The Current Density on the Fermi Surface for Superconductivity with d-wave Symmetry

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In this work, a theoretical model within the Generalized Hubbard Hamiltonian on a square lattice is considered to evaluate the current density $J(\boldsymbol{k}_F) = qn_s v_g(\boldsymbol{k}_F)$, at the Fermi Surface, for a superconductor wire, where q is electron charge, n_s the superconductor electronic density, and v_g the group velocity, which depends of $\boldsymbol{k}$. For an appropriate set of parameters of the Hamiltonian, to reach Tc=100K, the group velocity was evaluated at finite temperature within of superconducting state, and evaluated on the Fermi surface: The order of magnitude for J, depending of its temperature, can be variating from 1 MA/cm^2 to hundreds of MA/cm^2. This result is within the order of magnitude to the expected value for HTS, such as YBCO system.

Outline

- The Generalized Hubbard model in Real and Reciprocal space.
- The BCS coupled equations for d-wave symmetry.
- Criterium to choose the appropriate set of Hamiltonian parameters.
- The importance of optimal doping where T_c is máximum.
- The Current Density (J) as a function of QSPE.
- The J for the d-wave superconductor state on the FS.
- Conclusions .

Glossary of energies

- Kinetic energy of electrons; due the jump between sites in the crystalline lattice $\rightarrow$ Hoppings; t, t'.
- Potential energy or Coulombic interactions between the electrons; $v(\boldsymbol{r}-\boldsymbol{r}') \rightarrow$ interaction parameters; $U, V, \Delta t, \Delta t_3$.
- Permitted energies for the system of single particule, it is the dispersion relation as a function of electronic states $\rightarrow \varepsilon_{MF}(\boldsymbol{k})$.
- Binding energy for the Cooper pairs, it is the amplitude of superconducting gap $\rightarrow \Delta_d$
- Quasi particle energy, it is the dispersión relation for the Cooper pairs $\rightarrow E(\boldsymbol{k})$.
- Excitation of a single Cooper pair, it is the minimum energy necessary to break a Cooper pair, along of particular direction within of 1BZ $\rightarrow \Delta_0(\boldsymbol{k})$.
- The Fermi energy, the máximum energy of occupied states at T=0.

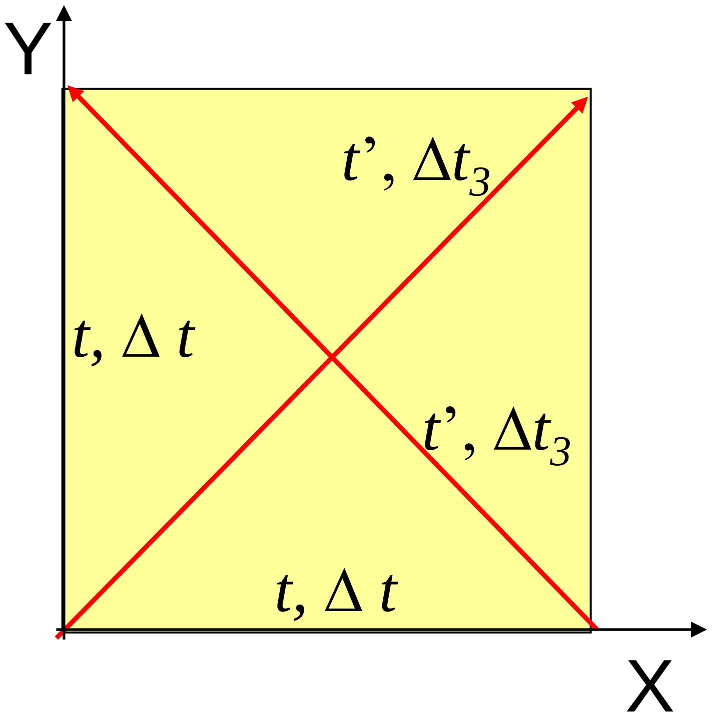
Hubbard model (Real space)

- We consider a single-band Hubbard model in a square lattice with first- (Δt) and second-neighbor (Δt_3) correlated hoppings, in addition to on site (U) and first-neighbor (V) Coulombic repulsions.

$$\hat{H} = t \sum_{<i,j>,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + t' \sum_{\ll i,j \gg,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j + \Delta t \sum_{<i,j>,\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{\substack{<i,l><j,l> \\ \ll i,j \gg,\sigma}} c_{i,\sigma}^{\dagger} c_{j,\sigma} n_l$$

- where $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$, and $c_{i,\sigma}^{\dagger}$ $\left(c_{i,\sigma}\right)$, is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i. $< i,j >$ and $<< i,j >>$ denote nearest-neighbour and next-nearest neighbour sites, respectively.

Definitions for the Hubbard model parameters



The hoppings to first and second neighbor in the square lattice.

Single-particle parameters

$t_{i,j} = \int d^3\mathbf{r}\, \varphi^*(\mathbf{r}-\mathbf{R}_i)\lfloor -\frac{\hbar^2\nabla^2}{2m} + u(\mathbf{r})\rfloor \varphi(\mathbf{r}-\mathbf{R}_i)$; $u(\mathbf{r})$ is the lattice periodic potential

$t = t_{i,j}$ for $< i,j >$

$t' = t_{i,j}$ for $\ll i,j \gg$

Electron-electron interaction parameters

$U_{ij}^{kl} = \int d^3\mathbf{r} d^3\mathbf{r}' \varphi^*(\mathbf{r}-\mathbf{R}_j)\varphi^*(\mathbf{r}'-\mathbf{R}_j) v(\mathbf{r}-\mathbf{r}')\varphi(\mathbf{r}-\mathbf{R}_k)\varphi(\mathbf{r}'-\mathbf{R}_l)$;

$v(\mathbf{r}-\mathbf{r}')$ is the interaction potential between two electrons in the lattice

$U = U_{ii}^{ii}$; $\Delta t = U_{ii}^{ij}$ with $< i,j >$; $\Delta t_3 = U_{lj}^{il}$ with $< i,l >, < j,l >$ and $\ll i,j \gg$

The Hubbard model (Reciprocal space)

After a Fourier transformation $c^{\dagger}_{\mathbf{k},\sigma} = \frac{1}{N_s} \sum_j \exp(i\mathbf{k} \cdot \mathbf{R}_j) c^{\dagger}_{j,\sigma}$

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{MF}(\boldsymbol{k}) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} V_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q},\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{q},\downarrow} c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}'+\mathbf{q},\uparrow}$$

Where :

$$V_{\mathbf{k},\mathbf{k}',\mathbf{q}} = U + V\beta(\mathbf{k} - \mathbf{k}') + \Delta t[\beta(\mathbf{k} + \mathbf{q}) + \beta(-\mathbf{k} + \mathbf{q}) + \beta(\mathbf{k}' + \mathbf{q}) + \beta(-\mathbf{k}' + \mathbf{q})] + \Delta t_3[\gamma(\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}) + \gamma(-\mathbf{k} + \mathbf{q}, -\mathbf{k}' + \mathbf{q})]$$

with

$$\beta(\mathbf{k}) = 2[cos(k_x a) + cos(k_y a)]$$

$$\gamma(\mathbf{k}.\mathbf{k}') = 4cos(k_x a)cos(k'_y a) + 4cos(k'_x a)cos(k_y a)$$

The Coupled Equation for *d-wave* Symmetry

1) Gap Δ_d : $$1 = -\frac{(V - 4\Delta t_3)a^2}{4\pi^2} \iint_{1BZ} \left\{ \frac{\left[\cos(k_x a) - \cos(k_y a)\right]^2}{2E(\boldsymbol{k})} \tanh\left(\frac{E(\boldsymbol{k})}{2k_B T}\right) \right\} dk_x dk_y$$

2) Chemical potential μ : $$n - 1 = -\frac{a^2}{4\pi^2} \iint_{1BZ} \frac{\varepsilon_{MF}(\boldsymbol{k}) - \mu}{E(\boldsymbol{k})} \tanh\left(\frac{E(\boldsymbol{k})}{2k_B T}\right) dk_x dk_y$$

The Mean Field (MF) Dispertion relation $$\varepsilon_{MF}(\boldsymbol{k}) = E_{MF} + t_{MF}\left[\cos(k_x a) + \cos(k_y a)\right] + 4t'_{MF}\cos(k_x a)\cos(k_y a)$$

With the MF hoppings $E_{MF} = \left(\frac{U}{2} + 4V\right)n,\quad t_{MF} = t + n\Delta t,\quad t'_{MF} = t' + 2n\Delta t_3.$

The QSPE $E(\boldsymbol{k}) = \sqrt{(\varepsilon_{MF}(\boldsymbol{k}) - \mu)^2 + \Delta^2(\mathbf{k})}$: $\Delta(\mathbf{k}) = \Delta_d\left[\cos(k_x a) - \cos(k_y a)\right]$

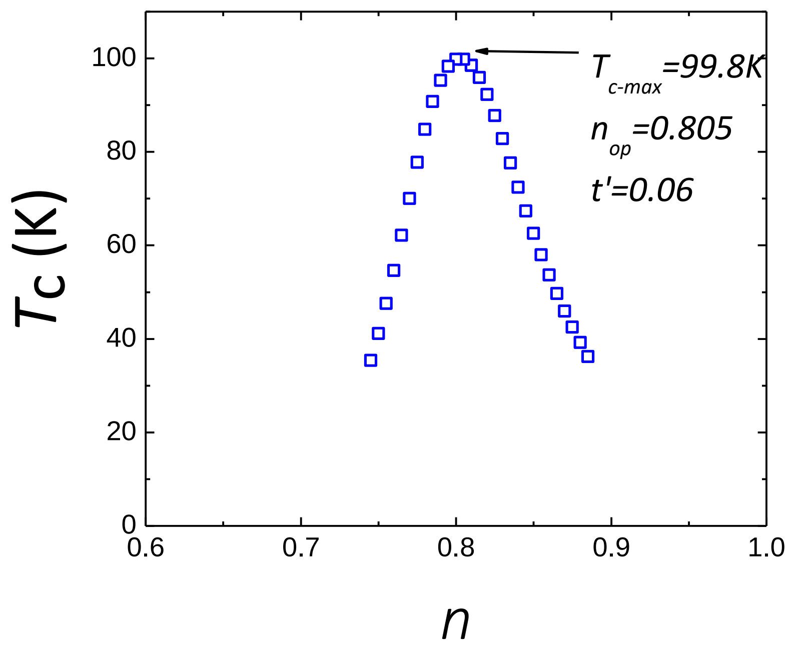
The ground state Energy $\left(E_g\right)$ by site

- Since the microscopic point of view for the superconductor state, the wave function is as a function of probability amplitudes to find states of pairs $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ occupied (un-occupied), and they are $v_{\boldsymbol{k}}(u_{\boldsymbol{k}})$, respectively;
- Therefore $\psi_g = \pi_{\boldsymbol{k}}\left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger}\right)|\varphi\rangle$ is the ground state BCS-like wavefunction, where:

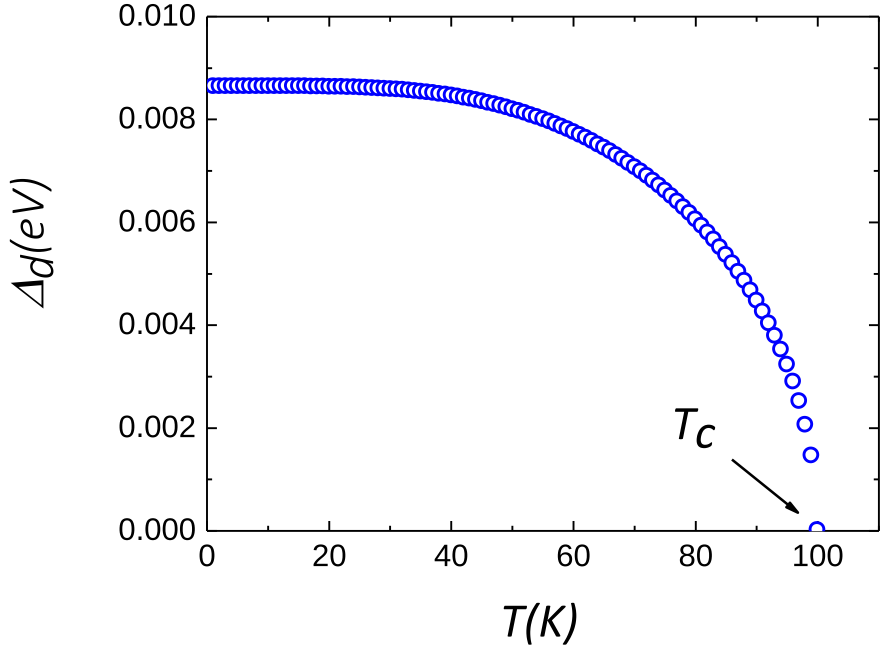
$$v_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_{MF}(\boldsymbol{k}) - \mu}{E(\boldsymbol{k})}\right)}, u_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_{MF}(\boldsymbol{k}) - \mu}{E(\boldsymbol{k})}\right)} \rightarrow u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2 = 1.$$

$$E_g = \langle \psi_g | \widehat{H} | \psi_g \rangle = \frac{1}{N_s} \sum_{\boldsymbol{k}} [\varepsilon_{MF}(\boldsymbol{k}) - E(\boldsymbol{k})] + \frac{\Delta_d^2}{4\Delta t_3 - V} + (n-1)\mu - \left(\frac{U}{4} + 2V\right) n^2$$

The *d-wave* behavior

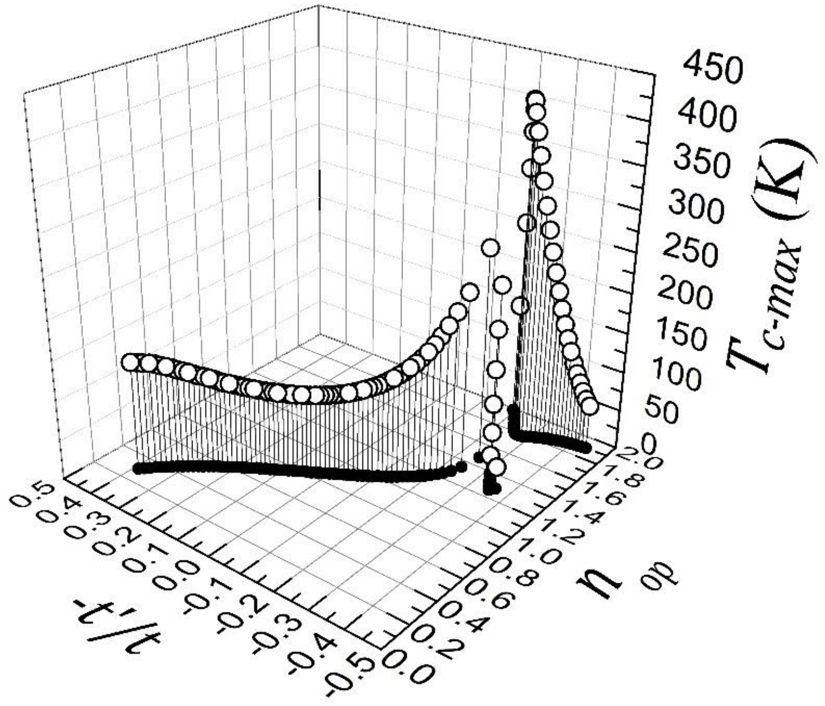


The critical temperature (T_c) against n with Δt=0.5$|t|$ and Δt_3=0.05$|t|$.

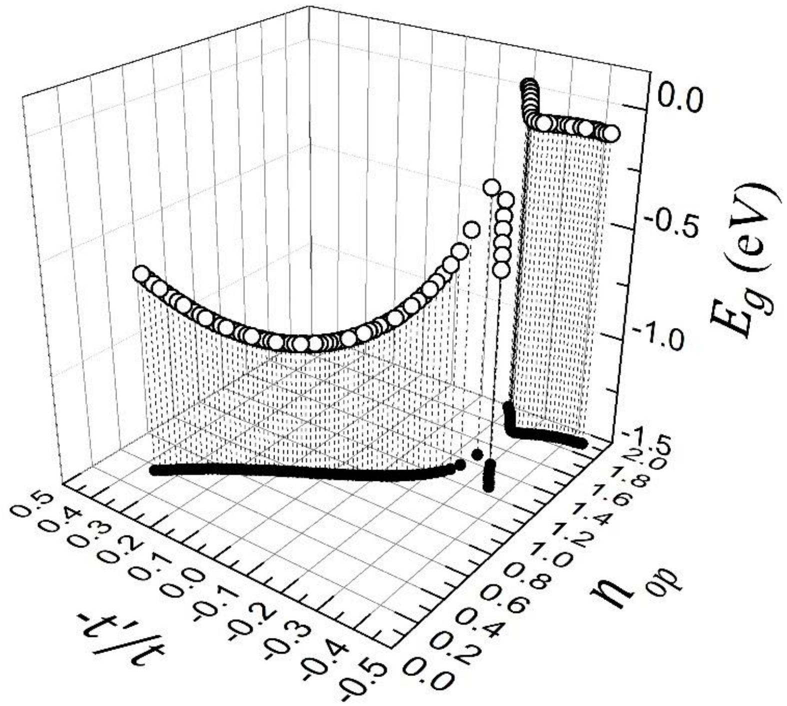


The SC gap (Δ_d) as a function of the temperature (T).

T_{c-max}

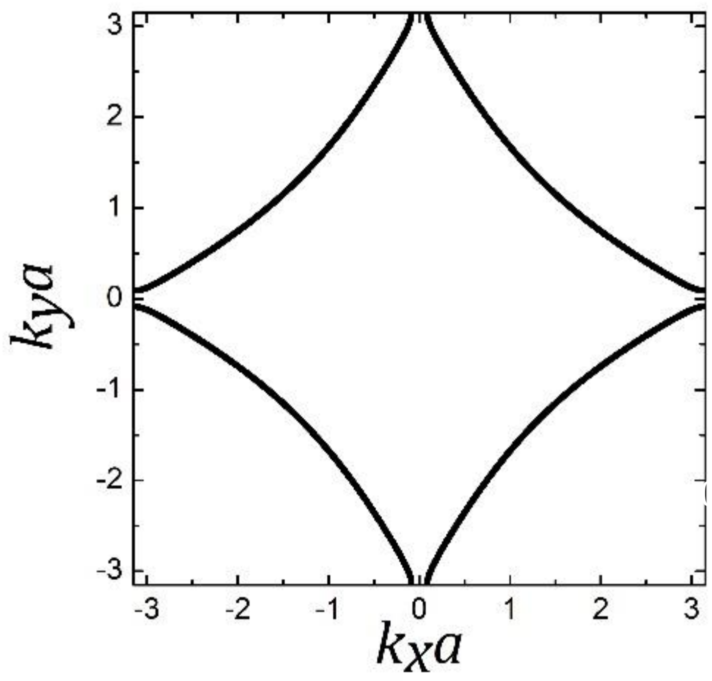


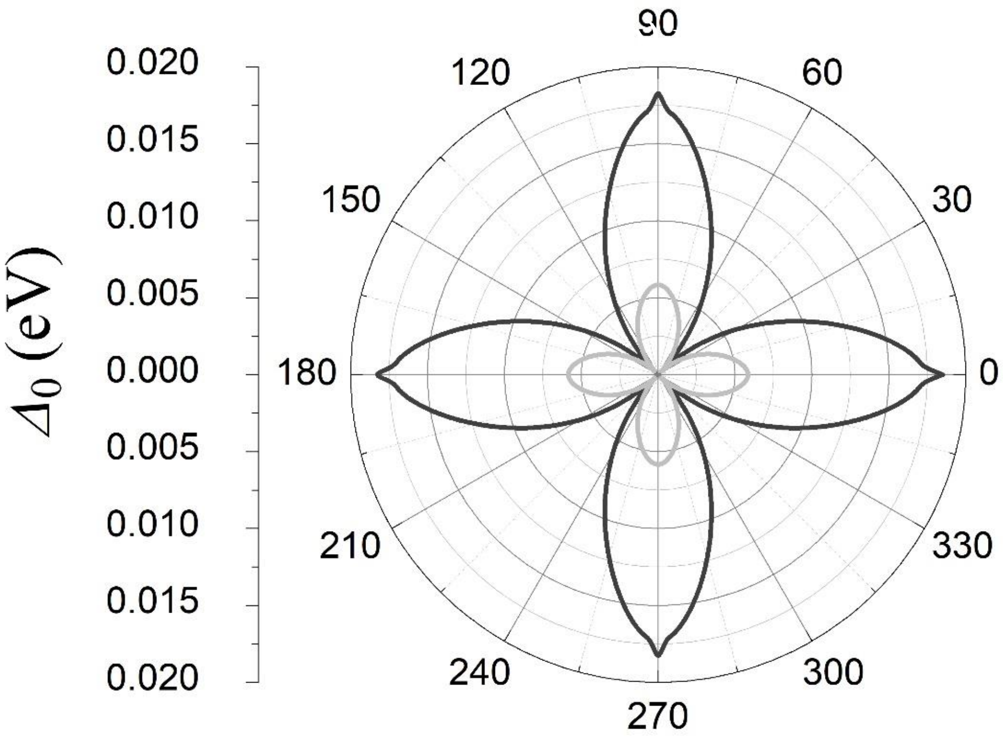
Ground state energy E_g



$U=V=0,\ \Delta t=0.5\ eV,\ \Delta t_3=0.05eV$

Fermi Surface and Δ_0





The evaluation for the FS considers the condition $\varepsilon_{MF}(\boldsymbol{k}_F) = \mu$

n=0.805, t'=0.06, Δ_d=8.634meV, $E_F = -555.325$meV.

Concept of the Current density J

- *Since the quantum mechanic point of view, the current density can be considered as the probability of radiant flux.*
- *If one thinks as a heterogeneous fluid, then the probability current is the rate of flow of this fluid.*
- *As an examples: Probability currents of mass in hydrodynamic, and charges in electromagnetism.*
- *In the superconductor state, the probability current is the rate of flow of Cooper´s pairs which form the superconductor condensate.*

Definition of J

- In one dimension, for a free particle with spin 0:

$$J = \frac{1}{2m}(\psi^* p_x \psi - \psi p_x^* \psi^*),$$

- where ψ is the wave function and $p_x = \left(\frac{\hbar}{i}\right)\frac{d}{dx}$ is the momentum operator
- In two or three dimensions, this generalizes to:

$$J = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*).$$

- But the last formula is equivalent to:

$$J = \frac{\rho}{m} v_g, \text{ where } \rho = |\psi|^2 \text{ and } v_g(\boldsymbol{k}) = \frac{1}{\hbar}|\nabla\, S(\boldsymbol{k})|$$

Equivalent formulas for radiant flux

Assume $\psi = Re^{iS/\hbar}$ where R, S are real functions of (r, t).

The density of probability is $\rho = \psi\psi^* = |\psi|^2 = R^2$.

The probabillity of current $J = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$ is:

$$J = \frac{\hbar}{2mi}\left(Re^{-iS/\hbar}\nabla Re^{iS/\hbar} - Re^{iS/\hbar}\nabla Re^{-iS/\hbar}\right)$$

$$=\frac{\hbar}{2mi}\left(Re^{-iS/\hbar}\left(e^{iS/\hbar}\nabla R + R\frac{i}{\hbar}e^{iS/\hbar}\nabla S\right) - Re^{iS/\hbar}\left(e^{-iS/\hbar}\nabla R - R\frac{i}{\hbar}e^{-iS/\hbar}\nabla S\right)\right)$$

$$= \frac{1}{m}R^2\nabla S \rightarrow J = \frac{1}{m}\rho\nabla S.$$

Gradient of E

- From $E(\boldsymbol{k}) = \sqrt{(\varepsilon_{MF}(\boldsymbol{k}) - \mu)^2 + \Delta^2(\mathbf{k})}$ we obtain $\nabla E(\boldsymbol{k})$:
- $\frac{\partial E}{\partial k_x} = \frac{1}{2}\left\{\frac{\begin{gathered}2a(\varepsilon_{MF}(\boldsymbol{k})-\mu)\left(-2t_{MF}\sin(k_x a)-4t'_{MF}\sin(k_x a)\cos\left(k_y a\right)\right)\\ +2\Delta_d^2 a\left(\cos(k_x a)-\cos\left(k_y a\right)\right)(-\sin(k_x a))\end{gathered}}{\sqrt{(\varepsilon_{MF}(\boldsymbol{k})-\mu)^2+\Delta^2(\mathbf{k})}}\right\}$
- $\frac{\partial E}{\partial k_y} = \frac{1}{2}\left\{\frac{\begin{gathered}2a(\varepsilon_{MF}(\boldsymbol{k})-\mu)\left(-2t_{MF}\sin\left(k_y a\right)-4t'_{MF}\sin\left(k_y a\right)\cos(k_x a)\right)\\ +2\Delta_d^2 a\left(\cos(k_x a)-\cos\left(k_y a\right)\right)\left(\sin\left(k_y a\right)\right)\end{gathered}}{\sqrt{(\varepsilon_{MF}(\boldsymbol{k})-\mu)^2+\Delta^2(\mathbf{k})}}\right\}$

The SC Current Density J

- For the current density is necessary to obtain the group velocity evaluated on the Fermi surface:

$$v_g(\boldsymbol{k}_F) = \frac{1}{\hbar} |\nabla\, E(\boldsymbol{k}_F)|$$

- The group velocity is $v_g(\boldsymbol{k}_F) = \frac{a\Delta_d}{\hbar}\sqrt{\sin^2(k_{xF}a) + \sin^2(k_{yF}a)}$, where a is the lattice parameter, and Δ_d the d-wave gap amplitude. Assuming $\rho = \frac{n}{V}$ and $q = 2e$, the final expression for the current density is:

$$J(\boldsymbol{k}_F) = \frac{n}{V} 2e \left(\frac{1}{\hbar} a\Delta_d \sqrt{\sin^2(k_{xF}a) + \sin^2(k_{yF}a)} \right)$$

Results

Considering $\Delta t_3 = 0.05\,\text{eV}$ and $\Delta t = 0.5\text{eV}$ as in Ref. [2] to apply the model into YBCO system, which requires $T_c \approx 100\,\text{K}$, the figure show the current density (J) along the Fermi surface.

The lattice parameters are $a = 3.82\text{Å}, b = 3.89\text{Å}, c = 11.68\text{Å}, V = 1.735 \times 10^{-22} cm^3$.

[2] B. Millán, L. A. Pérez and J. S. Millán, Revista Mexicana de Física 64, 233–239 (2018).

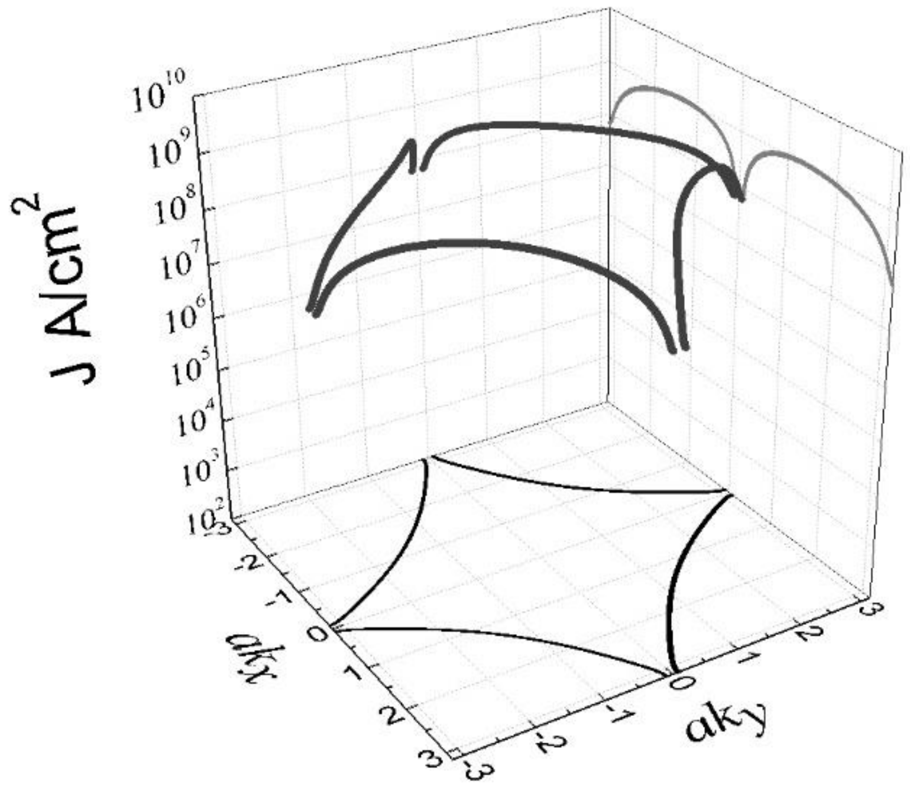


Figure 1. Current density (J) on the Fermi surface, for a set of Hamiltonian parameters with $-t'/t = 0.06$, $\Delta t = 0.5\text{eV}$, and $n = 0.805$.

J vs T

The figure 2 shows the current density as a function of temperature and the gap amplitude for the same system as figure 1 and two different $\boldsymbol{k}_F$ vectors:

Star: $\boldsymbol{k}_{F-1} = (1.323239, 1.319890)$,

$Circle$: $\boldsymbol{k}_{F-2} = (\pi, 0.087194)$.

$\boldsymbol{k}_{F-1} \rightarrow J \rightarrow$maximum.

$\boldsymbol{k}_{F-2} \rightarrow \boldsymbol{J} \rightarrow$minimum close to $(\pi, 0)$.

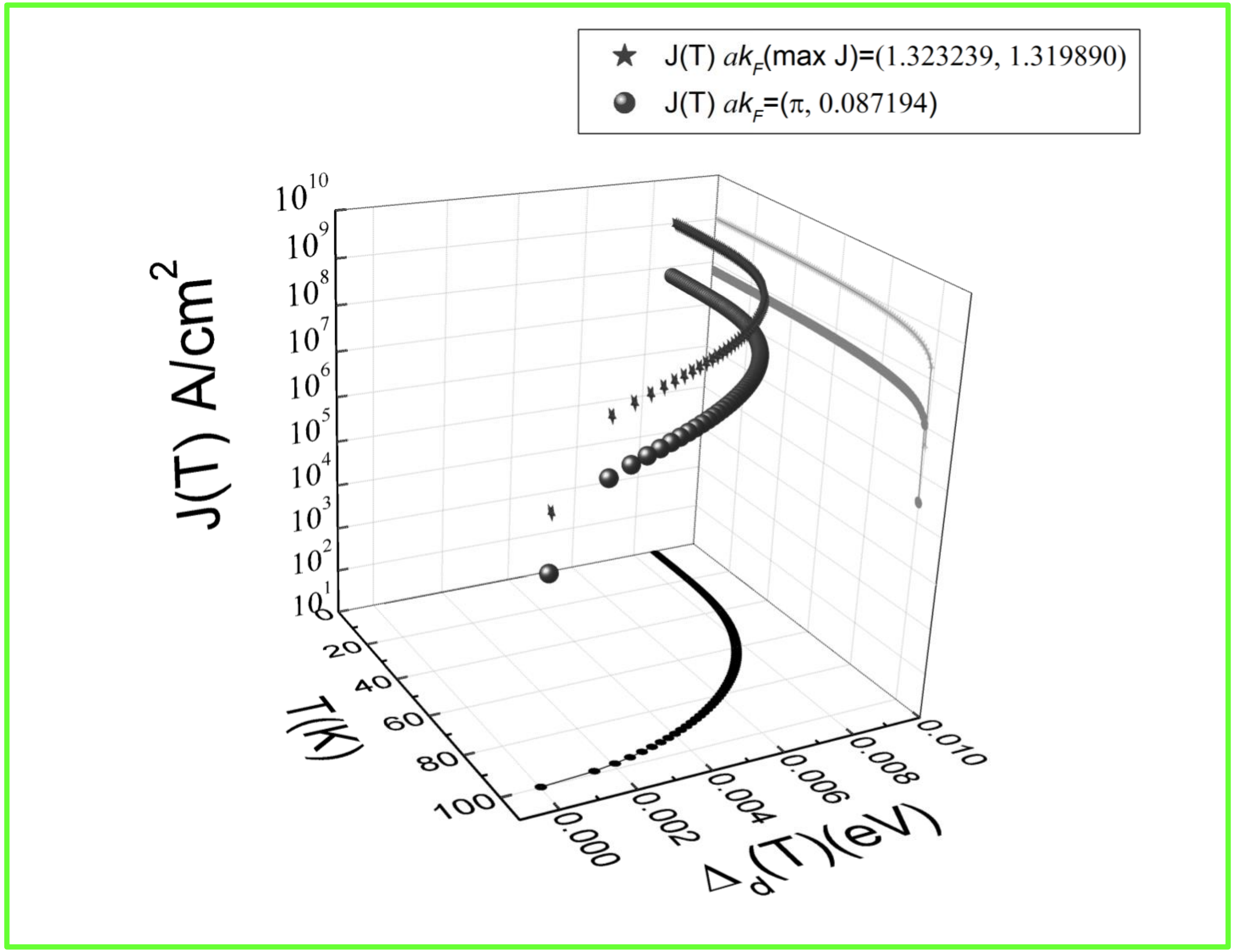


Figure 2. Current density as a function of temperature and gap amplitude for the same system as figure 1.

Applications

- For elements using coated cable superconductor, for example 2G American Superconductor of YBCO

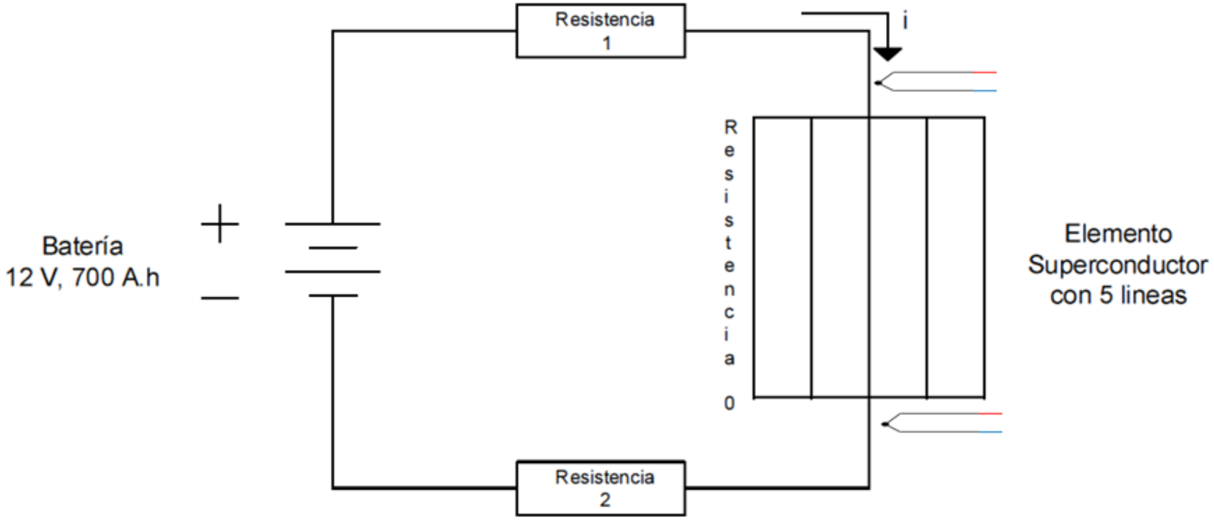


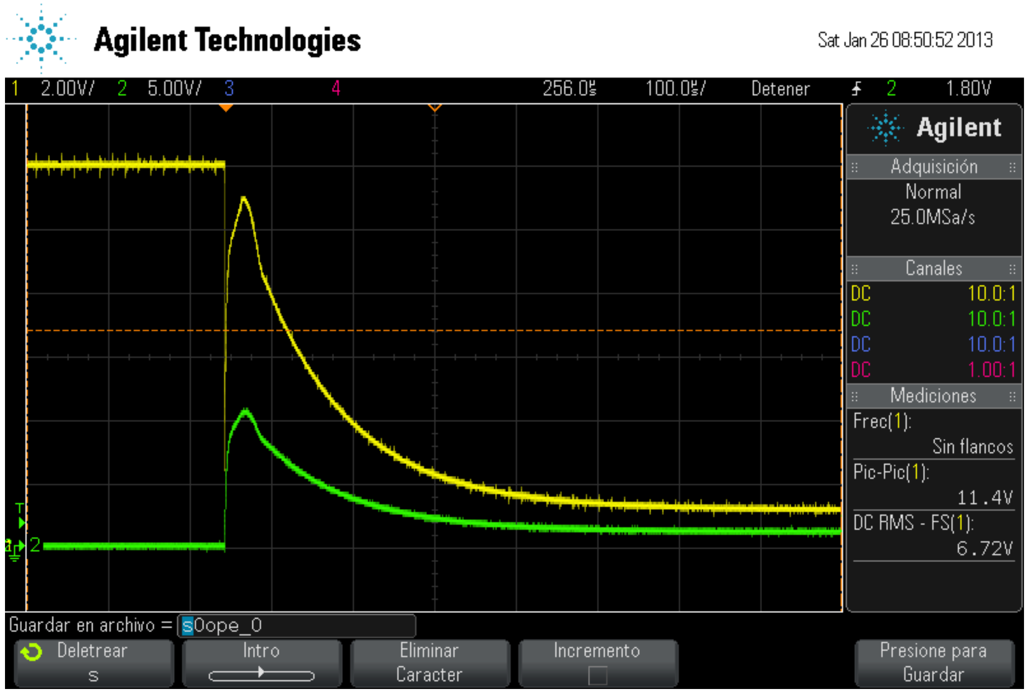
TABLE 1. CURRENT MEASUREMENT IN THE SUPERCONDUCTING STACKING

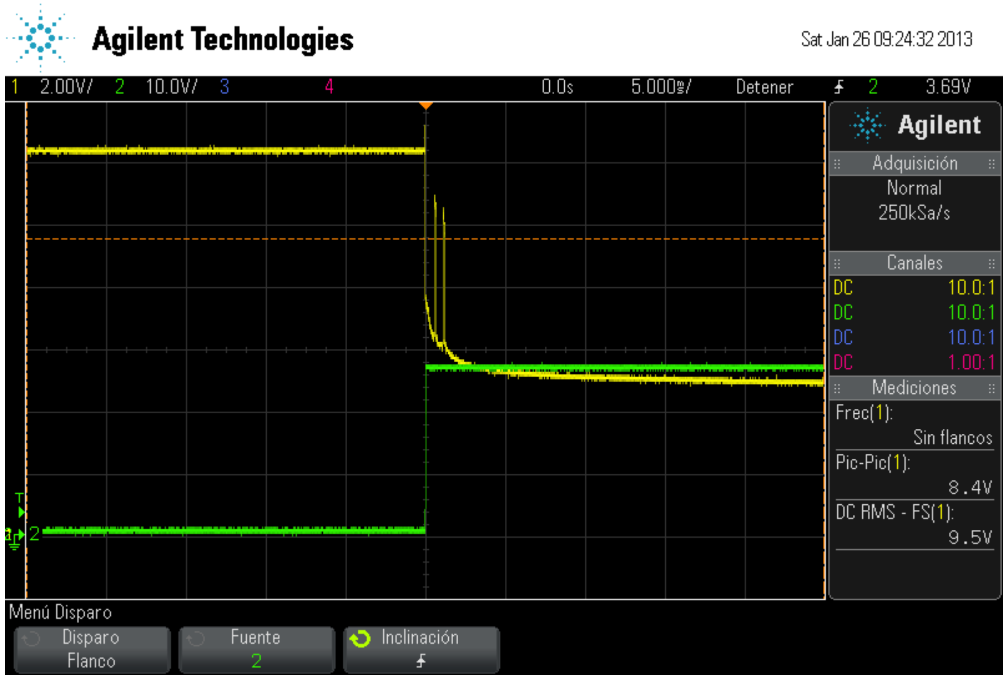
Data	*I (A)*	*J(MA/cm²)*
1	458	2.082
2	472	2.145
3	585	2.66
avg	**505**	**2.29**

Measure of current

Battery charge

Within the battery the current density (J_I) in terms of ionic mobility (μ_I) is given by $J_I = nqv_I$, with $v_I = \mu_I E$, $\mu_I = ZnqD$, and $D = \rho\frac{N}{r}$ is the factor of diffusion which depends of viscosity (ρ), the # of layers of solvation (N) and the ionic radio (r), Z is the valence of ion. Finally in ideal conditions the charge conservation requires the equation of continuity: $J = J_I$





Conclusions

- The Generalized Hubbard model that consider the correlated hopping interactions Δt and Δt_3 result a good aproximation to reproduce superconducting properties in materials with *d*-wave symmetry, which permit to estimate the appropriate set of Hamiltonian paremeters.
- The Quasi Particle Energy is an important parameter that permit study importants superconducting properties, such that the Current Density (J).
- For a set of Hamiltonian parameters choosed under the criterium of supreme in the space (t', n_{op}), J was calculated at two point of FS. The maximum value of J is directed along the diagonal in the 1BZ, while the minimal is along the axis K_x, K_y There are two orders of magnitud, $(10^7 - 10^9)\ \mathrm{A/cm^2}$ of difference between these points.
- The method proposed to calculate J for *d*-wave symmetry can be used for others symmetries like s^* and p-wave.
- The technological applications are many, for example, the performance of charging batteries.

Thank you for your kind attention

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