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Influence the on-site Coulomb interaction on parameters of the superconducting state in a two-dimensional lattice

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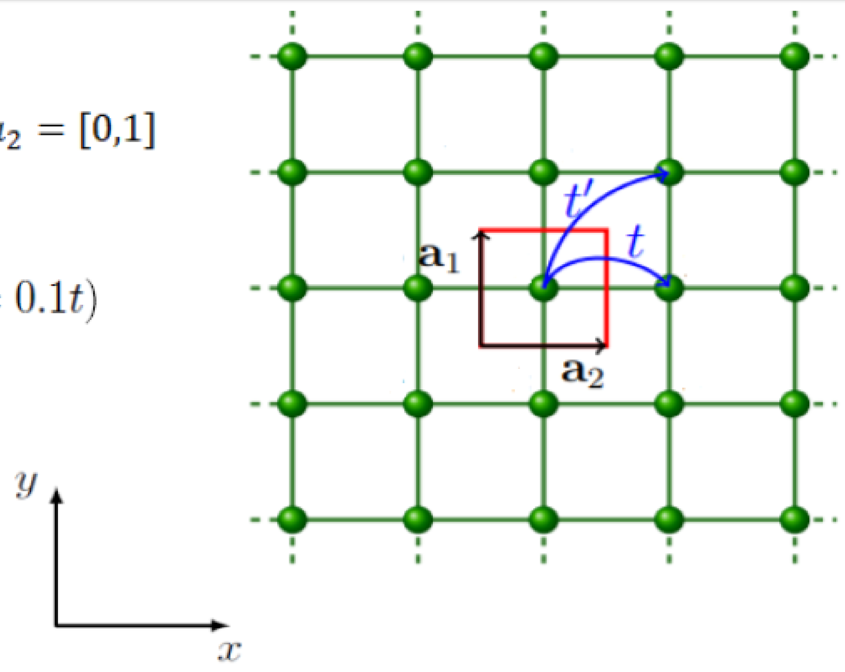
Abstract:

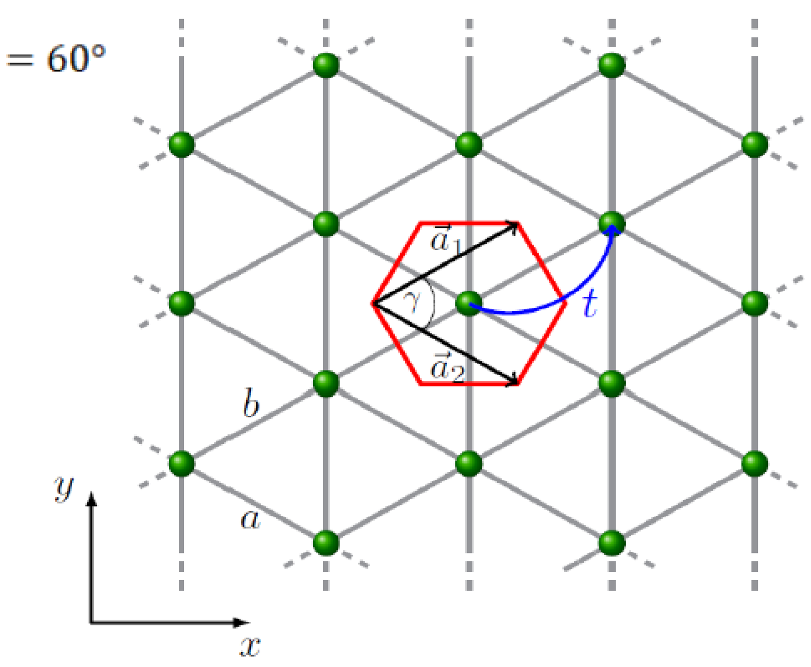
In the framework of the Eliashberg formalism has examined the efect of electron correlations characterized by the on-site Coulomb integral (U) on the electronic density of states and on the thermodynamic properties of the superconducting state in a model square and triangular lattice. We determined the electronic dispersion relation using the tight binding method. We included the U parameter in the calculations using the formalism of the thermodynamic Green functions of the Zubarev type. We determined the Eliashberg function using standard analytical formulas. In particular, we examined the the electronic density of states and the Eliashberg function as a function of U and analyzed the infuence of on-site electron correlations on the parameters of the superconducting state: the electron-phonon coupling constant and the critical temperature.

A square and trianular lattice:

$a_1 = [1,0]$ $a_2 = [0,1]$

$t = 1$ $(t' = 0.1t)$





$a = b = 1$

$\vec{a}_1 = \left[\frac{\sqrt{3}}{2}, \frac{1}{2}\right]$

$\vec{a}_2 = \left[\frac{\sqrt{3}}{2}, -\frac{1}{2}\right]$

$t = 1$

The electronic dispersion relation for the two-dimensional lattices:

$$\varepsilon_{\mathbf{k}} = -2t\left[\cos(k_x) + \cos(k_y)\right] + 4t'\cos(k_x)\cos(k_y) \qquad \varepsilon_{\mathbf{k}} = -2t\left[\cos(k_x) + 2\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right]$$

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{l}} c^{\dagger}_{\mathbf{k}+\mathbf{l}\uparrow} c_{\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}'+\mathbf{l}\downarrow}$$

where $c_{\mathbf{k}\sigma}$ ($c^{\dagger}_{\mathbf{k}\sigma}$) are the annihilation (creation) operators of the electronic state with momentum $\mathbf{k}$ and spin $\sigma \in \{\uparrow, \downarrow\}$

$$\varepsilon^{eff}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \frac{U}{2}\langle n \rangle$$

$\langle n \rangle = \frac{2}{N}\sum_{\mathbf{k}} \langle n_{\mathbf{k}\downarrow} \rangle$ $\qquad (\langle n \rangle = 1)$

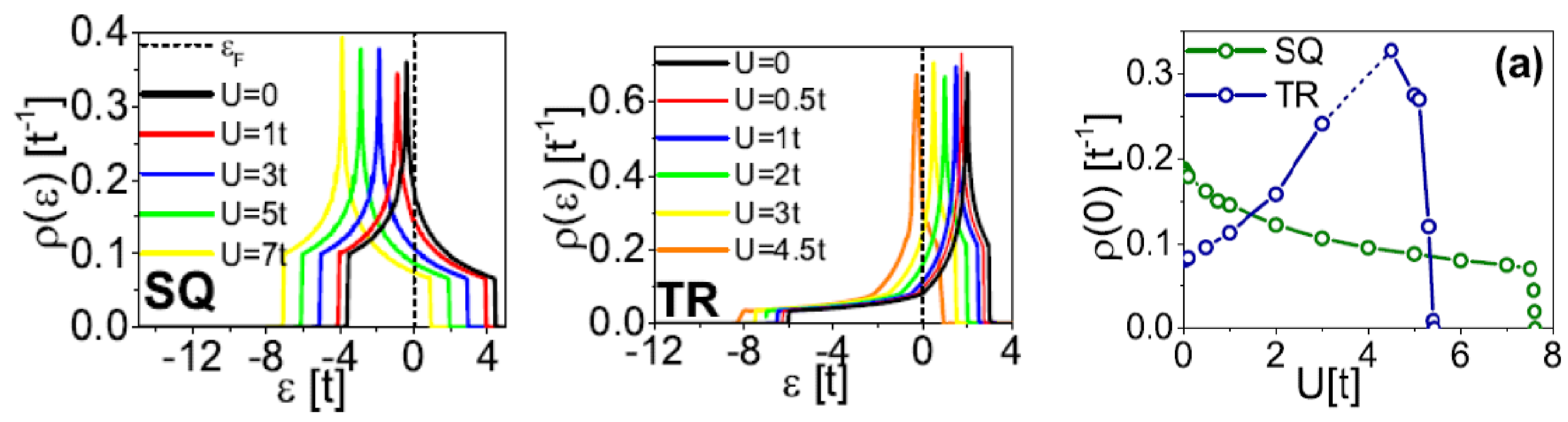
$\langle n_{\mathbf{k}\downarrow} \rangle = \left\langle c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} \right\rangle$ $\qquad (\mu = 0)$

The electron density function of states:

$$\rho(\varepsilon) = \frac{1}{N}\sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon^{eff}_{\mathbf{k}})$$

$\delta(x)$ symbol represents the Dirac distribution

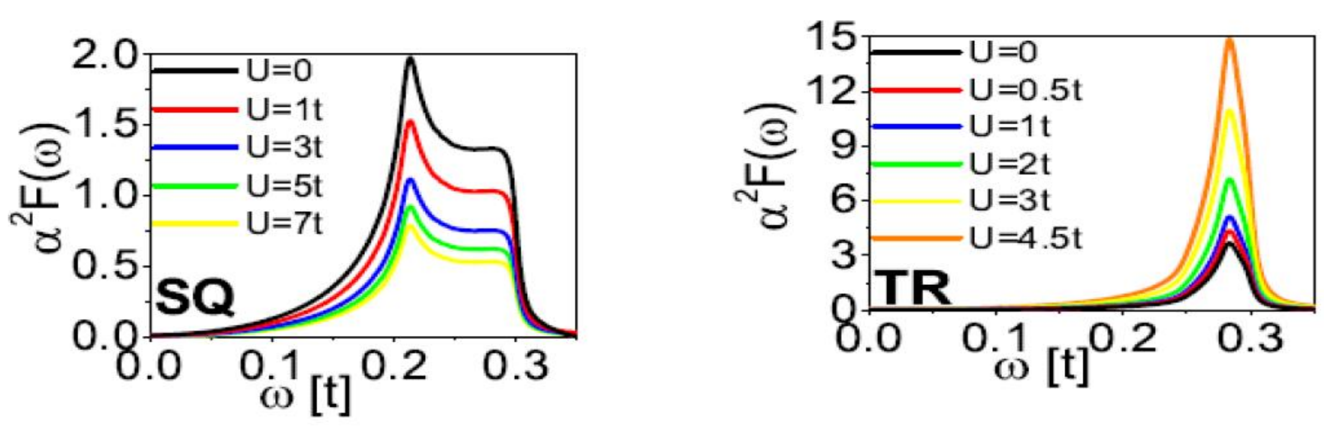
$\delta(x) = \lim_{a \to 0} \frac{1}{\pi}\frac{a}{a^2 + x^2}$



Theisotropic Eliashberg function:

$$\alpha^2 F(\omega) = \rho(0)\sum_{\mathbf{q}} g^2_{\mathbf{q}} \delta(\omega - \omega_{\mathbf{q}})$$

$g_{\mathbf{q}} = g_0|\mathbf{q}|\sqrt{1/\omega_{\mathbf{q}}}$ $\qquad \omega_0 = \{0.15, 0.2\}$ t, $\qquad g_0 = \{0.031, 0.03\}$ $t^{3/2}$



The parameters of the superconducting state:

$$\omega_{\ln} = \exp\left[(2/\lambda) \cdot \int_0^{\infty} d\omega (\alpha^2 F(\omega)/\omega) \ln(\omega)\right]$$

$$\lambda = 2\int_0^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega}$$

$$\Lambda_1 = 1.82(\sqrt{\omega_2}/\omega_{\ln})$$

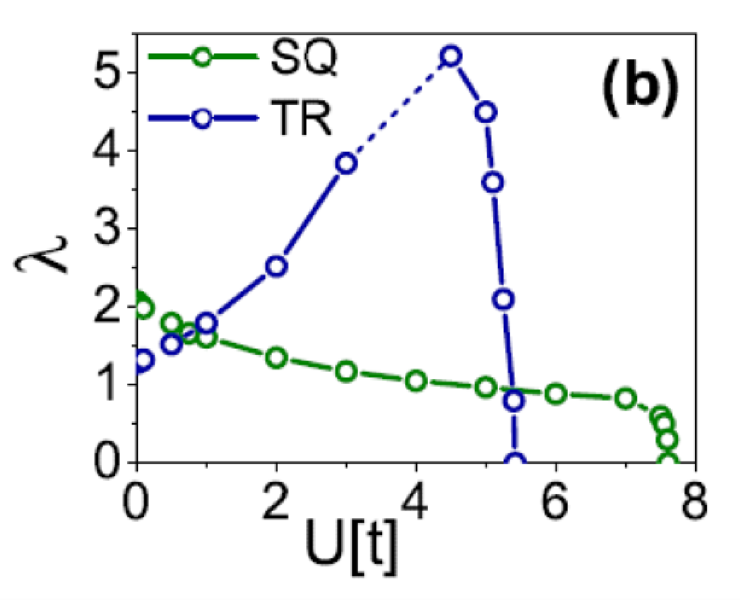
$$f_2 = 1 + ((\sqrt{\omega_2}/\omega_{\ln} - 1)\lambda^2) / (\lambda^2 + \Lambda^1_2)$$

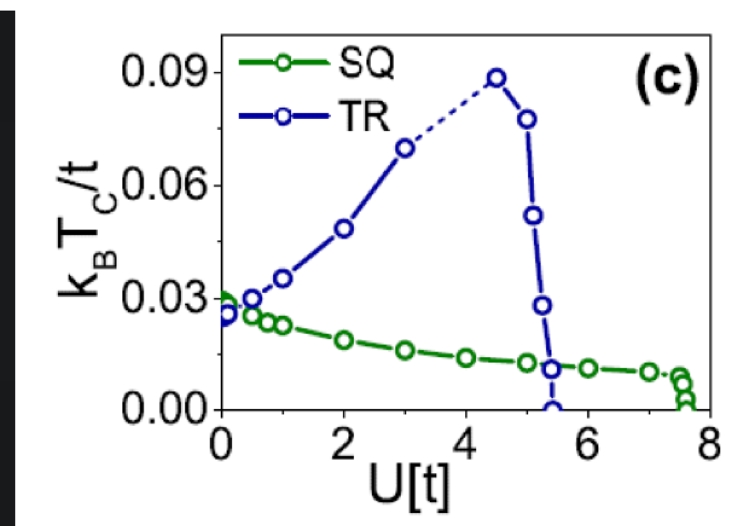
$$\sqrt{\omega_2} = \sqrt{(2/\lambda) \cdot \int_0^{\infty} d\omega \alpha^2 F(\omega)\omega}$$

$$k_B T_C = f_1 f_2 \frac{\omega_{\ln}}{1.2}\exp\left[\frac{-1.04(1+\lambda)}{\lambda}\right]$$

$$f_1 = \left[1 + \left(\frac{\lambda}{2.46}\right)^{3/2}\right]^{1/3}$$

The parameters of the superconducting state:





Conclusions:

- In conclusion, we found that in the square model the superconducting state disappears throughout the course of U, assuming the maximum $\lambda = 2.1$ and $T_c = 84.5$ K for U =0 and disappearing completely for $U_c = 7.61$ t.
- In a triangular lattice the superconducting state is amplied with increasing Coulomb interaction reaching $\lambda = 3.85$ and $T_c = 202.9$ K for U = 3 t. Furthermore, the superconducting state the triangular system tends to decrease in the range of $U \in (4.5, 5.42)$ t, assuming the maximum value of $\lambda = 5.22$ and $T_c = 257.2$ K for U= 4.5 t.

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