FROM THE BCS EQUATIONS TO THE ANISOTROPIC SUPERCONDUCTIVITY EQUATIONS

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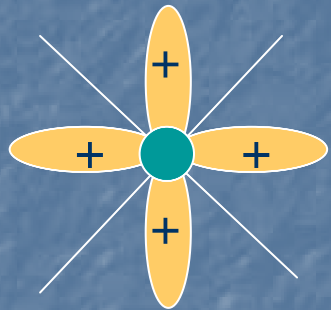
Outline

- MOTIVATION.
- THE GENERALIZED HUBBARD MODEL.
- TWO PARTICLES.
- THE BCS GENERALIZED EQUATIONS.
- THE *p* AND *d* COUPLED EQUATIONS.
- SUPERCONDUCTING PROPERTIES.
- CONCLUSIONS.

2D Superconducting Gap Symmetry

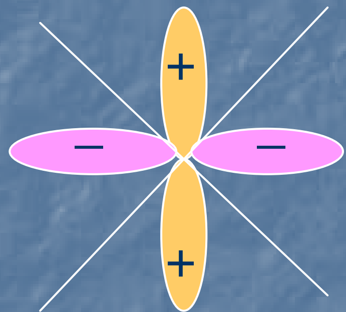
Extended *s** Symmetry



$$g_{s^*}(\mathbf{k}) = \cos(k_x a) + \cos(k_y a)$$

$$\Delta^{(1)}_{s^*}(\mathbf{k}) = \Delta_s + \Delta_{s^*}\, g_{s^*}(\mathbf{k})$$

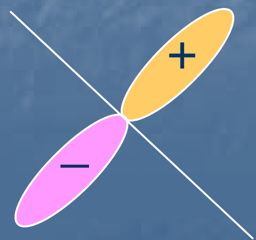
$d_{x^2-y^2}$ Symmetry



$$g_d(\mathbf{k}) = \cos(k_x a) - \cos(k_y a)$$

$$\Delta^{(1)}_{d}(\mathbf{k}) = \Delta_d\, g_d(\mathbf{k})$$

p Symmetry



$$g^{\pm}_{p}(\mathbf{k}) = \sin(k_x a) \pm \sin(k_y a)$$

$$\Delta^{(3)}_{p_\pm}(\mathbf{k}) = \Delta_p\, g^{\pm}_{p}(\mathbf{k})$$

The Pair Symmetry

Singlet (1): $\Phi_S(1,2) = \Psi_S(\mathbf{r}_1, \mathbf{r}_2)\left[\frac{1}{\sqrt{2}}\left(\alpha(1)\beta(2) - \beta(1)\alpha(2)\right)\right],$

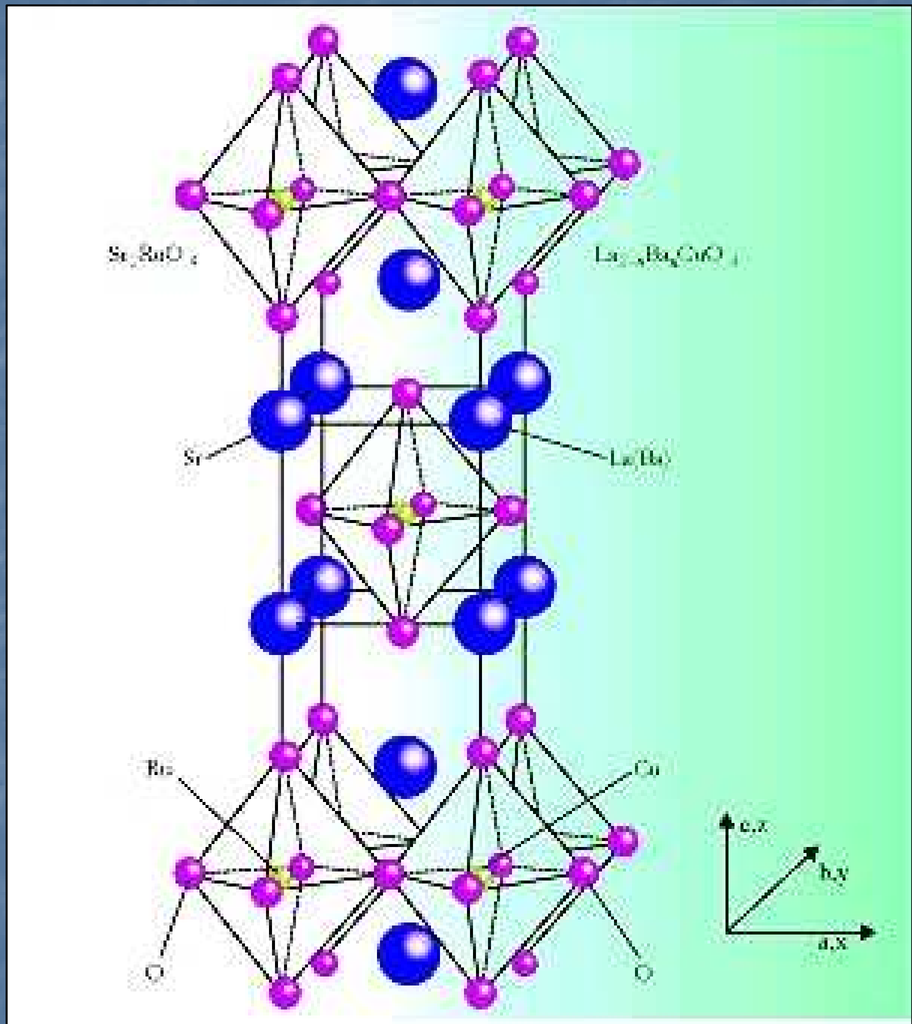
where $\Psi_S(\mathbf{r}_1, \mathbf{r}_2) = \Psi_S(\mathbf{r}_2, \mathbf{r}_1)$, with $\alpha \equiv \uparrow,\ \beta \equiv \downarrow$.

Triplet (3): $\Phi_T(1,2) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2)\left\{\begin{array}{l} \alpha(1)\alpha(2) \\ \beta(1)\beta(2) \\ \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] \end{array}\right\},$

where $\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = -\Psi_T(\mathbf{r}_2, \mathbf{r}_1)$.

The Crystal Structure

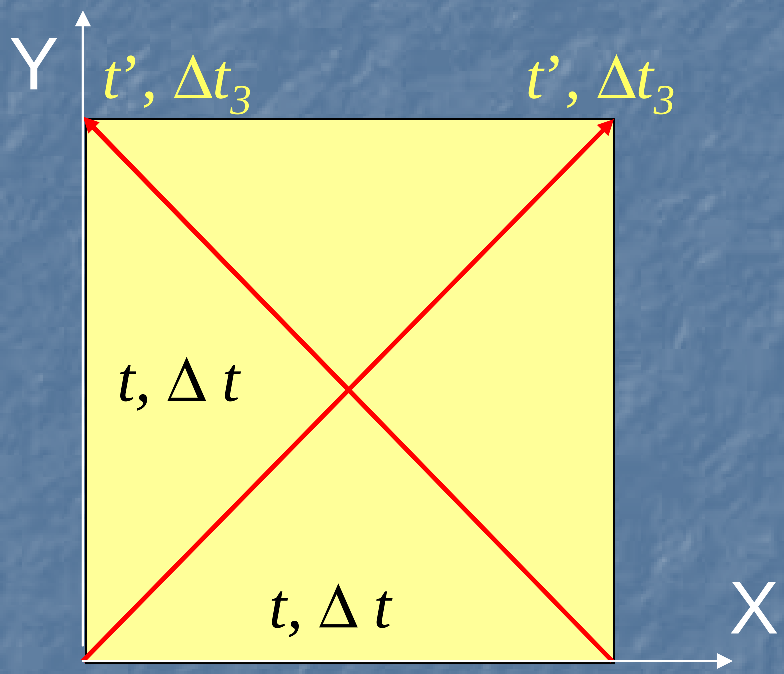
Ru-O planes



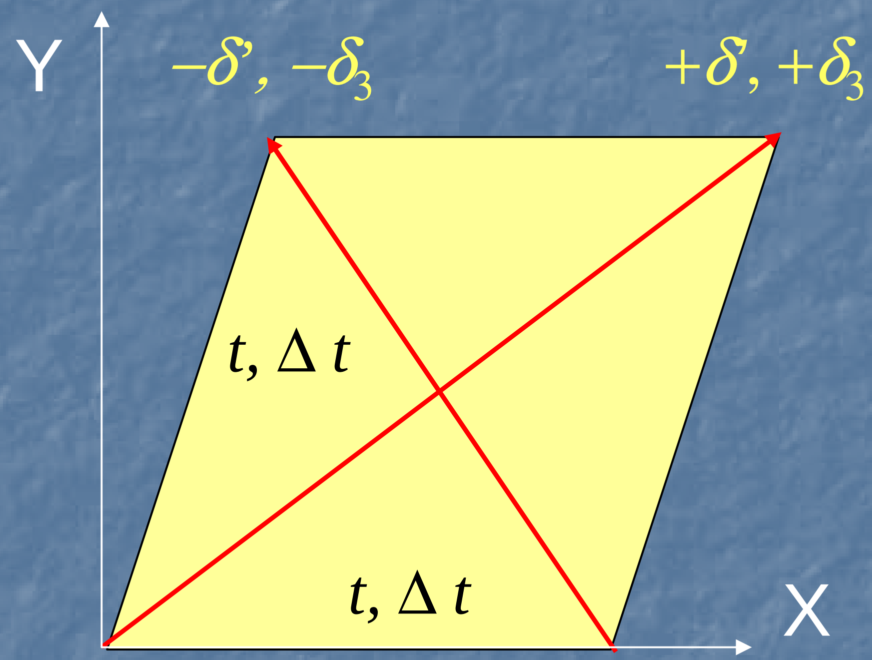
Cu-O planes

Similar Structure for Sr-Ru and La-Ba(Sr) systems

The Distortion of the Square Lattice



The hopping to first and seconds neighbors are the same in both directions



$$t'_{\pm} = t'_0 \pm \delta', \qquad \Delta t_3^{\pm} = \Delta t_3 \pm \delta_3$$

The hopping to seconds neighbors are different in **X+Y**, **X–Y** directions

The Experimental Evidence for a Distortion on the Surface

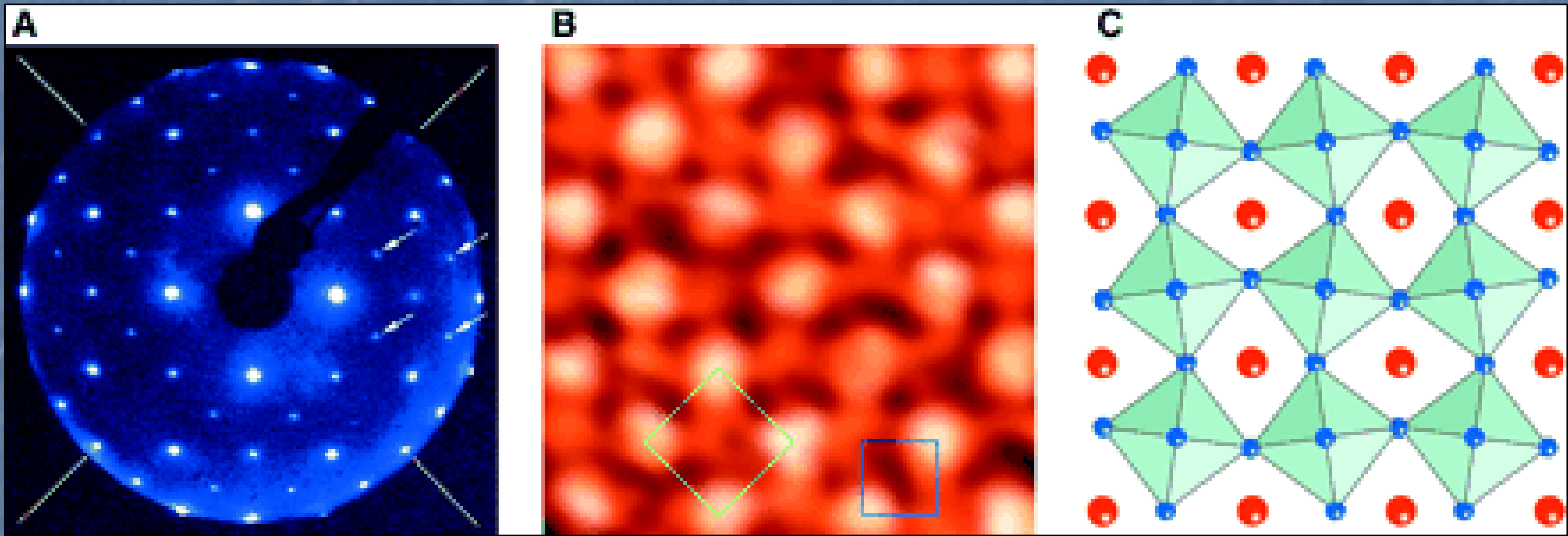


Image of the surface for Sr_2RuO_4 seeing from up of $Ru\text{-}O_2$ planes, where we can see a distortion of the octahedrons formed by oxygens.

Matzdorf, *et al.*, *Science* **289**, 746 (2000).

The Hubbard Model (Real Space)

$$\hat{H}=t_0\sum_{<i,j>\sigma}c^{+}_{i,\sigma}c_{j,\sigma}+t_0'\sum_{<<i,j>>\sigma}c^{+}_{i,\sigma}c_{j,\sigma}+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}+\frac{V}{2}\sum_{<i,j>}n_i n_j+$$

$$\Delta t\sum_{<i,j>,\sigma}c^{+}_{i,\sigma}c_{j,\sigma}(n_{i,-\sigma}+n_{j,-\sigma})+\Delta t_3\sum_{<<i,j>>;<i,l>,<j,l>}c^{+}_{i}c_{j}n_{l}$$

where $\quad n_i=n_{i,\uparrow}+n_{i,\downarrow},\ n_{i,\sigma}=c^{+}_{i,\sigma}c_{i,\sigma},$

$$t_{ij}\equiv\langle i|h|j\rangle=\int d^3r\,\varphi^{*}(\vec{r}-\vec{R}_i)\left[\frac{-\hbar^2\nabla^2}{2m}+u(\vec{r})\right]\varphi(\vec{r}-\vec{R}_j),$$

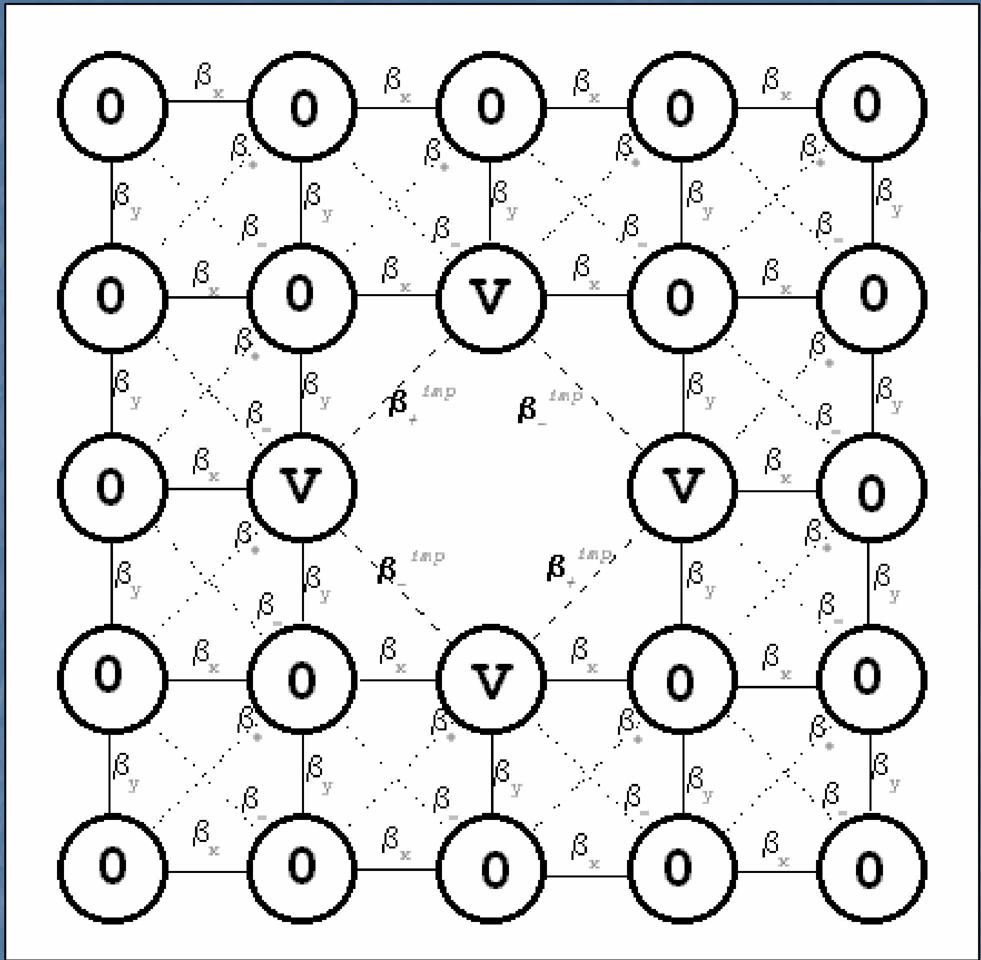
$$U=\langle ii|v|ii\rangle\approx 20\,eV,\ V=\langle ij|v|ij\rangle\approx 3\,eV,$$

$$\Delta t=\langle ii|v|ij\rangle\approx 0.5\,eV\ \ \mathrm{y}\ \ \Delta t_3=\langle ij|v|ik\rangle\approx 0.1\,eV.$$

The integrals of interaction between two electrons are:

$$\langle ij|v|kl\rangle=\int d^3r\,d^3r'\,\varphi^{*}(\vec{r}-\vec{R}_i)\varphi(\vec{r}-\vec{R}_l)v(\vec{r}-\vec{r}')\varphi^{*}(\vec{r}-\vec{R}_j)\varphi(\vec{r}-\vec{R}_k)$$

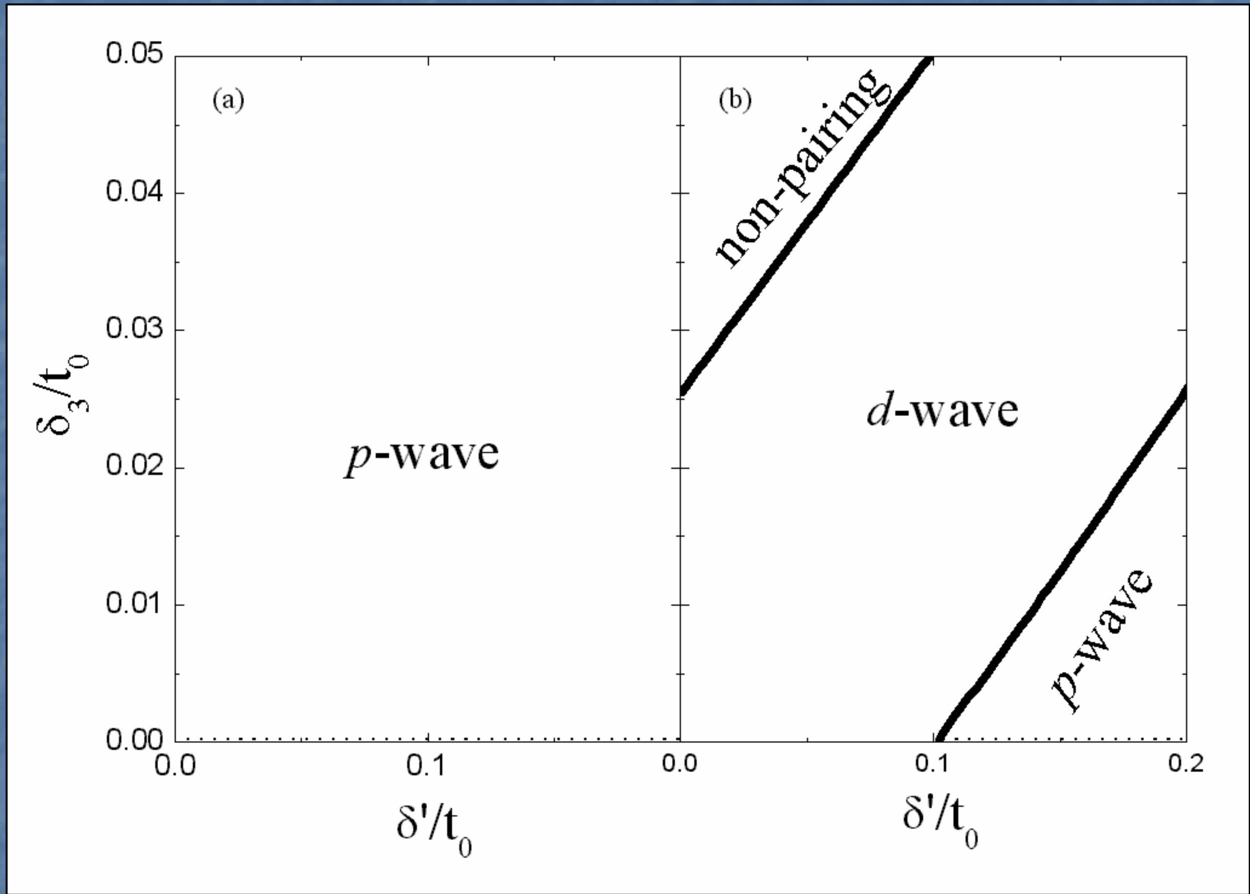
Maping Method to Space of States



$$\beta_x = 2t_0 \cos(K_x a/2)$$
$$\beta_y = 2t_0 \cos(K_y a/2)$$
$$\beta_\pm = 2t'_\pm \cos\left[\left(K_x \pm K_y\right)a/2\right]$$
$$\beta_\pm^{imp} = 2\left(t'_\pm + \Delta t_3^\pm\right)\cos\left[\left(K_x \pm K_y\right)a/2\right]$$
$$pairing \quad condition: \ \Delta_2 = 2E_1 - E_2 > 0$$

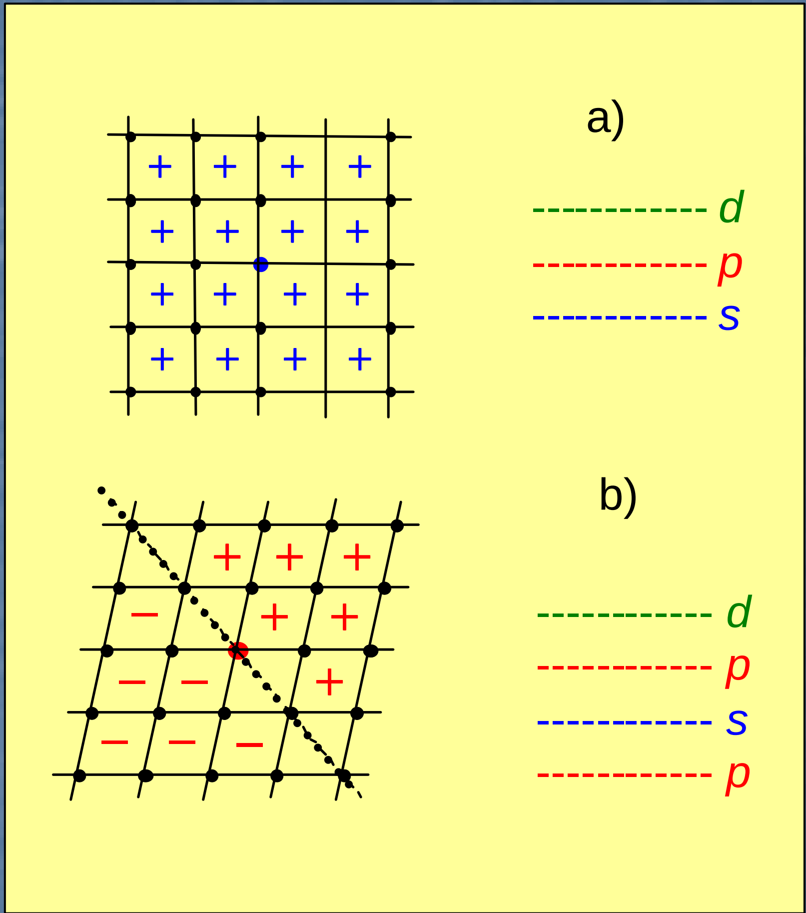
A proyected square lattice for 1742 two particles states with triplet spin corresponding to space of states for hypercube of dimension four. S Millán, *et al.*, Physica C **408**, 259 (2004).

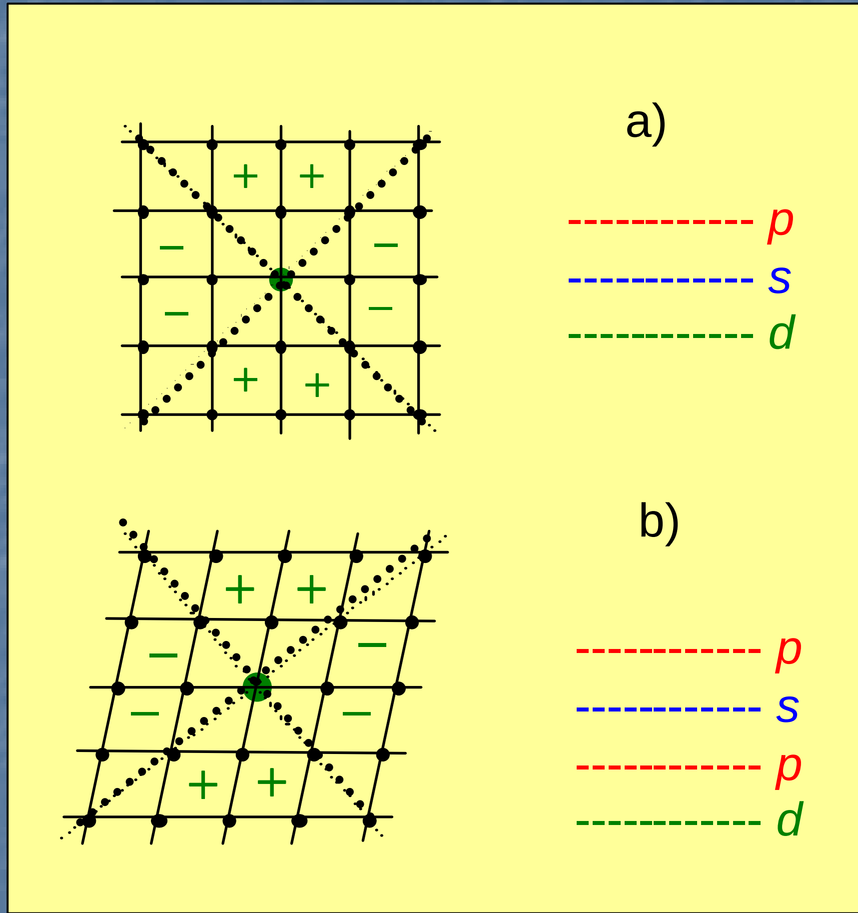
The Phase Diagram
(two particles)



(a) Two electrons t_0=-1, t'=0.45 t_0 (b) Two holes t_0=1, t'=0.45 t_0, both with U=6 $|t_0|$, V=0, Dt=0.5$|t_0|$ y Dt_3=0.1$|t_0|$.

The Electronic Levels





Two electrons

Two holes

The Generalized Hubbard Model

Real Space:

$$\hat{H} = t_0 \sum_{<i,j>\sigma} c^+_{i,\sigma} c_{j,\sigma} + t_0' \sum_{<<i,j>>\sigma} c^+_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j +$$

$$\Delta t \sum_{<i,j>,\sigma} c^+_{i,\sigma} c_{j,\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{<<i,j>>,<i,l>,<j,l>} c_i^+ c_j n_l$$

Reciprocal Space:

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

$$\xi(\mathbf{k}) = [\varepsilon_0(\mathbf{k}) - \mu] \qquad \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}',\sigma} W_{\mathbf{k},\mathbf{k}'} c^+_{\mathbf{k},\sigma} c^+_{-\mathbf{k}',\sigma} c_{-\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}$$

Potential Interaction with Antiparallel Spin:

$$V_{\mathbf{k},\mathbf{k}'} = U + V\beta(\mathbf{k} - \mathbf{k}') + \Delta t[\beta(\mathbf{k}) + \beta(-\mathbf{k}) + \beta(\mathbf{k}') + \beta(-\mathbf{k}')] + 2\Delta t_3^+[\gamma(\mathbf{k},\mathbf{k}')] + 2\Delta t_3^-[\varsigma(\mathbf{k},\mathbf{k}')]$$

Potential Interaction with Parallel Spin: $W_{\mathbf{k},\mathbf{k}'} = \frac{V}{2}\beta(\mathbf{k} - \mathbf{k}') + \Delta t_3^+ \gamma(\mathbf{k},\mathbf{k}') + \Delta t_3^- \varsigma(\mathbf{k},\mathbf{k}')$

where $\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)]$, $\quad \gamma(\mathbf{k},\mathbf{k}') = 2[\cos(k_x a + k'_y a) + \cos(k'_x a + k_y a)]$,

$$\varsigma(\mathbf{k},\mathbf{k}') = 2[\cos(k_x a - k'_y a) + \cos(k'_x a - k_y a)]$$

BCS Generalized Theory

$$\hat{H} = \sum_{\mathbf{k},\sigma} [\varepsilon_0(\mathbf{k}) - \mu] c^{+}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \sigma,\sigma'}} V_{\mathbf{k},\mathbf{k}'} c^{+}_{\mathbf{k},\sigma} c^{+}_{-\mathbf{k},\sigma'} c_{-\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma}$$

For the singlet case the spatial part of the energetic gap is

$$\Delta_{\eta}^{(1)}(\mathbf{k}) = -\sum_{\mathbf{k}'} V^{(e)}(\mathbf{k},\mathbf{k}') \frac{(1-2f_{\mathbf{k}'})}{2\sqrt{\xi^2(\mathbf{k}') + \Delta_{\eta}^2 |g_{\eta}(\mathbf{k}')|^2}} \Delta^{(1)}(\mathbf{k}')$$

where *η* =s, s*, d

$$g_{s*}(\mathbf{k}) = \Delta_s / \Delta_{s*} + [\cos(k_x a) + \cos(k_y a)]$$

$$g_d(\mathbf{k}) = [\cos(k_x a) - \cos(k_y a)]$$

while the triplet case

$$\Delta_{p_\pm}^{(3)}(\mathbf{k}) = -\sum_{\mathbf{k}'} V^{(o)}(\mathbf{k},\mathbf{k}') \frac{(1-2f_{\mathbf{k}'})}{2\sqrt{\xi^2(\mathbf{k}') + \Delta_{\eta}^2 |g_{\eta}^{\pm}(\mathbf{k}')|^2}} \Delta_{p_\pm}^{(3)}(\mathbf{k}')$$

with *η* =p

$$g_{\eta}^{\pm}(\mathbf{k}) = [\sin(k_x a) \pm \sin(k_y a)]$$

Millan, *et al.*, Physics Letters A **335**, 505 (2005).

The Coupled Equation for *p* and *d* Symmetry

p-Symmetry

$$1=-\frac{(V\pm 4\delta_3)}{N_s}\sum_{\mathbf{k}}\frac{\sin^2(k_x a)\pm\sin(k_x a)\sin(k_y a)}{E_p(\mathbf{k})}\tanh\frac{E_p(\mathbf{k})}{2k_B T},$$

where

$$E_p(\mathbf{k})=\sqrt{[\varepsilon_0(\mathbf{k})-\mu]^2+\Delta_p^2\left[\sin(k_x a)\pm\sin(k_y a)\right]^2},$$

d-Symmetry

$$1=-\frac{(V-4\Delta t_3)}{N_s}\sum_{\mathbf{k}}\frac{\cos^2(k_x a)-\cos(k_x a)\cos(k_y a)}{E_d(\mathbf{k})}\tanh\frac{E_d(\mathbf{k})}{2k_B T},$$

where

$$E_d(\mathbf{k})=\sqrt{[\varepsilon_0(\mathbf{k})-\mu]^2+\Delta_d^2\left[\cos(k_x a)-\cos(k_y a)\right]^2},$$

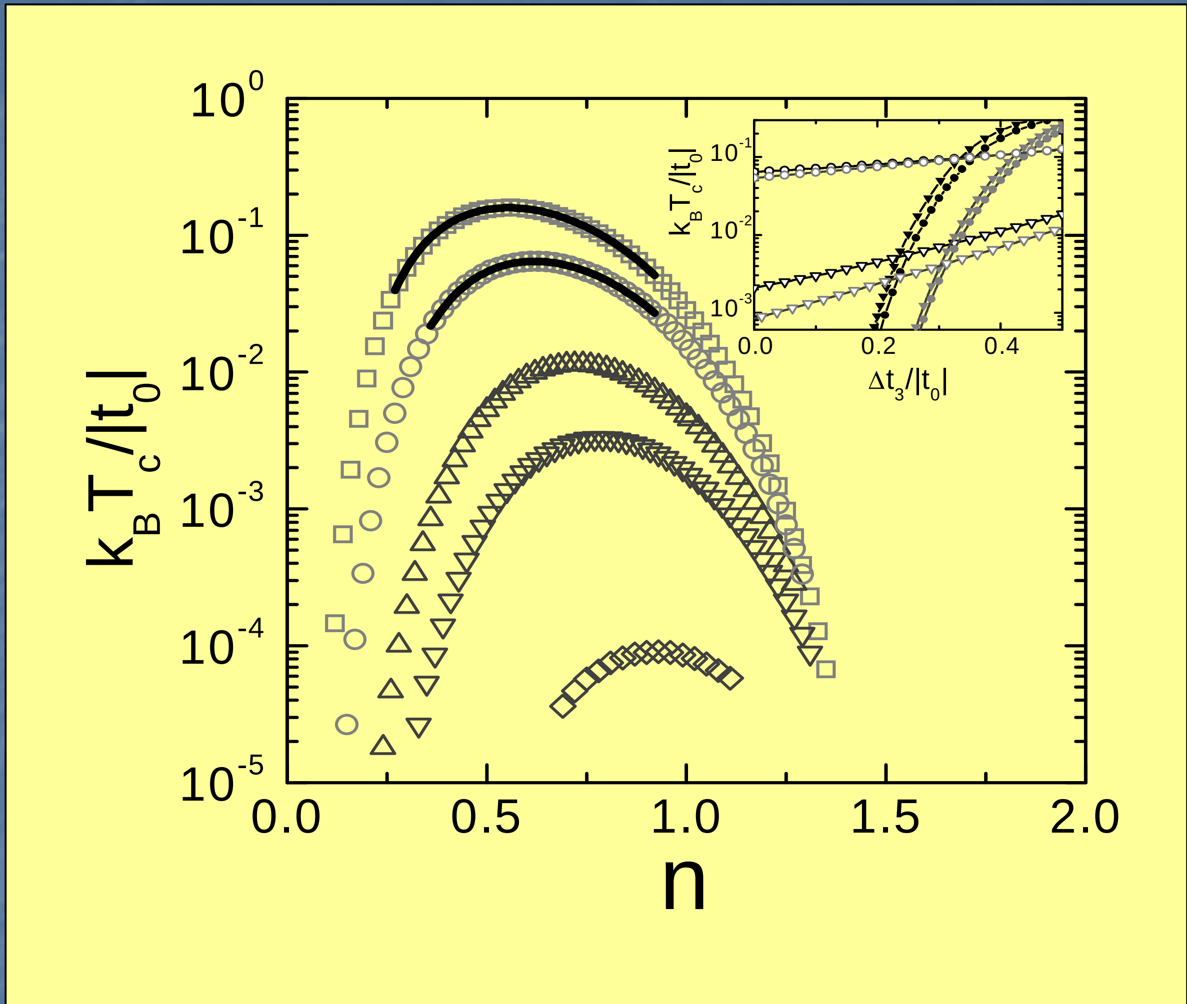
the Chemical Potential μ for the Superconductor State satisfied

$$n-1=-\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\varepsilon_0-\mu}{E_\eta(\mathbf{k})}\tanh\frac{E_\eta(\mathbf{k})}{2k_B T},\qquad\rightarrow\ n=\int_{-\infty}^{\mu}D(\varepsilon)\,d\varepsilon$$

and within the mean field aproximation:

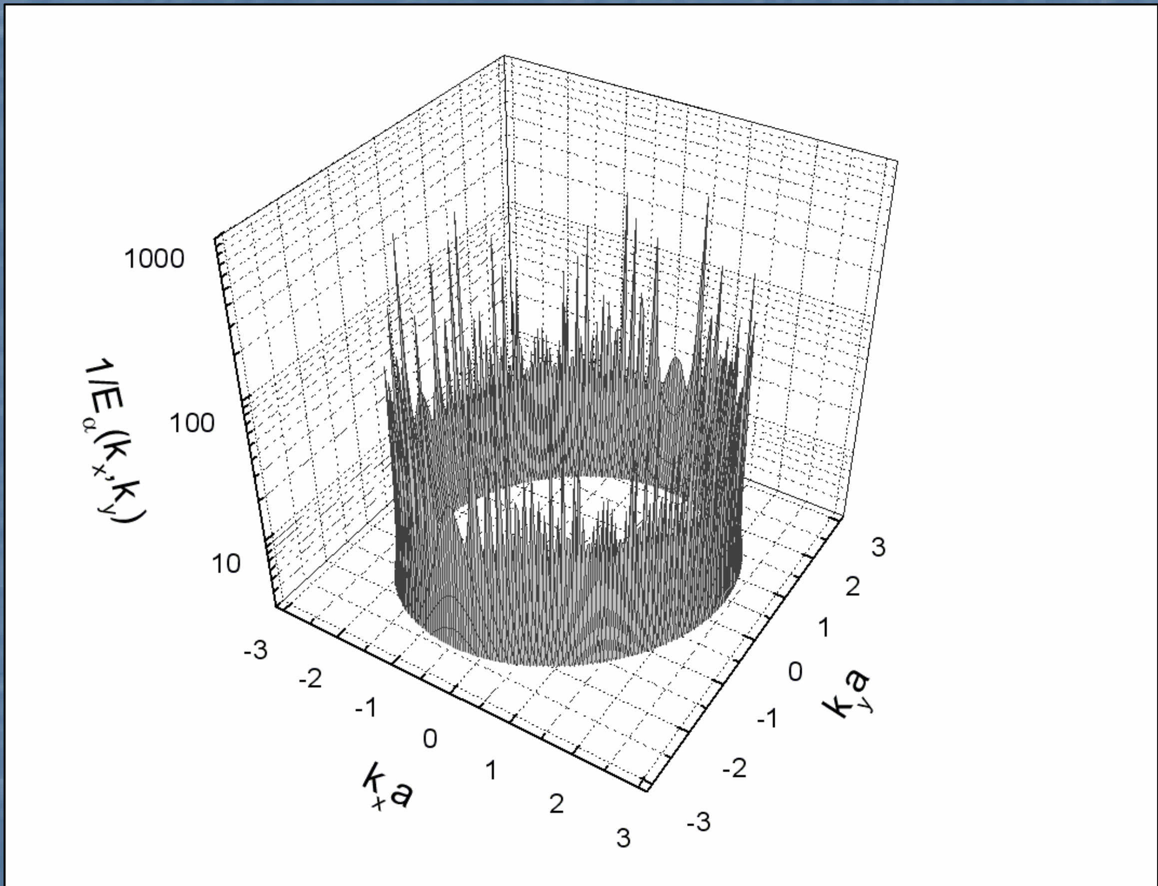
$$\varepsilon_0(\mathbf{k})=\left(\frac{U}{2}+4V\right)n+2(t_0+n\Delta t)\left[\cos(k_x a)+\cos(k_y a)\right]+2\left(t'_+ +2n\Delta t_3^+\right)\cos(k_x+k_y)+2\left(t'_- +2n\Delta t_3^-\right)\cos(k_x-k_y)$$

T_c vs n for d and p Symmetries



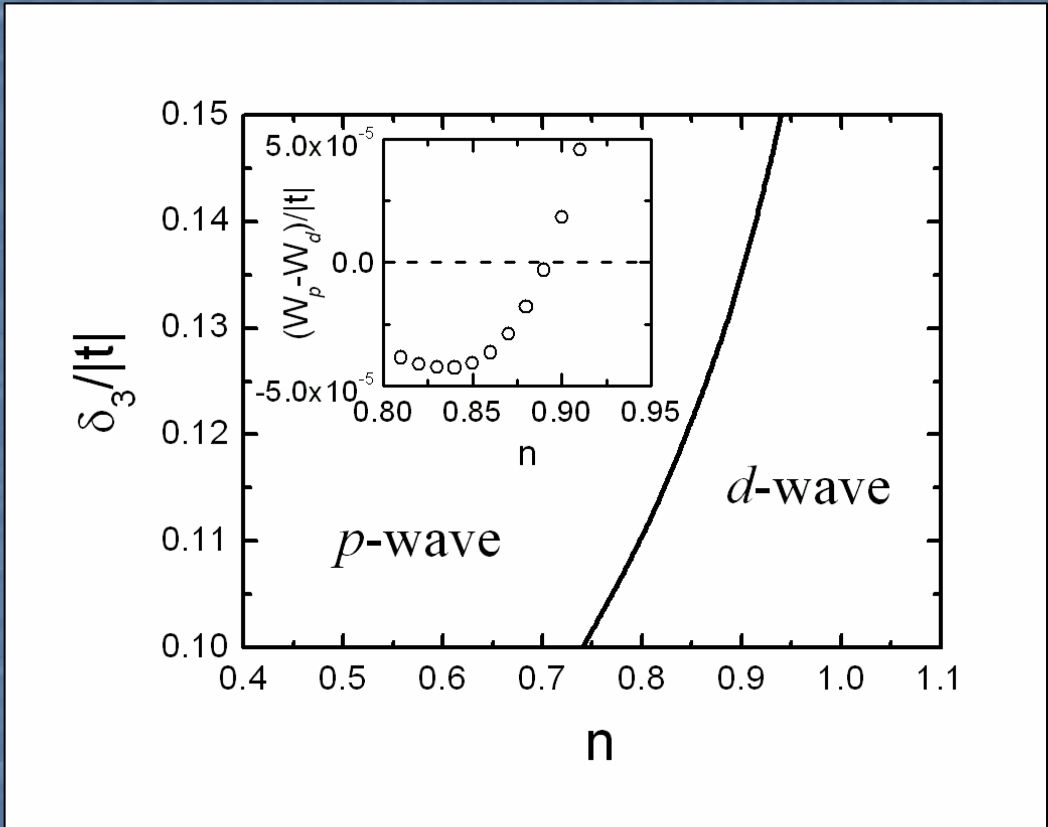
Systems with $U=V=\Delta t=\delta'=\Delta t_3=0$, $t'_0=-0.3|t_0|$, I. Mazin, *et al.*, Phys. Rev. Lett. **79** , 733 (1997), $\delta_3=0.5|t_0|$ (squares), $0.375|t_0|$ (circles), $0.25|t_0|$ (up triangles), $0.2|t_0|$ (down triangles) y $0.125|t_0|$ (rhombus). Inset: n=0.61 black, n=0.5 gray

The Fermi Surface



Integrand $1/E_p(\mathbf{k})$ plotted over the first Brillouin zone for $U=V=\delta=0$, $t'_0=-0.6|t_0|$, $\Delta t=0.5|t_0|$, $\Delta t_3=0.15|t_0|$, $\delta_3=0.11$ $|t_0|$, $n=0.8$, $\Delta_p=0.00154|t_0|$, $\mu_p=0.147|t_0|$.

The Superconductor Phase Diagram

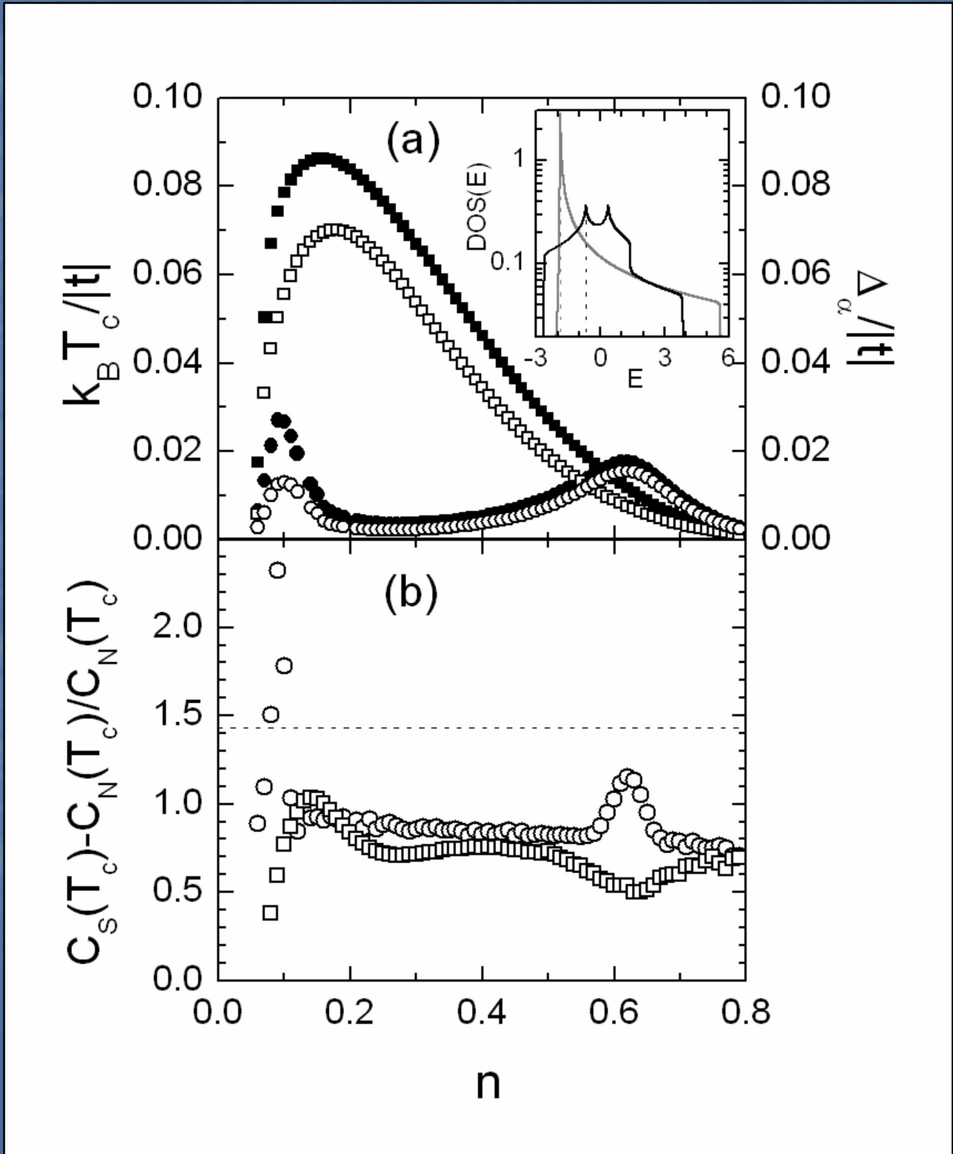


The superconductor ground state phase diagram in the space of electron density (n) and δ_3.

Inset: Difference of ground state energies (W_p-W_d) vs n

$$W_\eta = \sum\left[\varepsilon(\mathbf{k}) - E_\eta(\mathbf{k})\right] + \frac{\Delta_\eta^2}{4\Lambda - V} + (n-1)\mu_\eta - \left(\frac{U}{4} + 2V\right)n^2$$

The Jump of the Specific Heat

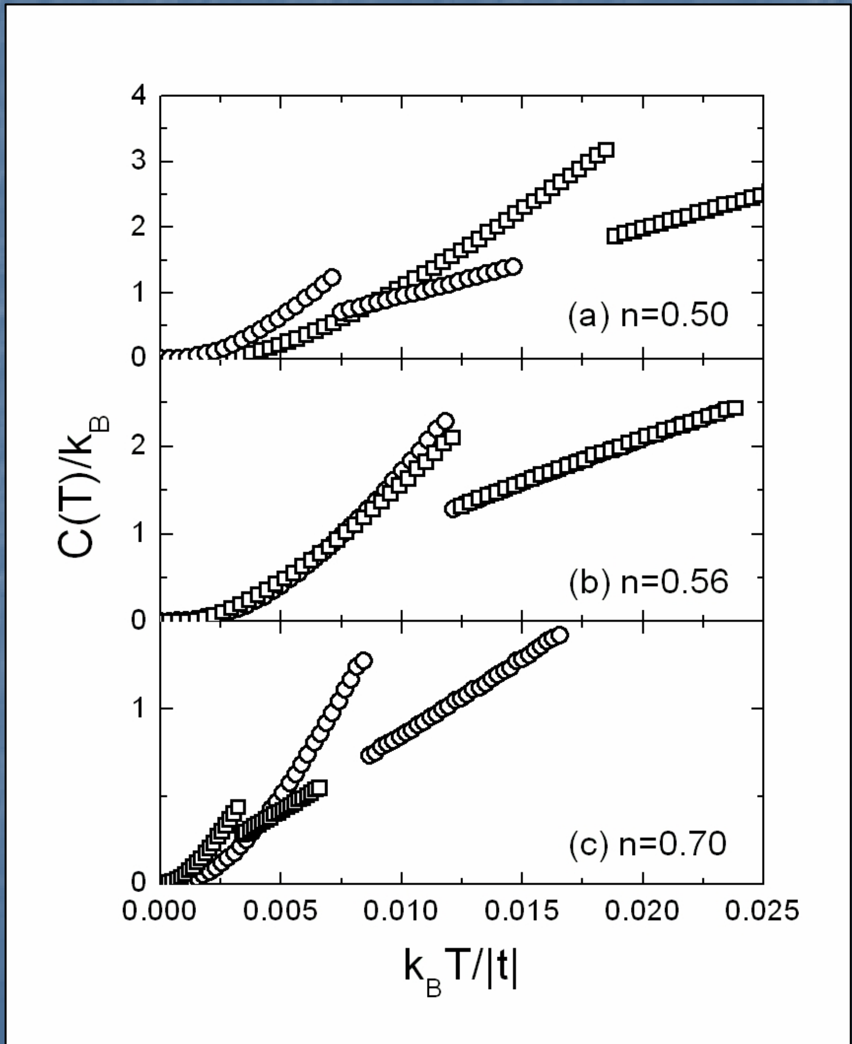


(a) Critical temperature vs *n,* for a system with arbitrary *U*, *V*=*δ*=*0*, *t'*$_0$=0.45|*t*$_0$|, Δ*t*=0.5|*t*$_0$|, Δ*t*$_3$=0.15|*t*$_0$|, *δ*$_3$=*0.1* |*t*$_0$|.

The inset show DOS vs *E*, for *n*=0.09 (grey line) and *n*=0.61 (black line).

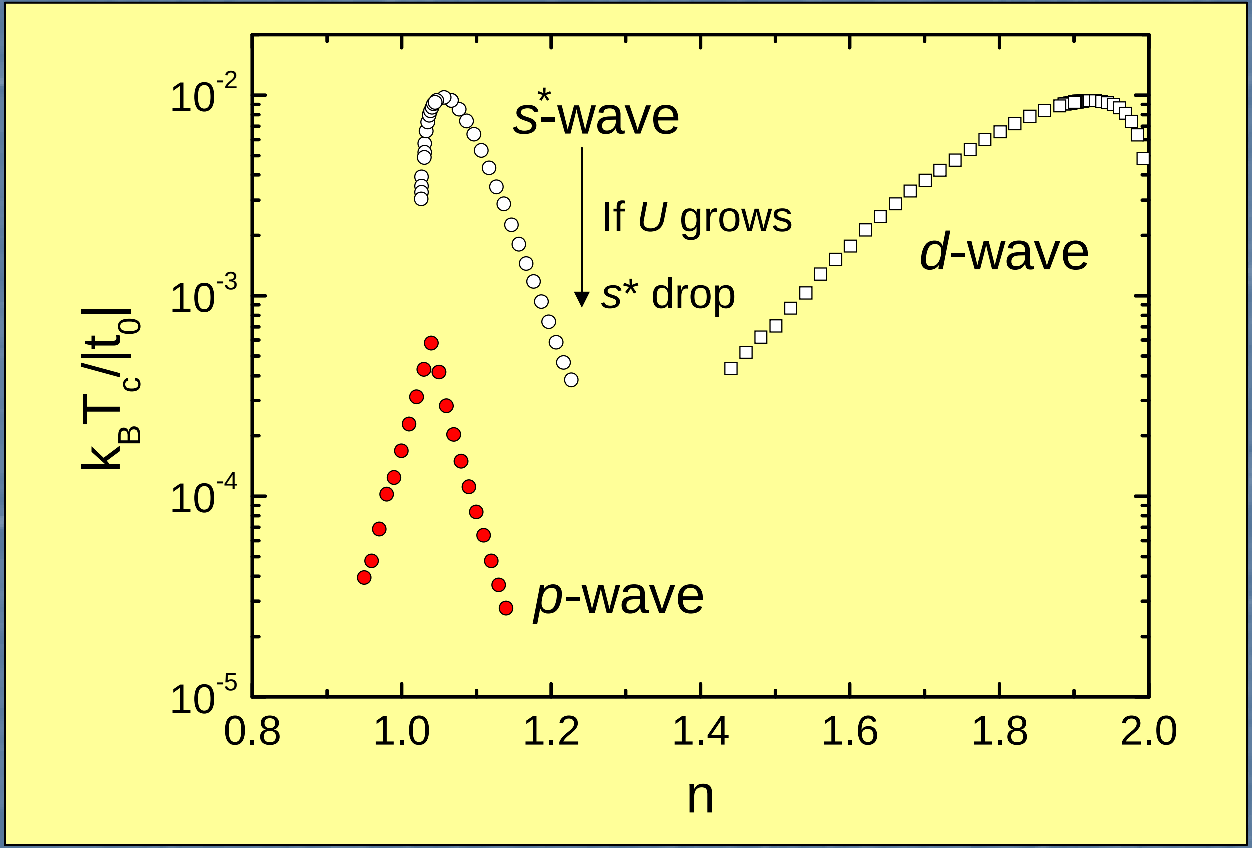
(b) The jump for *d* (squares) and *p* (circles) symmetries as a function of *n.*

Electronic Specific Heat vs *T*



In low temperatures the specific heat is very sensitive to the nodal lines *d* (squares) and *p* (circles) symmetries

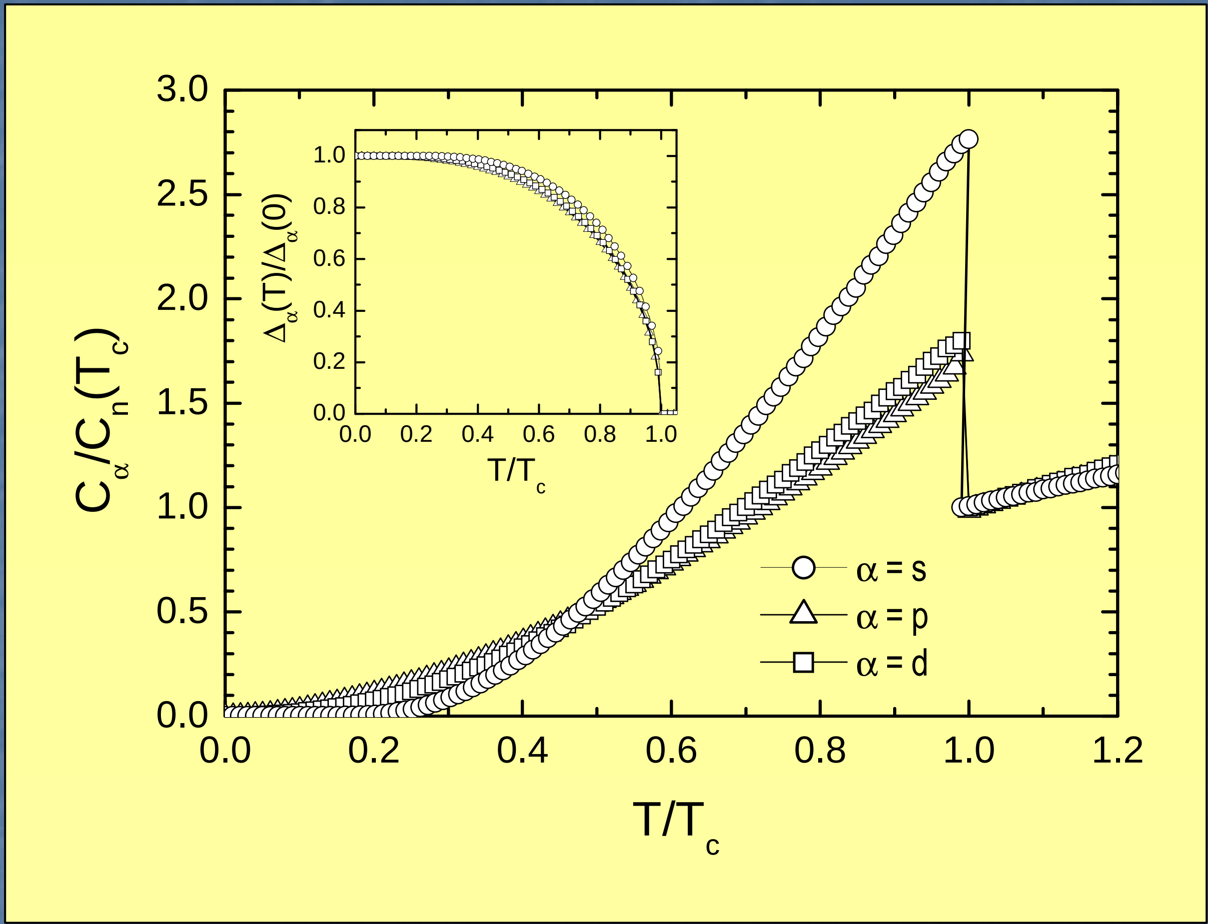
The Critical Temperature for the Anisotropic Superconductivity



L.A. Pérez, *et al.*, Physica B **359**, 569 (2005)

$V=\delta'=0$, $t'_0=-0.45\ |t_0|$, $\Delta t=0.5\ |t_0|$, $\Delta t_3=0.05\ |t_0|$, $\delta_3= 0.05\ |t_0|$ and $U=8\ |t_0|$.

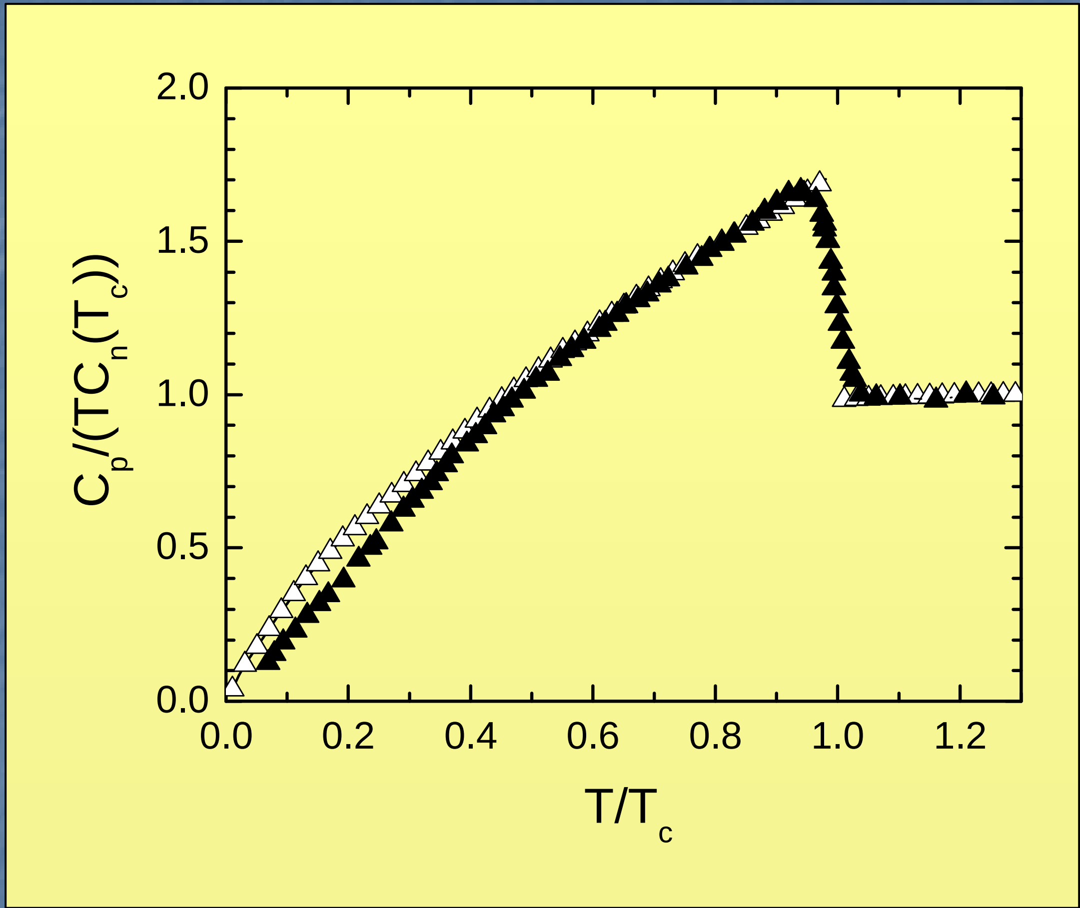
The Electronic Specific Heat



J.S. Millan, *et al.*, Proceedings of AIP **850**, 563 (2006).

V=*δ*=0, *t'*$_0$=-0.45 |*t*$_0$|, *Δt*=0.5 |*t*$_0$|, *Δt*$_3$=0.15 |*t*$_0$| , *δ*$_3$= 0.1 |*t*$_0$|, *n*=1 (*p*) and 1.4 (*d*). The *s* symmetry with *U*=-1.3 |*t*$_0$| y *t'*$_0$=-0.45 |*t*$_0$|.

Comparison of Theory and Experiment

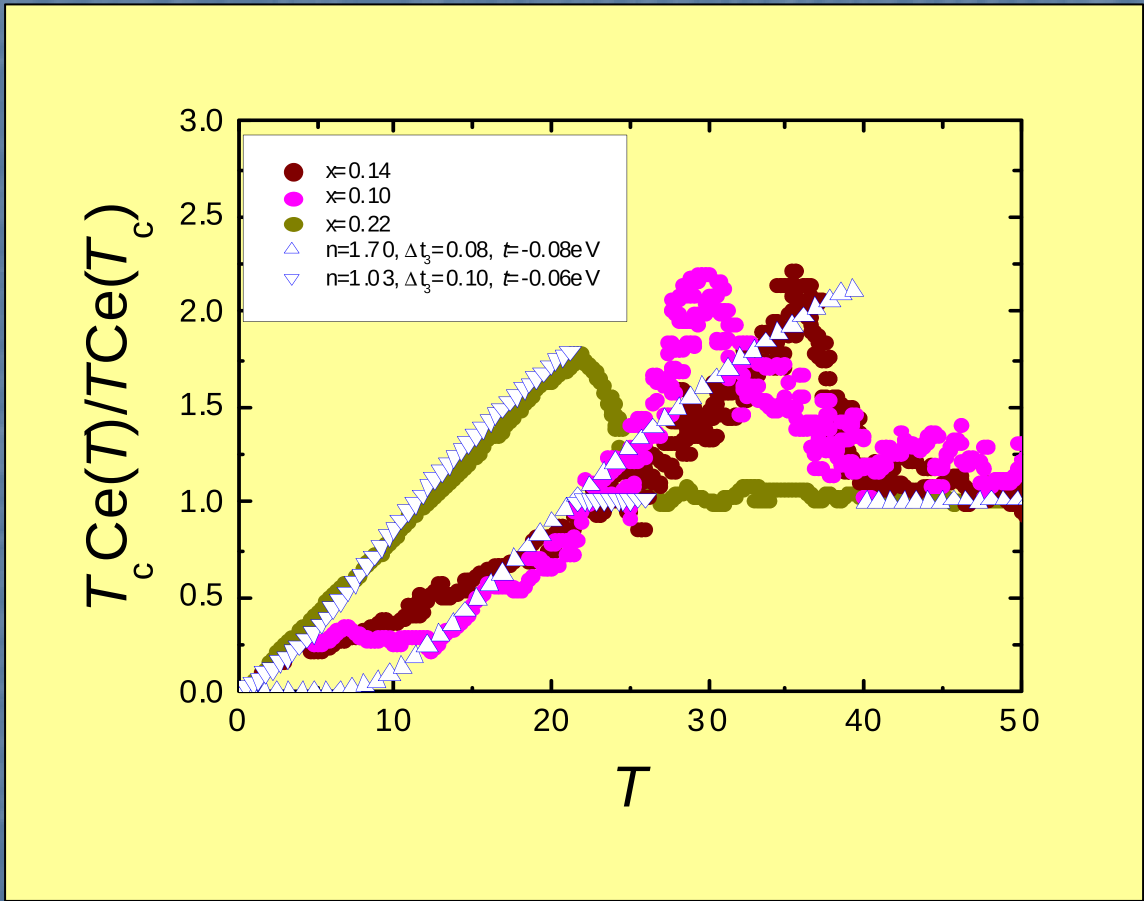


J.S. Millan, *et al.*, Proceedings of AIP **850**, 563 (2006).

S.Nishizaki, et al., *J. Phys. Soc. Jpn.* **69**, 572-578 (2000).

Adjust for *p* symmetry with $V=\delta'=0$, $t'_0=-0.45\ |t_0|$, $\Delta t=0.5\ |t_0|$, $\Delta t_3=0.15\ |t_0|$, $\delta_3=0.1\ |t_0|$ *and* $n=1$ with the experimental data (solid triangles) of Sr_2RuO_4.

Comparison of Theory and Experiment



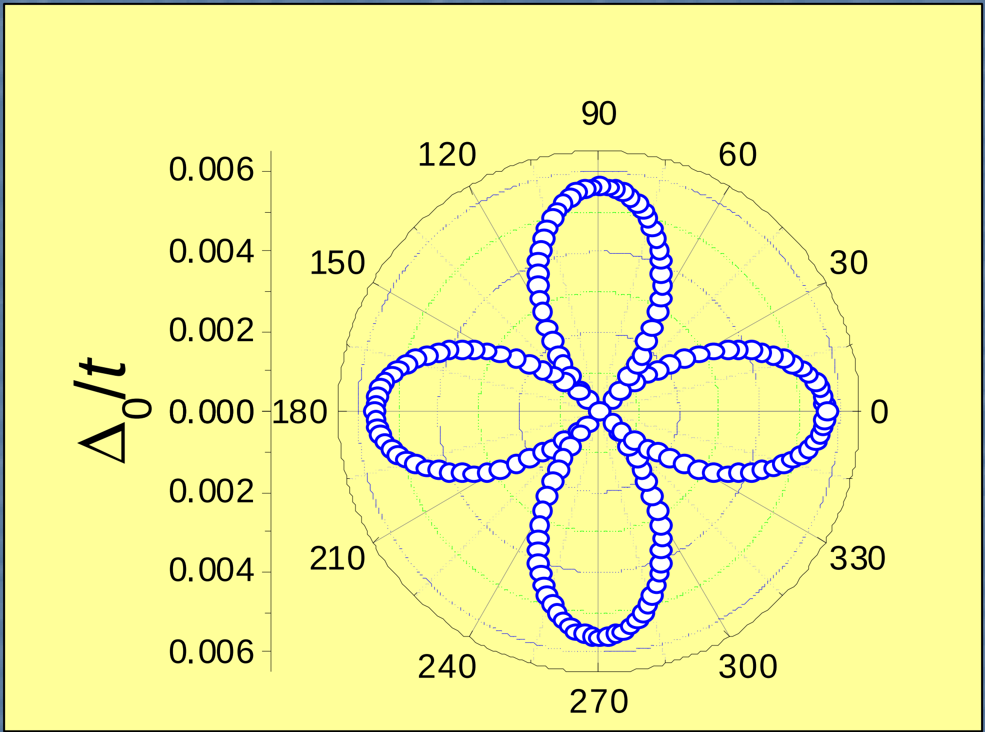
$La_{2-x}Sr_xCuO_4$,

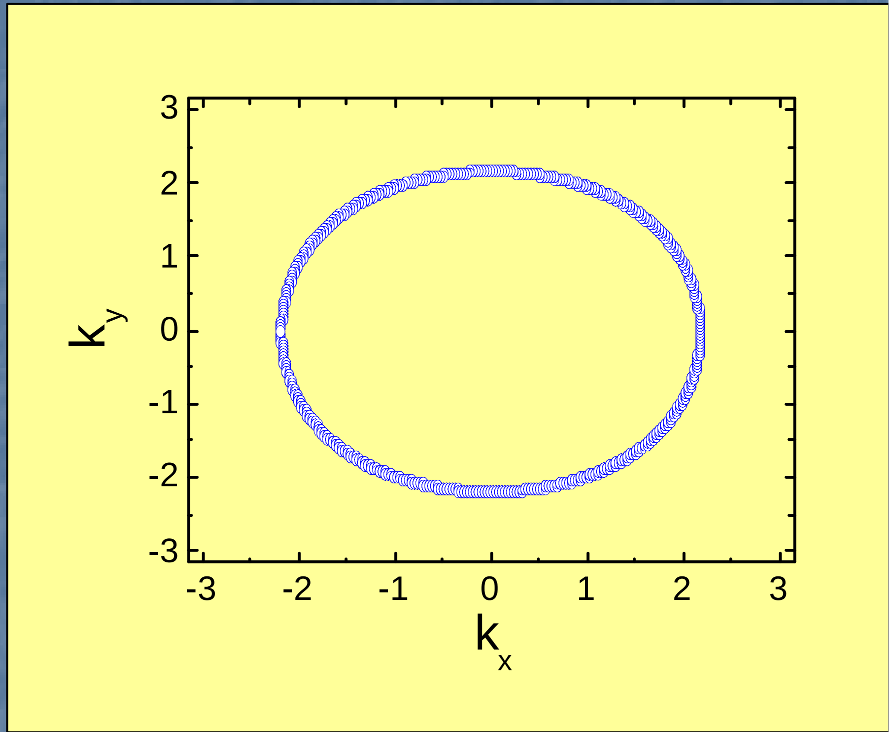
T. Matsuzaki, N. Momono, M. Oda, and M. Ido, J. Phys. Soc. Jpn. 73 (2004) 2232

dw-wave for

$U=V=\delta'=\delta_3=0$, $t'_0=-0.45|t_0|$, $\Delta t=0.5|t_0|$.

The Single Particle Excitation Energy Gap (Δ_0)





The double of the minimal energy in order to break a Cooper pair (Δ_0) as a function of polar angle $\theta=\tan^{-1}(k_y / k_x)$ for *dw*-wave with $U=V=\delta'= \delta_3 =0$, $t'_0=-0.45|t_0|$, $\Delta t =0.5 |t_0|$, $\Delta t_3=0.14|t_0|$, $n=$ 0.78 and the corresponding Fermi Surface.

CONCLUSIONS

1. The research of singlet and triplet superconductivity suggests the posibility of a unified theory about the **Anisotropic Superconductivity** for *p* and *d* symmetries in a square lattice.
2. The *p*- and *d*-wave superconductivity are respectively enhance in the low and high electronic density regime.
3. We can find appropriate set of Hamiltonian parameters in order to find the electronic specific heat that matches very well with experimental data.
4. Then, we have now the possibility to associate theory and experiments of some materials.