 January 1997 by C.N.R. Rao)

The superconducting gap for 2D electron gas in a superlattice of quantum stripes with a finite 1D periodic potential barrier is calculated. The resonant enhancement of the superconducting gap is found when the Fermi level is tuned near the bottom of the nth superlattice subband with $n \approx 2$. The critical charge density $\rho_c$ for maximum $T_c$ at the $n = 2$ resonance is mainly determined by the stripe width $L$ and vice versa, while it is nearly independent on the amplitude of the potential barrier. The width of the resonance is determined by the interaction cutoff $\hbar \omega_0$ and its shape by the ratio $\Delta E_{nL}/\hbar \omega_0$, where $\Delta E_{nL}$ is the transversal energy dispersion of the $n$ subband due to the transverse hopping between stripes. © 1997 Elsevier Science Ltd. All rights reserved

1. INTRODUCTION

Recently a particular heterostructure of the superconducting CuO$_2$ plane in high $T_c$ superconductors [1] has been found at the mesoscopic scale length: a superlattice of quantum stripes [2–6]. Quantum size effects appear because of the finite mesoscopic width $L \approx 15$ Å of each stripe. Quantum size effects modify the two dimensional electronic structure giving superlattice subbands. The superconducting critical temperature $T_c$ reaches a maximum when the Fermi level is tuned near the bottom of a superlattice subband i.e. at a “shape resonance”. This resonance provides not only a possible mechanism for understanding the amplification of the critical temperature from the low to the high temperature range in cuprate superconductors [7], but also an approach to synthesize new superconductors with high critical temperature made of heterostructures of metallic stripes at the atomic limit [8]. A calculation of the amplification of the critical temperature going from a homogeneous 2D plane to a superlattice of quantum stripes has been reported in a recent paper in which only the case of an infinite potential barrier was considered [9]. In this simple case no single particle transverse hopping between stripes is allowed and the Josephson coupling between stripes was required to suppress quantum fluctuation in 1D.

In this communication we report a calculation of the amplification of superconducting gap in a superlattice of quantum stripes with finite hopping between the stripes. A generic case of a two dimensional (2D) free electron model with a 1D periodic barrier has been considered to investigate the basic physical properties of the system. The structural and electronic parameters for superlattice are chosen close to the experimental values observed in the cuprate superconductors. The results can be easily extended to any superconducting superlattice of quantum stripes.

The “shape resonance” for the superconducting gap appears when the transverse energy dispersion ($\Delta E_{nL}$) of the nth superlattice subband due to single particle hopping between stripes, is lower than the energy cutoff for the interaction, i.e. $\Delta E_{nL}/\hbar \omega_0 < 1$. We consider the case of $n = 2$ “shape resonance” for an electron gas in a mesoscopic superlattice where the condition $\Delta E_{nL}/\hbar \omega_0 < 1$ is verified also for a small potential barrier of the order of few hundreds of meV as expected if it is due both to the magnetic interaction $J \sim 0.1$ eV and to the local lattice distortions that are associated with 1D charge ordering in cuprate superconductors [4–6].

2. THE ELECTRONIC STRUCTURE

We consider the superlattice of quantum stripes of
The coefficients \( \alpha, \beta, \gamma \) and \( \delta \) are obtained by imposing the Bloch conditions with periodicity \( \lambda_p \), and the continuity conditions of the wave function and its derivative at \( L/2 \) and finally by normalization in the surface unit.

The solution of the eigenvalue equation for \( E \) gives the electronic dispersion for the \( n \) subbands with energy \( e_n(k_x,k_y) = e(k_x) + E_n(k_y) \) where \( e(k_x) = (\hbar^2/2m)k_x^2 \) is the free electron energy dispersion in the \( x \) direction and \( E_n(k_y) \) is the dispersion in the \( y \) direction. The solution of the implicit equation derived by the Bloch conditions in the superlattice is given as [10]:

\[
\cos(k_y\lambda_p) = \cos(k_W L) \cdot \cos(k_b W) - \frac{1}{2}\left( \xi + \frac{1}{\xi} \right) \cdot \sin(k_W L) \cdot \sin(k_b W)
\]

where

\[
k_b = \sqrt{2m_e E_n(k_x)/\hbar^2}
\]

\[
k_W = \sqrt{2m_e (E_n(k_y) + V_b)/\hbar^2}
\]

\[
\xi = \frac{k_b}{k_W}
\]

We have derived \( N_b \) solutions for \( E_n(k_x) \) (1 \( \leq n \leq N_b \)) for each \( k_y \) in the Brillouin zone of the superlattice giving dispersion in the \( y \) direction of the first \( N_b \) subbands with \( k_x = 0 \). The dispersion of the superlattice subbands in the \( y \) direction for \( V_b = 150 \) meV is shown in Fig. 2(a). There are two subbands with negative energy. The second subband is dispersing in the transverse \( y \) direction from its energy top \( E_{2b} = -18 \) meV at \( k_y = 0 \), to its energy bottom \( E_{2b} = -43 \) meV at \( k_y = \pi/\lambda_p \), therefore the total dispersion in the transversal direction is \( \Delta E_{2b} = E_{2b} - E_{2b} = 25 \) meV. The corresponding density of states (DOS) as a function of the chemical potential \( \mu \) is shown in Fig. 3(a). The DOS shows a sharp step increases at the energy \( E_{2b} \) and a peak at \( E_{2b} \). The jump at \( E_{2b} \) is determined by the threshold of the contribution of the partial density of states of the second subband to the total density of states. The peak at \( E_{2b} \) is due to an anisotropic Van Hove singularity. The total energy dispersion of the \( n \) subband \( \Delta E_{n,2b} \) in the transversal direction determines the energy separation between the peak and the step edge. In the energy range \( E_{2b} < E < E_{2b} \) the electronic structure is like that of an anisotropic 2D electron gas, while the 1D character appears at higher energy \( E > E_{2b} \).

The bottom of the first superlattice subband is at \( E_{1b} = -120 \) meV, i.e. 30 meV above the bottom of the potential well and its superlattice transversal energy dispersion \( \Delta E_{1b} \) is 3 meV. The DOS of first subband in Fig. 3(a) shows a difference of only 3 meV between the
with a negligible transversal hopping between stripes $t_\perp$ in comparison with the longitudinal hopping in the stripe direction $t_\parallel$.

We find three subbands in the negative energy range for the larger potential barrier $V_b = 450$ meV shown in Fig. 2(b). The first and second subbands with their bottom at $E_{1b} = -407$ meV and $E_{2b} = -284$ meV are nearly 1D subbands with a superlattice dispersion of $\Delta E_{1\perp} = 0.5$ meV and $\Delta E_{2\perp} = 3$ meV respectively. Therefore the lineshape of the partial DOS for these subbands in Fig. 3(b) show the nearly 1D divergence. On the contrary third subband at $E_{3b} = -103$ meV has a sizable transversal energy dispersion $\Delta E_{3\perp} = 16$ meV therefore the separation between the step edge and the van Hove peak can be seen in the DOS in Fig. 3(b).

The chemical potential as a function of the charge density for the two cases shown here is plotted in Fig. 4. Steps appear at the bottom of each subband as in the case of a single stripe [9]. The chemical potential is tuned at the bottom of the second subband at an electron number density in the range of $7 \times 10^{-3}$ Å$^2$ in the superlattice considered here. This charge density is determined by the stripe width $L$ and it is a weak function of the amplitude of the potential barrier as can be seen in Fig. 4.

3. THE SUPERCONDUCTING GAP

The calculation of the superconducting gap at $T = 0$ K is carried out using the BCS approach. We have solved the BCS equations for the gap as a function of the chemical potential in a self consistent manner. A generic cutoff energy $\hbar \omega_0$ for the effective pairing interaction of any magnetic, charge or phonon nature has been considered. The coupling term has been calculated following the approach of Blatt and Thompson [11] taking into account the interference effects between the

---

**Fig. 2.** The dispersion of the superlattice subbands in the $y$ direction for the case $V_b = 150$ meV (panel a) and $V_b = 450$ meV (panel b).

**Fig. 3.** The density of states as a function of the chemical potential for a periodic potential barrier $V_b = 150$ meV (panel a) and $V_b = 450$ meV (panel b).

**Fig. 4.** The chemical potential as a function of the electron number density for the periodic potential barrier $V_b = 150$ meV and $V_b = 450$ meV. The relative variation of the chemical potential going from the superconducting to the metal phase is the case of $V_b = 150$ meV is shown. The arrows indicate the bottom of the second subband.
wave functions of the pairing electrons in the different subbands,

\[ V_0 = V_{n,k_x,k_y} \theta(\hbar \omega_0 - |\epsilon_n(k_x, k_y) - \mu|) \theta(\hbar \omega_0 - |\epsilon_n'(k_x', k_y') - \mu|) \]  

(4)

where

\[ V_{n,k_x,k_y'} = -J \int \frac{dxdy}{S} \psi_{n,-k_x}(x,y) \psi_{n',k_y'}(x,y) \times \psi_{n,k_x}(x,y) \psi_{n',k_y'}(x,y) \]

\[ = -J \int \frac{dxdy}{S} |\psi_{n,k_x}(x,y)|^2 |\psi_{n',k_y'}(x,y)|^2 \]  

(5)

with \( J = \lambda N_0 \) where \( N_0 = (1/(4\pi))(2m/\hbar^2) \) is the two dimensional free electron density of states and \( \lambda \) is the effective coupling parameter for the ideal homogeneous material \( (V_0 = 0) \); \( n \) and \( n' \) are the subband indexes. \( k_x \) (\( k_y \)) is the component of the wavevector in the stripe direction (or longitudinal direction) and \( k_{y'} \) (\( k_y' \)) is the superlattice wavevector (in the transversal direction) of the initial (final) state in the pairing process, and \( \mu \) the chemical potential.

In the BCS approximation, i.e. a separable kernel, the gap parameter has the same energy cut off \( \hbar \omega_0 \) as the interaction. Therefore it has a value \( \Delta_n(k_y) \) around the Fermi surface in a range \( \hbar \omega_0 \) depending from the subband index and the superlattice wave vector \( k_y \).

The self consistent equation for the gap \( \Delta_n(k_y) \) is:

\[ \Delta_n(\mu, k_y) = -\frac{1}{2N} \sum_{n'k_y'k_y'} \frac{V_0 \Delta_{n'}(k_y')}{\sqrt{\epsilon_{n'}(k_y') + \epsilon_{n'k_y'} - \mu^2 + \Delta_{n'}^2(k_y')}} \]  

(6)

where \( N \) is the total number of momenta. This equation has been solved iteratively, with the convergence criterion fixed for a relative gap variation less than \( 10^{-6} \). We obtain an anisotropic gap strongly dependent on the subband index and weakly dependent on the superlattice wave vector \( k_y \). We have considered the case for \( \lambda = 0.25 \) and \( \hbar \omega_0 = 600 \) K.

The charge density \( \rho \) and the chemical potential in the superconducting phase are related by:

\[ \rho = \frac{1}{S} \sum_n \sum_{k_y} \left( 1 - \frac{\epsilon_n(k_x, k_y) - \mu}{\sqrt{\epsilon_n(k_x, k_y) - \mu^2 + \Delta_n^2(k_y)}} \right) \]  

\[ \rho = \frac{\Delta(k_y)}{2\pi} \sum_{n=1}^{N_n} \sum_{k_y=0}^{\frac{\pi}{\lambda}} \left[ \int_0^{\epsilon_{n\mu}} \frac{d\epsilon}{L_x} N(\epsilon) + 2 + \int_{\epsilon_{\text{min}}}^{\epsilon_{n\mu}} \frac{d\epsilon}{L_x} N(\epsilon) \right] \]  

\[ \times \left( 1 - \frac{E_n(k_y) + \epsilon - \mu}{\sqrt{(E_n(k_y) + \epsilon - \mu)^2 + \Delta_n^2(k_y)}} \right) \]  

(7)

where

\( \epsilon_{\text{min}} = \max[0, \mu - \hbar \omega_0 - E_n(k_y)] \)

\( \epsilon_{\text{max}} = \max[0, \mu + \hbar \omega_0 - E_n(k_y)] \)

\[ N(\epsilon) = \frac{L_y}{2\pi} \frac{1}{\sqrt{(\hbar^2/2m\epsilon)}} \]

and \( N_b \) is the number of the occupied subbands; \( L_x \) and \( L_y \) are the size of the considered surface \( S \); and the increment in \( k_y \) is taken as \( \Delta k_y = 2\pi/L_y \).

Figure 4 shows the variation of the chemical potential going from the superconducting to the normal phase \( (\mu_n - \mu_n) / \mu_n \) at the \( n = 2 \) resonance for the periodic potential barrier \( V_0 = 150 \) meV where \( \mu_n \) is the chemical potential in the superconducting (normal) phase. The chemical potential shows a blue shift in the superconducting phase above the peak of the van Hove singularity at \( E > E_{\text{in}} \) and a red shift near the bottom of the subband \( E \sim E_{\text{in}} \) as it was already found in the case of an infinite potential barrier [9].

We have found in cuprate superconductors that at the optimum doping giving the maximum \( T_c \) the Fermi level is tuned at the \( n \approx 2 \) "shape resonance" [2–8]. The superconducting gap at the \( n = 2 \) shape resonance both for a periodic potential barrier of amplitude \( V_0 = 150 \) and 450 meV are plotted in Fig. 5 as a function of the electron number density, for the effective coupling term \( \lambda = 0.25 \). The results show that the critical charge density for maximum \( T_c \) is \( \rho_c = 8.5 \times 10^{-3} \) Å\(^{-2} \) and is not dependent on the potential barrier.

This value is in qualitative agreement with the charge density in superconducting cuprate superconductors. In
fact the curve of the critical temperature versus doping \( T_c(\delta) \) in all cuprate superconductors shows a critical doping \( \delta_c \) in the range 0.12–0.15 holes per Cu site for maximum \( T_c \) [12]. The density of itinerant charges contributing to the transport properties in the underdoped regime, \( \delta < \delta_c \), is close to the doping therefore the maximum gap is expected in the cuprates for the critical doping \( \delta_c = \rho_c \) \( 3.8^2 = 0.12 \) electrons or holes per Cu site in qualitative agreement with experimental data.

The width of the resonance in Fig. 5 is about \( 7 \times 10^{-2} \) Å that agrees with the experimental width \( \Delta_3 \) of the experimental \( T_c(\delta) \) curve in cuprate superconductors ~0.1 holes per Cu site.

The amplitude of the gap resonance for \( V_b = 450 \) meV is close to that found for an infinite potential barrier and it decreases with increasing transversal hopping as can be seen in Fig. 5. Beyond the reduction of the amplification going from a potential barrier \( V_b \) of 450 meV to 150 meV, a variation of the shape of the resonance is observed. The separation between the maximum amplification and the drop at the left side of the resonance, \( \rho < \rho_c \), increases with decreasing potential barrier.

In the hole doped cuprate superconductors the so called overdoped regime for high hole density \( \delta > \delta_c \) [12] where \( T_c \) drops with increasing hole density corresponds with the regime of the shape resonance in a free electron gas for the low electron density \( \rho < \rho_c \) [4]. The data in the Fig. 5 predict that the range of the overdoped regime is larger for families with lower potential barrier and lower maximum \( T_c \). This effect is determined by the finite dispersion \( \Delta E_{n,\perp} \) of the superlattice subband in the direction transversal to the stripe direction. The origin of this effect can be understood by plotting in Fig. 6 the gap amplitude \( \Delta_2 \) at \( n = 2 \) resonance as a function of the energy separation from the bottom of the second subband \( E_{2b} \), in units of the energy cutoff \( \hbar \omega_0 \) for \( V_b = 150 \) meV (panel a) and \( V_b = 450 \) meV (panel b). In this scale the width of the “shape resonance” for the superconducting gap is ~1. Clearly the wide range for the overdoped regime is due to a relevant hopping between stripes \( \Delta E_{2\perp}/\hbar \omega_0 = 0.5 \) in panel (a), while a sharp drop of the resonance in the overdoped regime, recovering the shape of the 1D resonance for the case of zero single particle hopping between the stripes [9], is shown in panel (b) with \( \Delta E_{2\perp}/\hbar \omega_0 = 0.06 \).

4. CONCLUSIONS

We have shown presence of a “shape resonance” for the superconducting gap in a superlattice of mesoscopic quantum stripes when the condition \( \Delta E_{2\perp}/\hbar \omega_0 < 1 \) between the transversal superlattice dispersion and the energy cutoff for the interaction is satisfied. A small potential barrier of few hundreds meV is enough to give the quasi 1D confinement for an electron gas with effective mass \( m^* = 2.5 \), potential barrier width \( W = 10 \) Å and stripe width \( L = 15 \) Å as it has been recently found in cuprate superconductors.

The critical charge density for maximum gap amplification is in qualitative agreement with experimental values of doping in cuprate superconductors \( \delta_c \sim 0.12 \) hole per Cu site and it is mainly determined by the stripe width \( L \). Also the calculated range of charge density giving the width of the resonance is in agreement with experimental values by assuming an energy cutoff for the interaction \( \hbar \omega_0 = 600 \) K.

The gap resonance shows a first regime in the high charge density range \( \rho > \rho_c \) where the DOS shows a 1D behavior and the blue shift of the chemical potential in the superconducting phase. We have associated this regime with the underdoped regime in cuprate superconductors.
The gap resonance shows a second regime in the low charge density range $\rho < \rho_c$ where the DOS shows a 2D behavior and a red shift of the chemical potential in the superconducting phase is predicted. We have associated this regime with the overdoped regime in cuprate superconductors. The width of the overdoped regime increases with the transversal hopping between stripes. From these results a different shape of the Fermi surface and electronic behavior is predicted for the underdoped vs the overdoped regime.

Acknowledgements—This work was partially founded by Istituto Nazionale di Fisica Nucleare, Consiglio Nazionale delle Ricerche and Istituto Nazionale di Fisica della Materia.

REFERENCES