# Correlation of $T_c$ with copper 4s level revealing the mechanism of high-$T_c$ superconductivity

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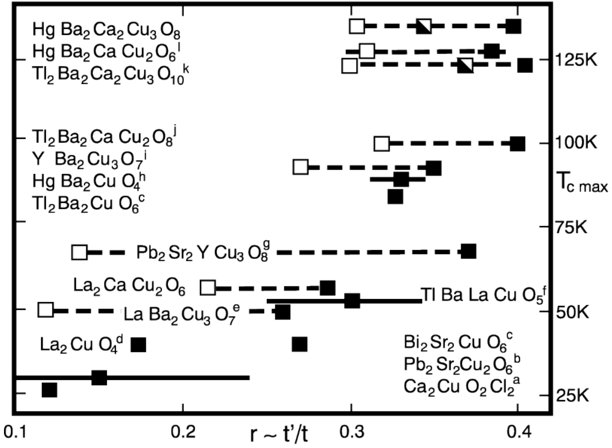
International Conference on Physics in Memoriam
Acad. Prof. Matey Mateev, 10–12 April 2011, Sofia

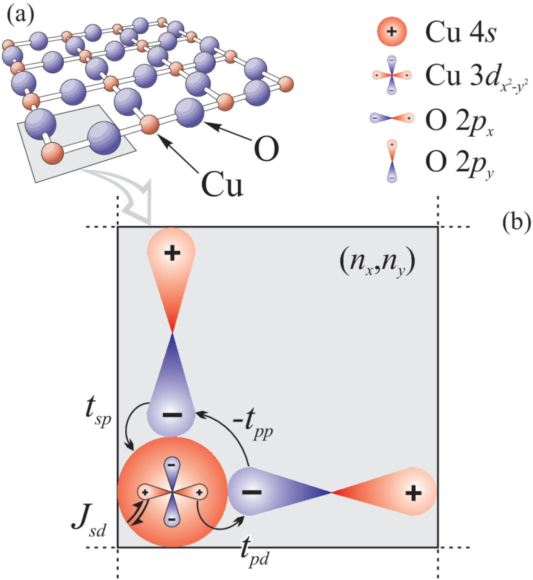
# Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\ max}$

E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001)

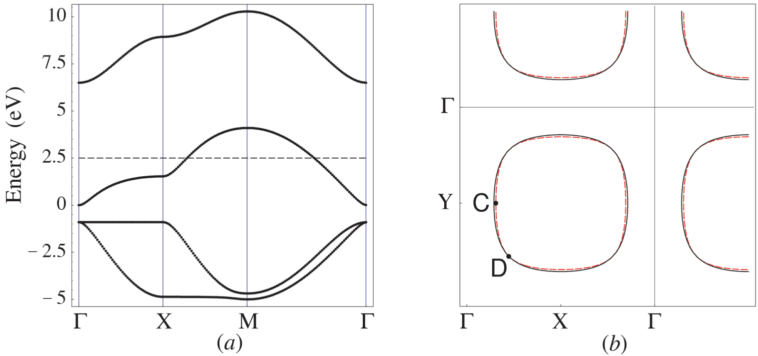



Maximal critical temperature $T_{c\ max}$ versus range parameter $r$

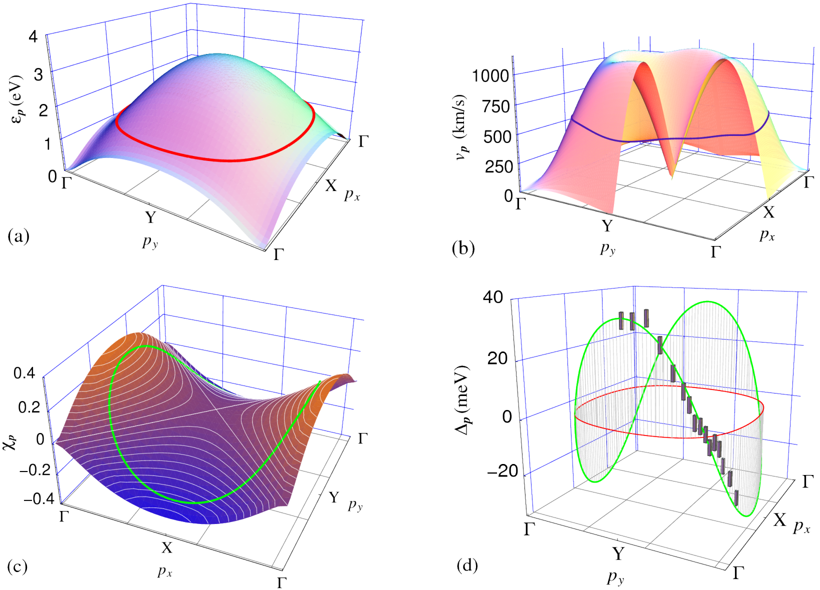
# The 3d-to-4s-by-2p highway to superconductivity
## T.M. Mishonov, J.O. Indekeu, and E.S. Penev
## J.Phys.: Condens. Matter 15 (2003) 4429–4456



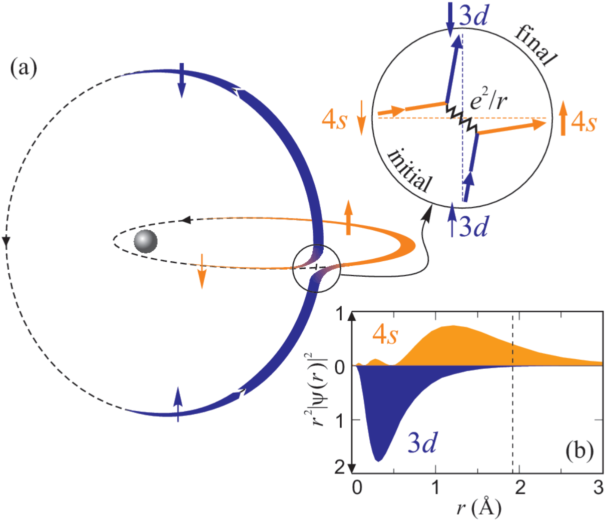
# Band Structure



# (a) conduction band, (b) velocity
# (c) superconducting gap, (d) ARPES data



# Supercoductivity of Overdoped Cuprtes: The Modern Face of the Ancestral Two-Electron s-d Exchange



# LCAO Secular Equation

$$s(E_{\mathrm{F}}) = (\epsilon_{\mathrm{s}} - E_{\mathrm{F}})(E_{\mathrm{F}} - \epsilon_{\mathrm{p}})/(2t_{\mathrm{sp}})^2. \qquad (1)$$

$$\tilde{s} = \frac{t_{\mathrm{sp}}}{t_{\mathrm{pd}}} s; \qquad \frac{1}{\tilde{s}(\epsilon)} = \frac{4 t_{\mathrm{pd}} t_{\mathrm{sp}}}{(\epsilon_{\mathrm{s}} - \epsilon)(\epsilon - \epsilon_{\mathrm{p}})}, \qquad (2)$$

$$\begin{pmatrix} \epsilon_{\mathrm{d}} & 0 & t_{\mathrm{pd}} s_x & -t_{\mathrm{pd}} s_y \\ 0 & \epsilon_{\mathrm{s}} & t_{\mathrm{sp}} s_x & t_{\mathrm{sp}} s_y \\ t_{\mathrm{pd}} s_x & t_{\mathrm{sp}} s_x & \epsilon_{\mathrm{p}} & t_{\mathrm{pp}} s_x s_y \\ -t_{\mathrm{pd}} s_y & t_{\mathrm{sp}} s_y & -t_{\mathrm{pp}} s_x s_y & \epsilon_{\mathrm{p}} \end{pmatrix} \begin{pmatrix} D_{\mathbf{p}} \\ S_{\mathbf{p}} \\ X_{\mathbf{p}} \\ Y_{\mathbf{p}} \end{pmatrix} = \epsilon_{\mathbf{p}} \begin{pmatrix} D_{\mathbf{p}} \\ S_{\mathbf{p}} \\ X_{\mathbf{p}} \\ Y_{\mathbf{p}} \end{pmatrix}, \qquad (3)$$

$$D_{\mathbf{p}}^2 + S_{\mathbf{p}}^2 + X_{\mathbf{p}}^2 + Y_{\mathbf{p}}^2 = 1.$$

$\epsilon_{\mathrm{d}}$ - Energy Cu 3d, $\epsilon_{\mathrm{s}}$ - Energy Cu 4s, $\epsilon_{\mathrm{p}}$ - Energy O 2p,
$E_{\mathrm{F}}$ - Fermi enegy, $t_{\mathrm{sp}}$ - Hopping integral Cu 4s – O 2p.

# Perturbative Bloch Functions and Gap Equation

$$\begin{pmatrix} D_{\mathbf{p}} \\ S_{\mathbf{p}} \\ X_{\mathbf{p}} \\ Y_{\mathbf{p}} \end{pmatrix} \approx \begin{pmatrix} 1 \\ \left(s_x^2 - s_y^2\right)/4\tilde{s}(\epsilon) \\ \dfrac{t_{\mathrm{pd}}}{\epsilon - \epsilon_{\mathrm{p}}} s_x \\ -\dfrac{t_{\mathrm{pd}}}{\epsilon - \epsilon_{\mathrm{p}}} s_y \end{pmatrix}, \tag{4}$$

$$s_x = 2\sin(p_x/2), \qquad s_y = 2\sin(p_y/2),$$

$$\Delta_{\mathbf{p}}(T) = \Xi(T)\chi_{\mathbf{p}}, \qquad \chi_{\mathbf{p}} \equiv S_{\mathbf{p}} D_{\mathbf{p}}. \tag{5}$$

$$E_{\mathbf{p}} \equiv (\eta_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2)^{1/2}, \qquad \eta_{\mathbf{p}} \equiv \epsilon_{\mathbf{p}} - E_{\mathrm{F}}, \tag{6}$$

$$2J_{\mathrm{sd}} \left\langle \frac{\chi_{\mathbf{p}}^2}{2E_{\mathbf{p}}} \tanh\left(\frac{E_{\mathbf{p}}}{2k_{\mathrm{B}}T}\right) \right\rangle = 1, \quad \langle f_{\mathbf{p}} \rangle \equiv \int_0^{2\pi}\int_0^{2\pi} \frac{dp_x\, dp_y}{(2\pi)^2} f(\mathbf{p}). \tag{7}$$

$$\left\langle \frac{\chi_{\mathbf{p}}^2}{\eta_{\mathbf{p}}} \tanh\left(\frac{\eta_{\mathbf{p}}}{2k_{\mathrm{B}}T_{\mathrm{c}}}\right)\right\rangle = \frac{1}{J_{\mathrm{sd}}}. \qquad (8)$$

$$k_{\mathrm{B}}T_{\mathrm{c}} \approx 1.14\,\hbar\omega_{\mathrm{D}}\mathrm{e}^{-1/N(0)V}. \qquad (9)$$

$$V = J_{\mathrm{sd}}\frac{4t_{\mathrm{pd}}t_{\mathrm{sp}}}{(\epsilon_{\mathrm{s}} - E_{\mathrm{F}})(E_{\mathrm{F}} - \epsilon_{\mathrm{p}})} = J_{\mathrm{sd}}/\tilde{s}(E_{\mathrm{F}}). \qquad (10)$$

$$\boxed{\ln(T_{\mathrm{c}}) \approx \ln(1.14\omega_{\mathrm{D}}) - \tilde{s}(E_{\mathrm{F}})/[N(E_{\mathrm{F}})J_{\mathrm{sd}}],} \qquad (11)$$

$$f = \langle\theta(\epsilon_{\mathbf{p}} > E_{\mathrm{F}})\rangle\,, \quad \text{where} \quad \theta(\epsilon_{\mathbf{p}} > E_{\mathrm{F}}) = \begin{cases} 1 & \text{if } E_{\mathbf{p}} > E_{\mathrm{F}}, \\ 0 & \text{if } E_{\mathbf{p}} < E_{\mathrm{F}}. \end{cases} \qquad (12)$$

# Choice of parameters

$$\epsilon_{\rm s} = 5.4, \quad \epsilon_{\rm p} = -1, \quad \epsilon_{\rm d} = 0, \qquad (13)$$
$$t_{\rm sp} = 2, \quad t_{\rm pd} = 1.5, \quad t_{\rm pp} = 0.2.$$

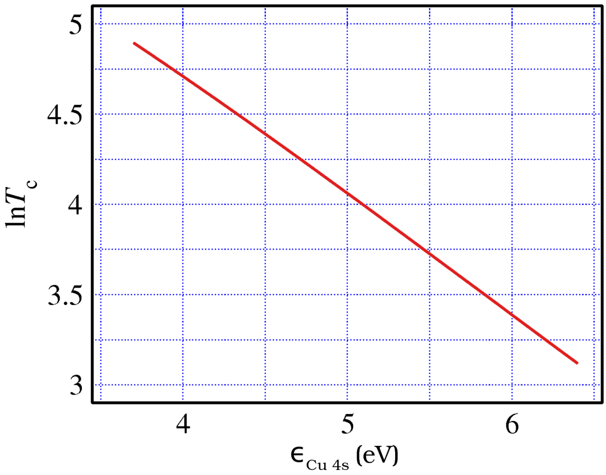
$$r \equiv \frac{1}{2(1+s)}. \qquad (14)$$

$$-2t(\epsilon)[\cos(p_x) + \cos(p_y)] + 4t'(\epsilon)\cos(p_x)\cos(p_y) = q(\epsilon), \qquad (15)$$

$$\frac{t'(E_{\rm F})}{t(E_{\rm F})} \propto r(E_{\rm F}), \qquad (16)$$

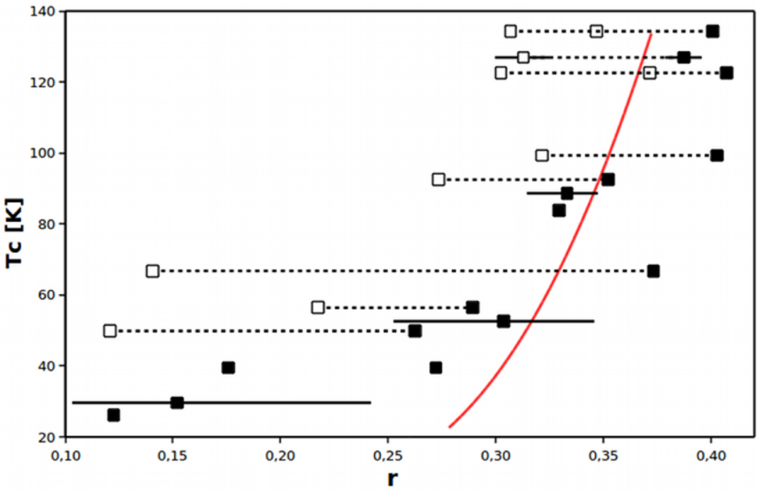
$$f_{\rm max} = 0.66$$

# Science Starts with the Simplicity - Brainwashed by Feynman




$$\ln(T_c) \approx \ln(1.14\omega_D) - \tilde{s}(E_F)/[N(E_F)J_{sd}]$$

# Red curve s-d theory after Pavarini *et al.* correlation.




Maximal critical temperature $T_{\mathrm{c\ max}}$ versus range parameter $r$.
Waiting for alternative explanations!