Two-component physics of charge carriers and the superconductor-insulator transition

M. Saarela
University of Oulu, Finland

F. V. Kusmartsev
Loughborough University, UK

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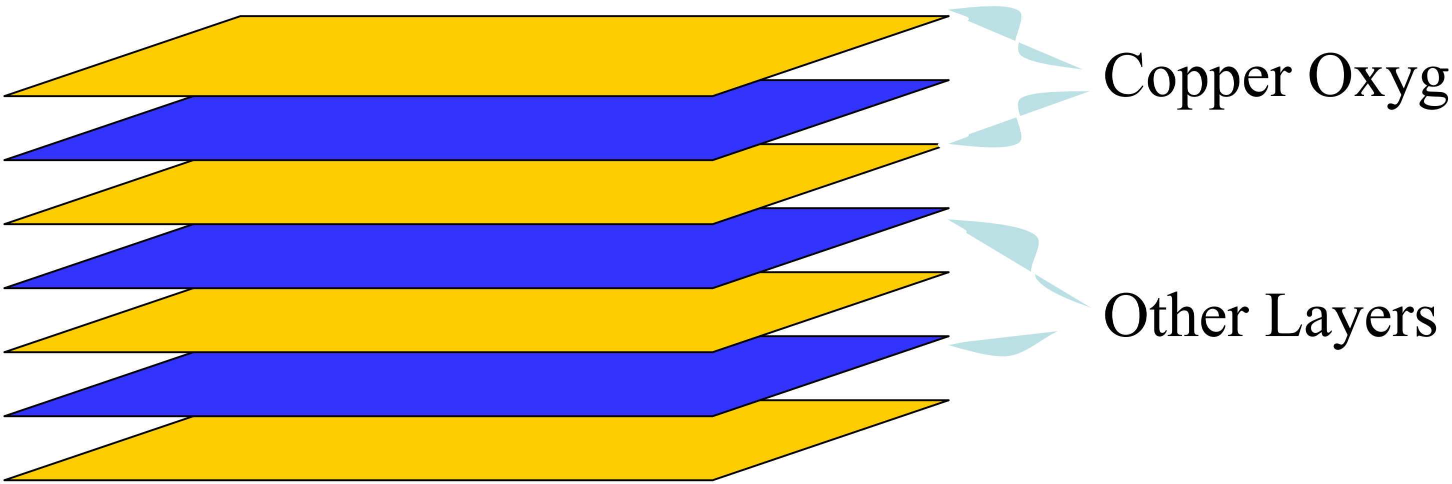
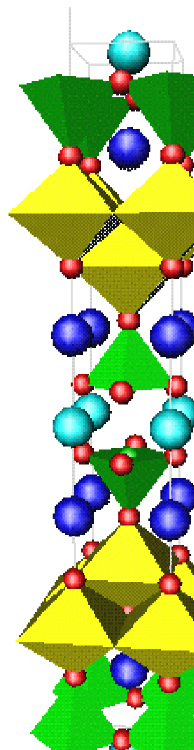
Outline of the talk

- Motivation: Experiments on superconductor-insulator transition in layered superconductors
- Coupling superconducting particles to charged impurities
- Over-screening of the Coulomb interaction
- Clustering of charge carriers around impurities → Coulomb bubbles
- Origin of the pseudogap
- Quantum phase transition from superconducting to insulating phase

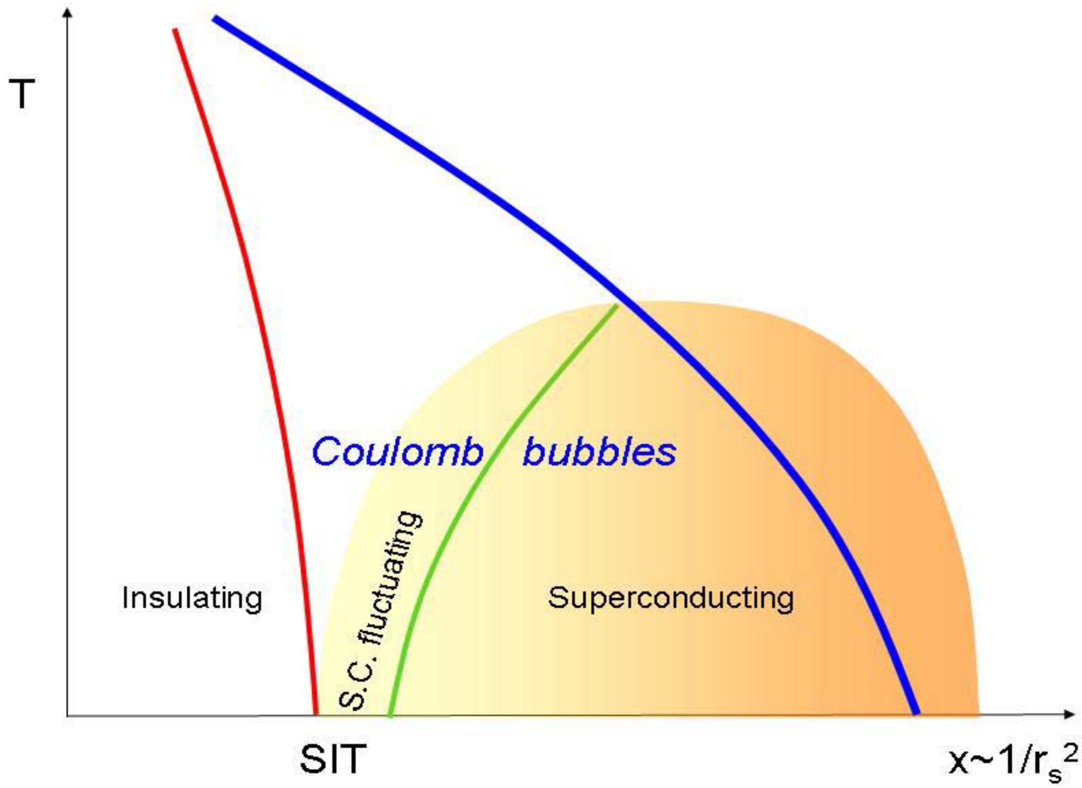
Layered Superconductor





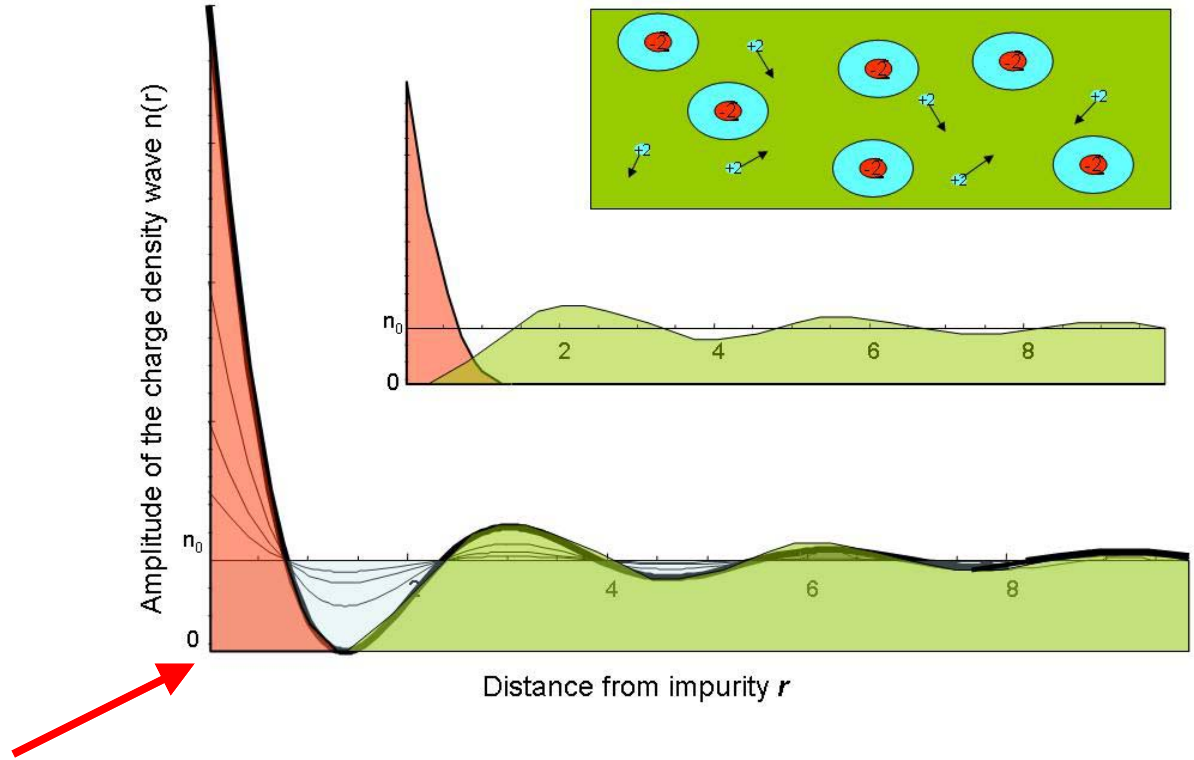
Layered structure → quasi-2D system

Phase Diagram



Coulomb bubble

Impurity is located at the origin and its charge is opposite to the charge of the superconducting particles



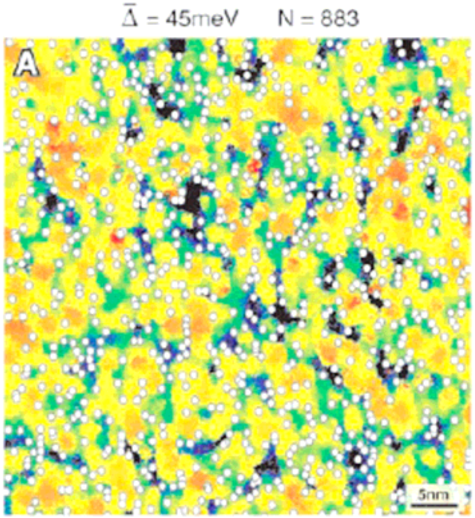
Impurity at the origin

High Tc Cuperates – STM gap map

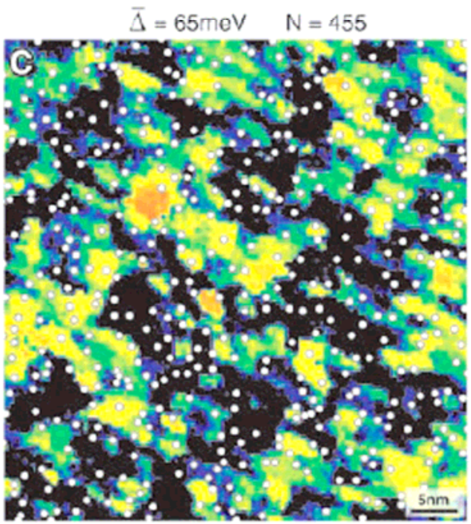
Atomic-Scale Sources and Mechanism of Nanoscale Electronic Disorder in $Bi_2Sr_2CaCu_2O_{8+\delta}$

K. McElroy,[1,2] Jinho Lee,[1] J. A. Slezak,[1] D.-H. Lee,[2] H. Eisaki,[3]
S. Uchida,[4] J. C. Davis[1*]

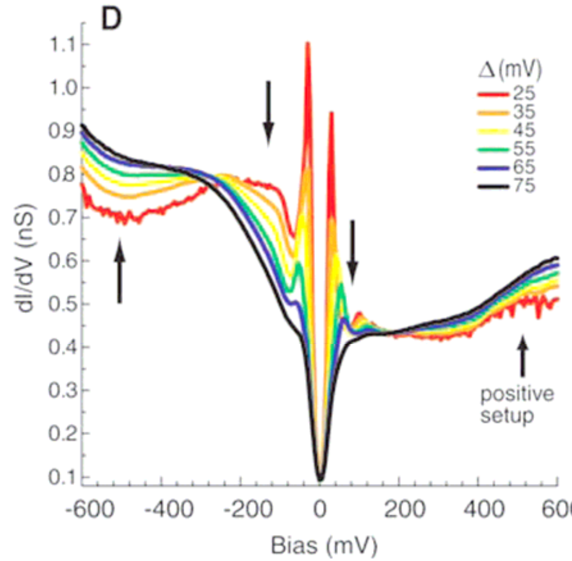
Science 309, 1048 (2005)



Overdoped region



Underdoped region



- **Strong variations in the superconductivity**
- **Black areas no superconductivity**
- **Impurities (white circles) are closely connected with the variations**

PRL **96,** 107003 (2006)

Doping Controlled Superconductor-Insulator Transition in $Bi_2Sr_{2-x}La_xCaCu_2O_{8+\delta}$

Seongshik Oh,* Trevis A. Crane, D.J. Van Harlingen, and J.N. Eckstein
Department of Physics, University of Illinois, Urbana, Illinois 61801, USA
(Received 20 September 2005; published 14 March 2006)

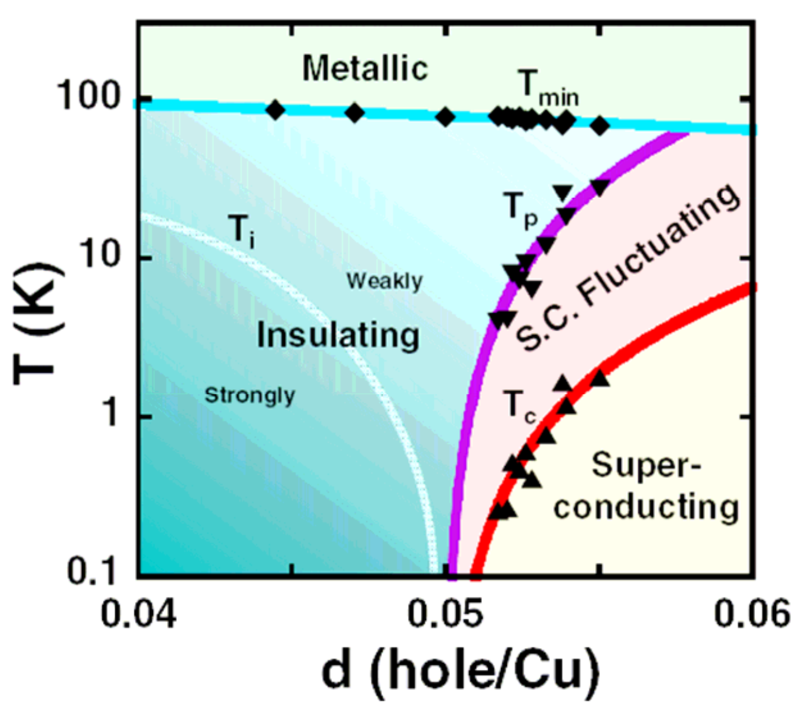


FIG. 4 (color online). (T, d) phase diagram near the critical doping. T_p and $T_{\min}$ are determined by the resistance data, and T_c is evaluated as $0.065 \times T_p$ according to the scaling analysis. Fitting curves for each of these crossover temperatures are plotted as well. Unlike other crossover temperatures, T_i is only

Free boson gas

Controlling parameter is r_s, which determines the distance between particles

$r_0 = r_s r_B$

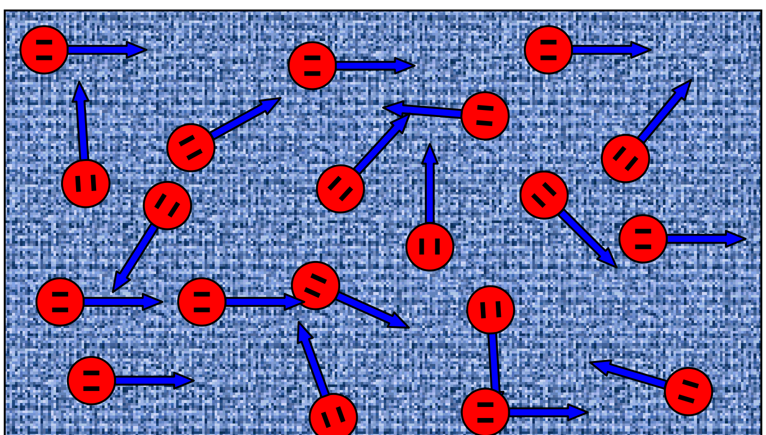
with the Bohr radius r_B

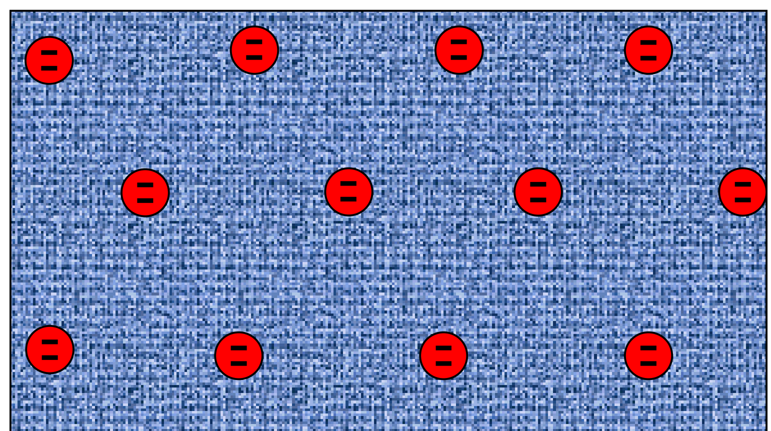
Gas | **Strongly correlated fluid** | **Wigner crystal**

~ 1 $\qquad$ ~ 50 $\qquad$ r_s

superconductor $\qquad$ *Insulator*

strength of interactions increases





Why charged bosons?

- Bose - condensation of charged bosons
- BEC with a long range order creates a superconducting state
- Local pairs on BEC side of the BEC-BCS crossover are charged bosons
- bi-polarons, RVB, etc…

- The energy hierarchy in HTSC: Coulomb ~0.4-1 eV, Spin ~0.2 eV, Phonon~0.04 eV,

→ Coulomb forces dominate

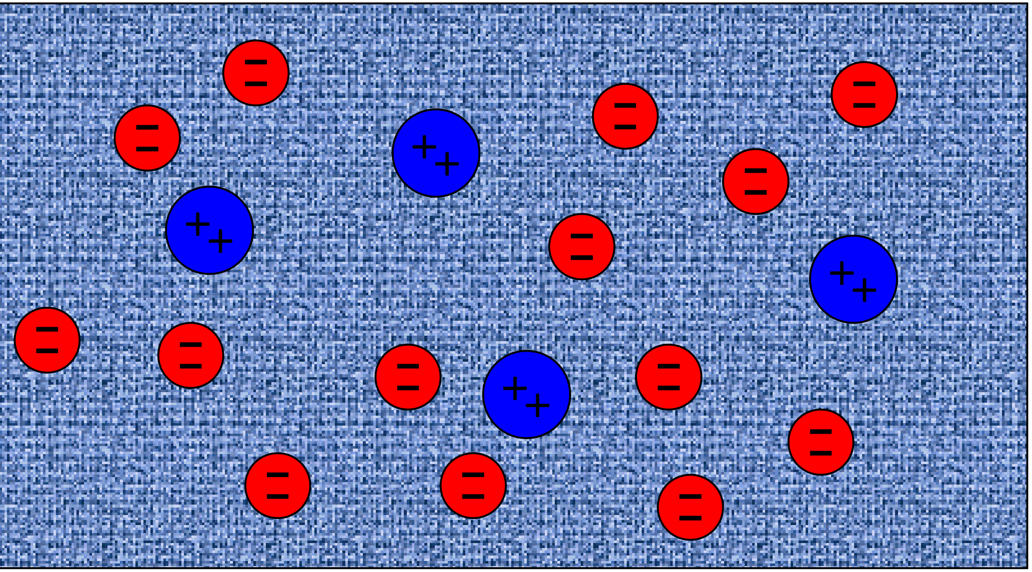
Jellium model with impurities

-Bosons are made of electron (hole) pairs

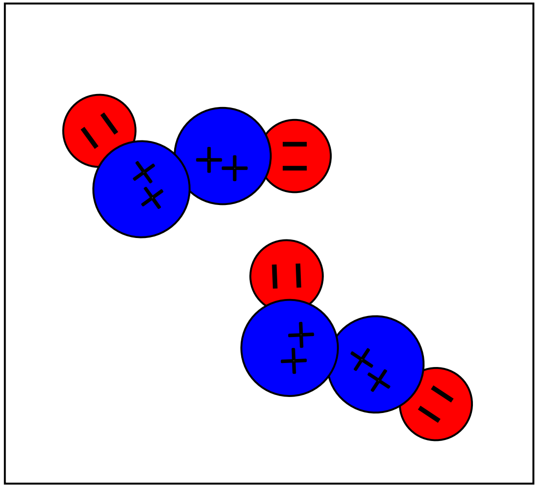
-Smooth, structureless background neutralizes the fluid

-Random impurities with opposite charge to bosons and heavy mass

t high densities bosons are free to move



In free space impurities bind into hydrogen like molecules.



Variational theory of quantum fluids

The Hamiltonian of the charged boson fluid with a charged impurity.

$$H = H_b + H_I = -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}{\sum_{i,j=1}^{N}}' \frac{e_b^2}{\varepsilon_b|\mathbf{r}_i - \mathbf{r}_j|} - \frac{\hbar^2}{2M}\nabla_0^2 + \sum_i^N \frac{e_I e_b}{\varepsilon_I|\mathbf{r}_0 - \mathbf{r}_i|}$$

Subindices b and I refer to the bosons and the impurity. Their interactions are Coulombic and the masses are m and M, respectively.

The variational wave functions contain boson-boson and boson-impurity correlation functions.

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = e^{\frac{1}{2}\sum_{i,j=1}^{N} u^{bb}(|\mathbf{r}_i - \mathbf{r}_j|)}$$

$$\Psi^I(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_N) = e^{\frac{1}{2}\sum_{i=1}^{N} u^{Ib}(|\mathbf{r}_0 - \mathbf{r}_i|)}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

Optimal correlations

The variational problem is divided into two parts. For the purely bosonic part we search for the optimal correlation function by minimizing the expectation value of the Hamiltonian without the impurity.

$$\frac{\delta}{\delta u^{bb}(\mathbf{r}_i, \mathbf{r}_j)} \frac{\langle \Psi | H_b | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$$

The impurity-boson distribution function is solved by minimizing the impurity chemical potential

$$\mu^I = E_{N+1} - E_N = \frac{\langle \Psi^I | H_I | \Psi^I \rangle}{\langle \Psi^I | \Psi^I \rangle} - \frac{\langle \Psi | H_b | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad ; \quad \frac{\delta \mu^I}{\delta u^{Ib}(|\mathbf{r}_0 - \mathbf{r}_i|)} = 0$$

Diagrammatic hyper-netted summations are needed to calculate distributio and correlation functions. This results into a system of equations for a pair correlation functions g(r) for bosons.

System of nonlinear equations

Define radial distribution functions

$$\rho^{bb}(|\mathbf{r}_1-\mathbf{r}_2|) = \rho_0^2 g^{bb}(|\mathbf{r}_1-\mathbf{r}_2|) = N(N-1)\frac{\int d^2r_3\ldots d^2r_N\,|\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2}{\langle\Psi|\Psi\rangle}$$

$$\rho^{I}(|\mathbf{r}_0-\mathbf{r}_2|) = \frac{1}{\Omega}\rho_0 g^{Ib}(|\mathbf{r}_0-\mathbf{r}_1|) = N\frac{\int d^2r_2\ldots d^2r_N\,\left|\Psi^I(\mathbf{r}_0,\ldots,\mathbf{r}_N)\right|^2}{\langle\Psi^I|\Psi^I\rangle}$$

Solve non-linear Euler-equations

$$-\frac{\hbar^2}{m}\nabla^2\sqrt{g^{bb}(r)}+\left[\frac{e_b^2}{\varepsilon_b}\frac{1}{r}+w_{\rm ind}^{bb}(r)\right]\sqrt{g^{bb}(r)}=0$$

$$-\frac{\hbar^2}{2m_{\rm red}}\nabla^2\sqrt{g^{Ib}(r)}+\left[\frac{e_Ie_b}{\varepsilon_I}\frac{1}{r}+w_{\rm ind}^{Ib}(r)\right]\sqrt{g^{Ib}(r)}=0$$

with the induced potentials

$$\tilde{w}_{\rm ind}^{bb}(k)=-\frac{\hbar^2k^2}{4m}\frac{(S^{bb}(k)-1)^2}{(S^{bb}(k))^2}\left[2S^{bb}(k)+1\right]$$

$$\tilde{w}_{\rm ind}^{Ib}(k)=-\frac{\hbar^2k^2}{4m}\frac{S^{Ib}(k)(S^{bb}(k)-1)}{(S^{bb}(k))^2}\left[\frac{m}{m_{\rm red}}S^{bb}(k)+1\right]$$

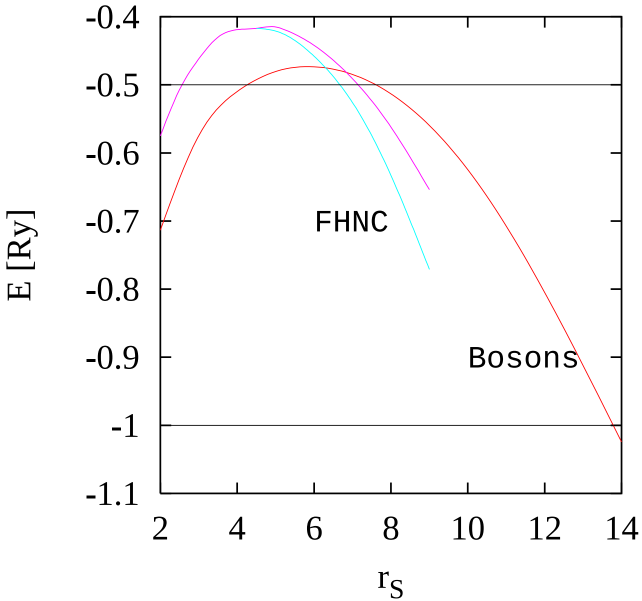
and the static structure factors

$$S^{bb}(k) = 1+\rho_b\int d^2r\, e^{i\mathbf{k}\cdot\mathbf{r}}[g^{bb}(r)-1]$$

$$S^{Ib}(k) = \rho_b\int d^2r\, e^{i\mathbf{k}\cdot\mathbf{r}}[g^{Ib}(r)-1]\,.$$

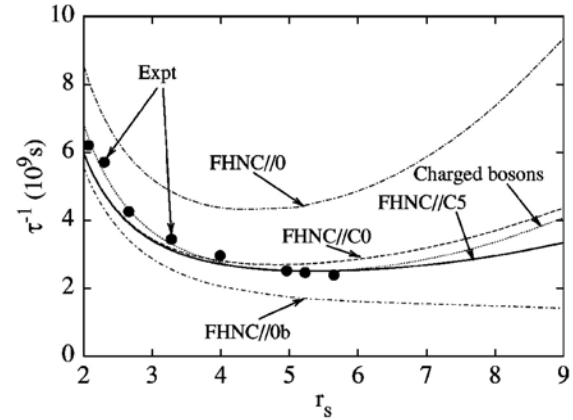
Mott instability and positron annihilation in 3D

Positron chemical potential

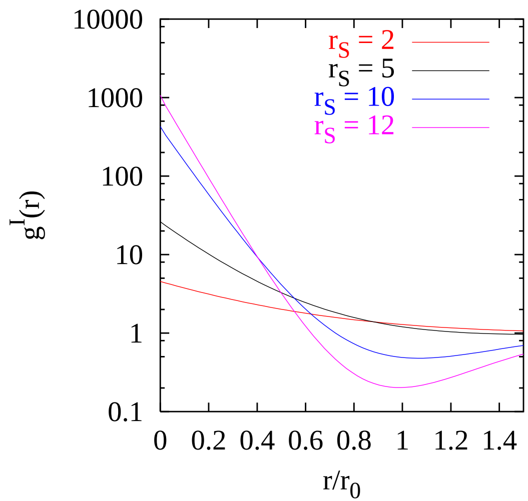


Correlation energies by Apaja et al. PRB 68 (0195118 (2003).
Red curve with bosonic electrons M.S. et al. J. Phys. A 36, 9223 (2003)

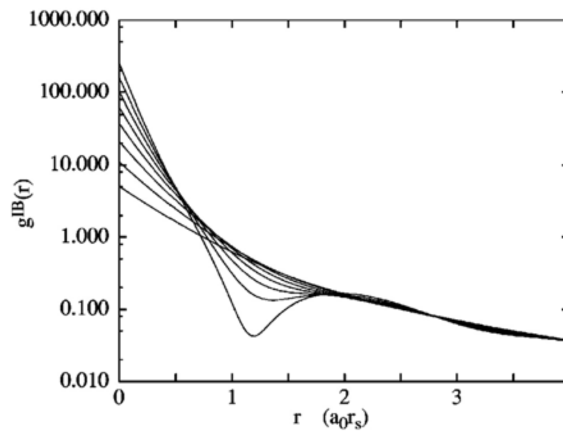
Positron annihilation rates



Radial distributions

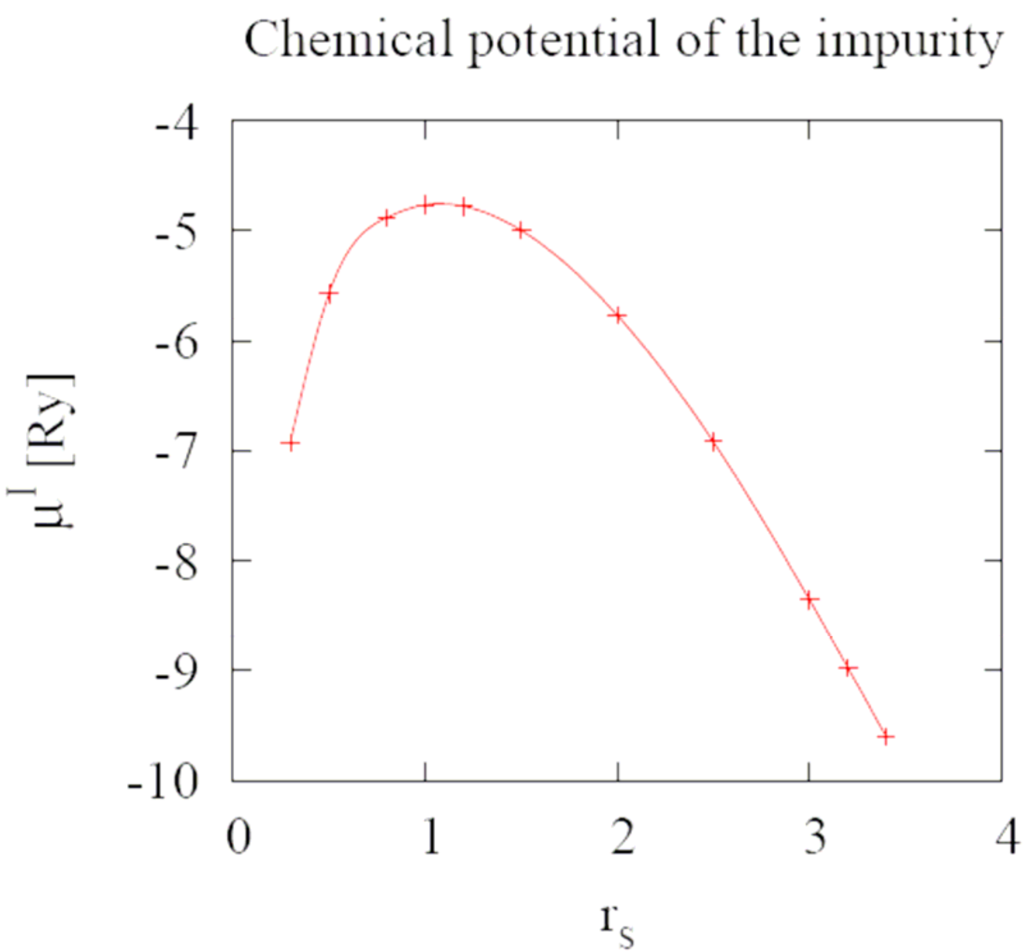


Positive impurity in the charged Bose gas



Positron in the electron gas

Chemical potential of a heavy, charged impurity in 2D



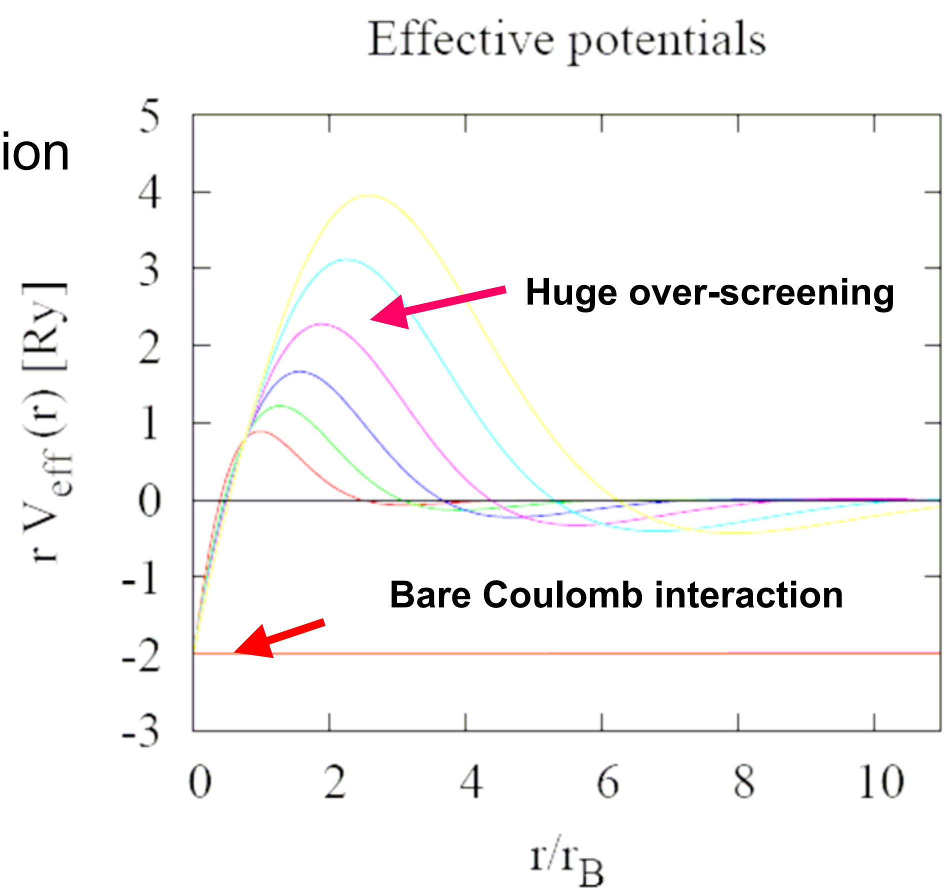
In free space the impurity-boson binding is -4 Ry.

Over-screening of the Coulomb interaction in 2D

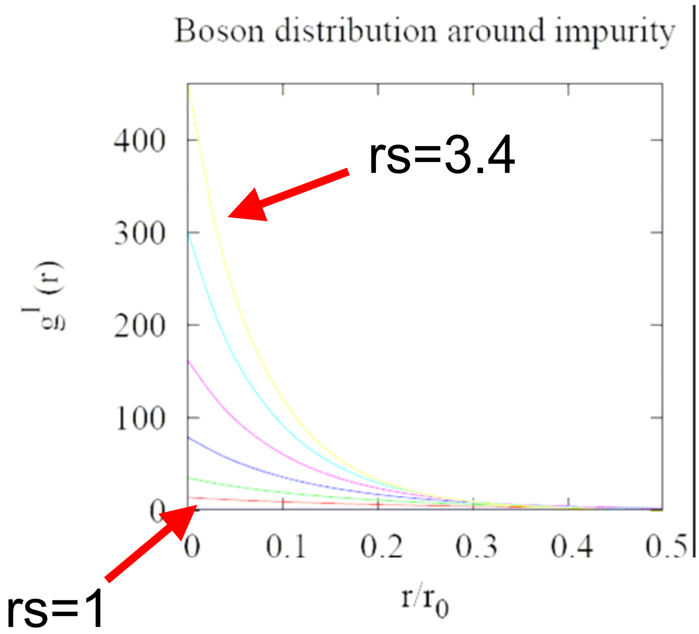
he effective boson-impurity interaction

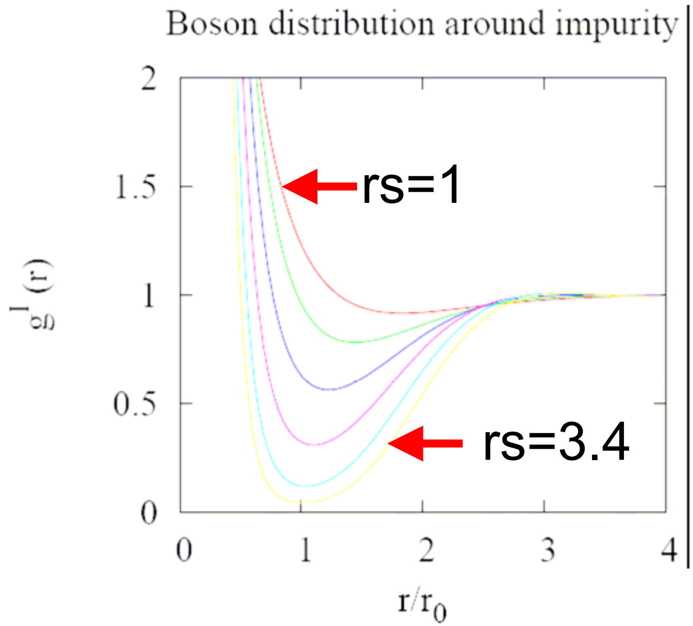
$$V_{\text{eff}}(r) = \frac{e_I e_b}{\varepsilon_I} \frac{1}{r} + w_{\text{ind}}^{Ib}(r)$$

The 6 curves are for rs= 1, 1.5, 2, 2.5, 3 and 3.4. The highest peak corresponds to the highest rs value.



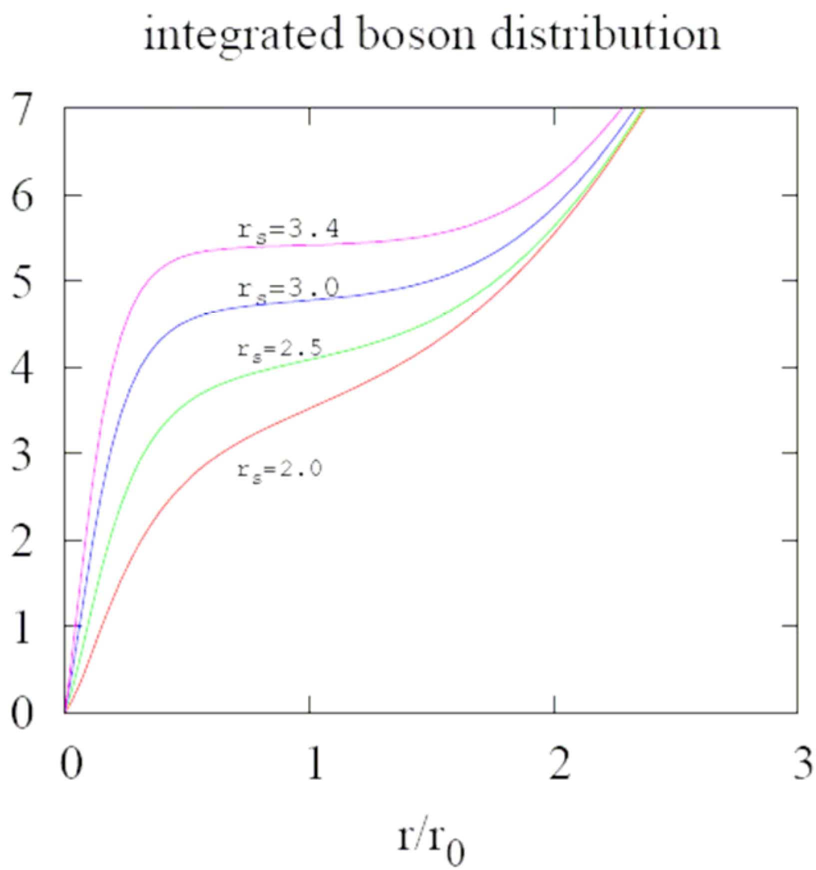
Boson distribution around the impurity



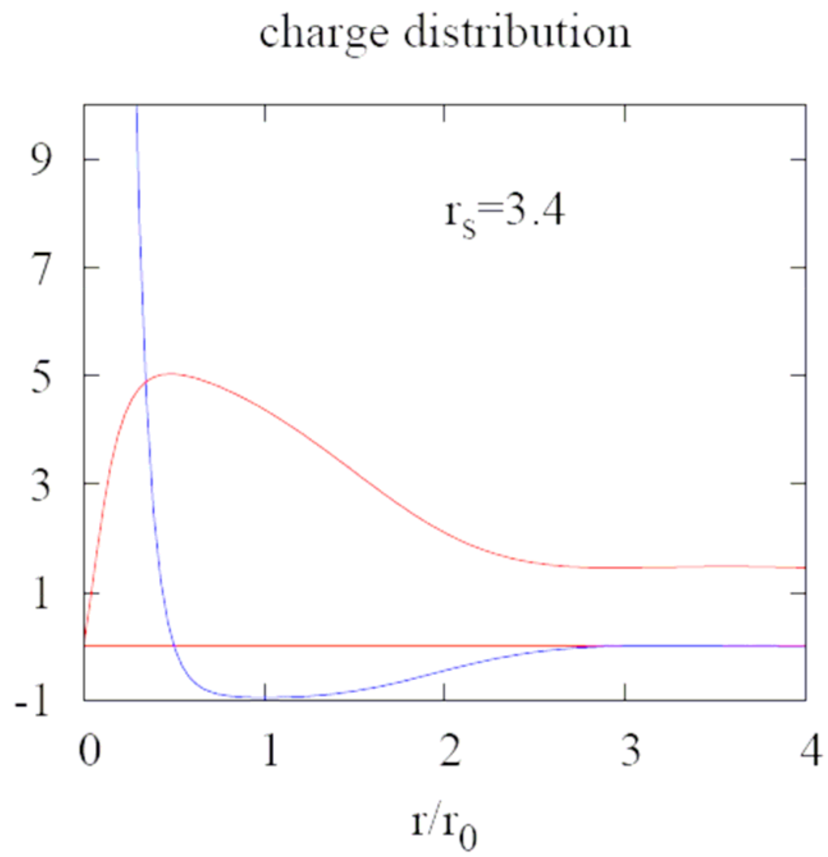


Boson distribution with r_s=1, 1.5, 2., 2.5, 3. ,3.4

Number of bosons around the impurity



$$\int_0^r g^I(r')d^2r'$$



$$\int_0^r (g^I(r') - 1)d^2r'$$

Coulomb bubbles emerge $r_s > 2$

The variational wave function of the fluid with bubbles contains boson-boson, trapped boson-impurity and non-trapped boson-impurity correlation functions.

$$\Psi^{IM}(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_N) = e^{\frac{1}{2}\sum_{i=1}^{M} u^{It}(|\mathbf{r}_0 - \mathbf{r}_i|)} e^{\frac{1}{2}\sum_{i=M+1}^{N} u^{In}(|\mathbf{r}_0 - \mathbf{r}_i|)} \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \, .$$

We minimize the bubble chemical potential, which determines the unknown correletion functions.

$$\mu^{IM} = \frac{\langle \Psi^{IM} | H_I | \Psi^{IM} \rangle}{\langle \Psi^{IM} | \Psi^{IM} \rangle} - \frac{\langle \Psi | H_e | \Psi \rangle}{\langle \Psi | \Psi \rangle} - M E_{\mathrm{bin}} \Bigg|$$

Express everything in terms of distribution functions

$$\mu^{IM} = n_0 \int d^2 r \left[-\frac{e^2}{\varepsilon} \frac{1}{r} \left(g^{It}(r) + g^{In}(r) - 1 \right) + \frac{\hbar^2}{2m} |(\nabla \sqrt{g^{It}(r)}|^2 + |\nabla \sqrt{g^{In}(r)}|^2) \right] + \frac{1}{2} \int \frac{d^2 k}{(2\pi)^2 n_0} S^{IM}(k) \; \tilde{w}^{IM}_{\mathrm{ind}}(k) - M E_{\mathrm{bin}}$$

Solve the resulting Euler equations

$$-\frac{\hbar^2}{2m}\nabla^2\sqrt{g^{It}(r)}+\left[-\frac{e^2}{\varepsilon r}+w_{\rm ind}^{IM}(r)\right]\sqrt{g^{It}(r)} = E_{bin}\sqrt{g^{It}(r)}$$

$$-\frac{\hbar^2}{2m}\nabla^2\sqrt{g^{In}(r)}+\left[-\frac{e^2}{\varepsilon r}+w_{\rm ind}^{IM}(r)\right]\sqrt{g^{In}(r)}=0$$

With the same induced potentials

$$\tilde{w}_{\rm ind}^{IM}(k)=\frac{\hbar^2k^2}{4m}S^{IM}(k)\left[\frac{1}{(S^{bb}(k))^2}-1\right]$$

$$S^{IM}(k)=n_0\int d^2re^{ik\cdot r}(g^{It}(r)+g^{In}(r)-1)$$

Use the normalizations

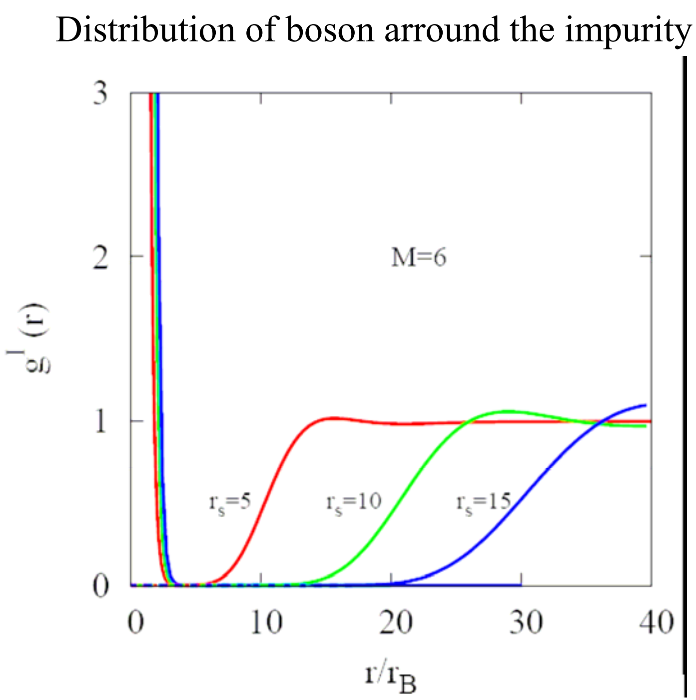
$$\int d\mathbf{r}\rho^I(r)=\frac{N}{\Omega}$$

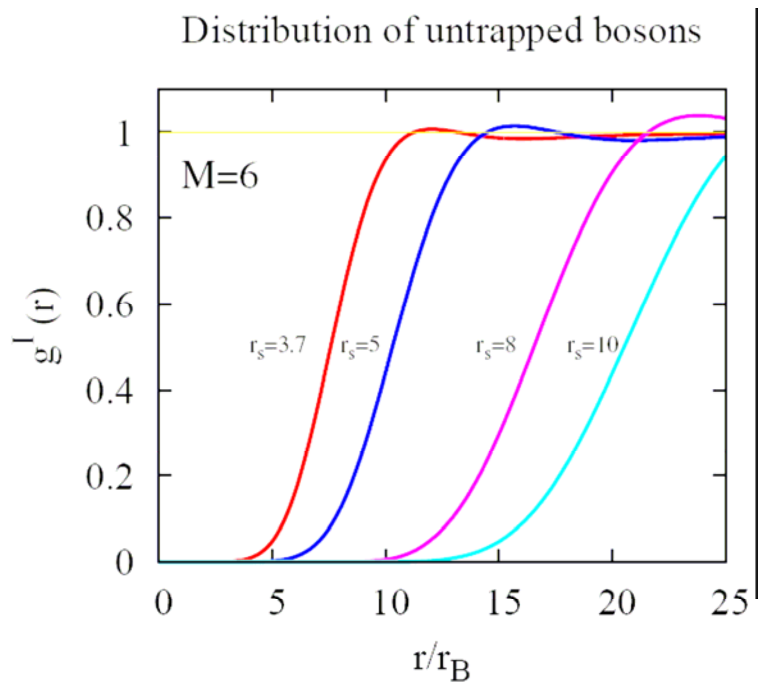
$$n_0\int d\mathbf{r}g^{It}(r)=M$$

$$n_0\int d\mathbf{r}[g^{In}(r)-1]=1-M$$

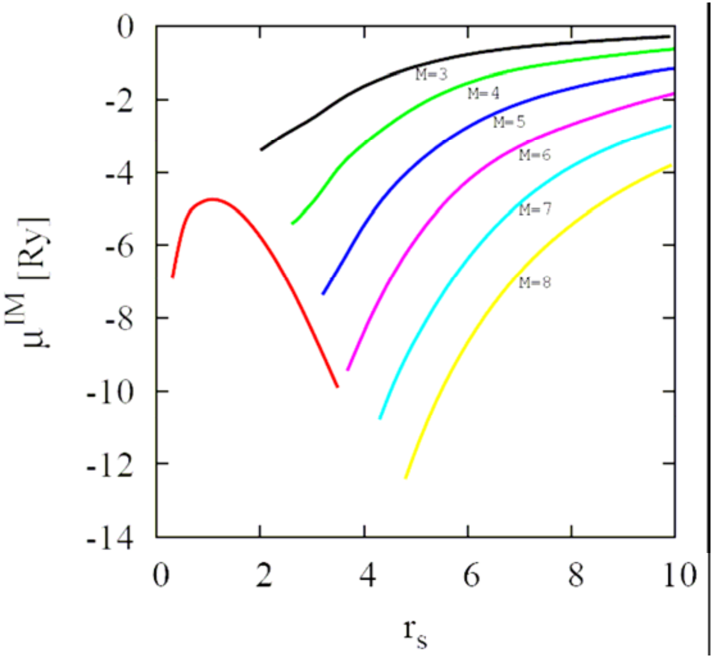
Coulomb bubble and proximity effect

At r_s >2 the boson fluid can break into two fractions. Bound particles form the Coulomb bubble and the unbound particles remain superconducting.

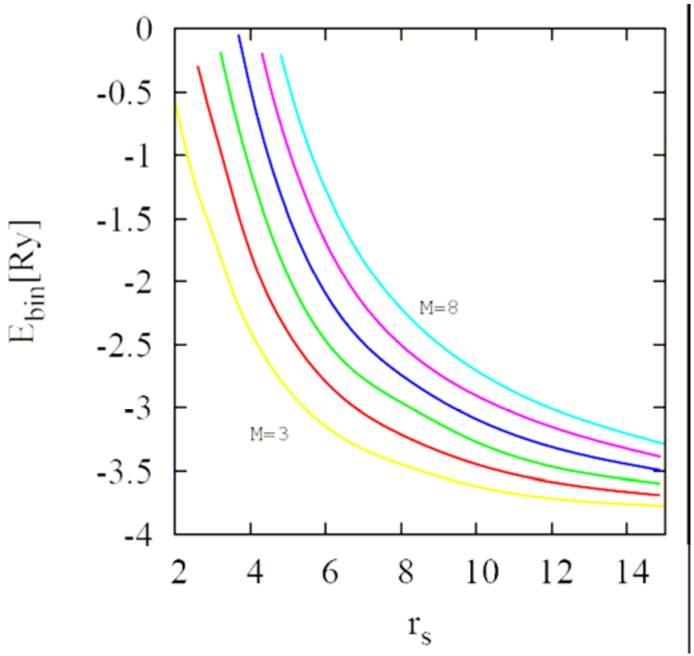




Chemical potentials with the Coulomb bubble and the Pseudogap



nergy required to create the bubble

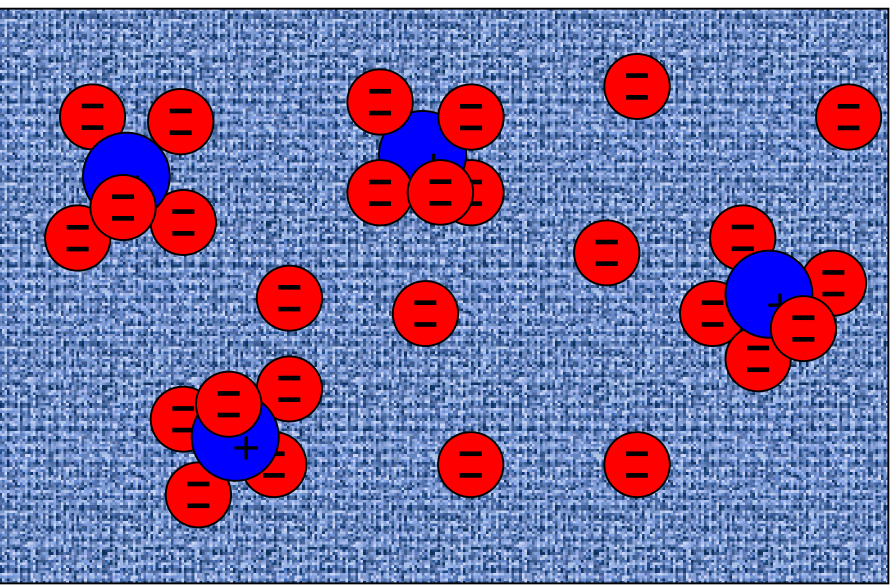


Binding energy of bosons in the bubble defines the pseudogap

Localization and superconductor-insulator transition

First step

Localization of bosons to impurities decrease the density of carrier bosons



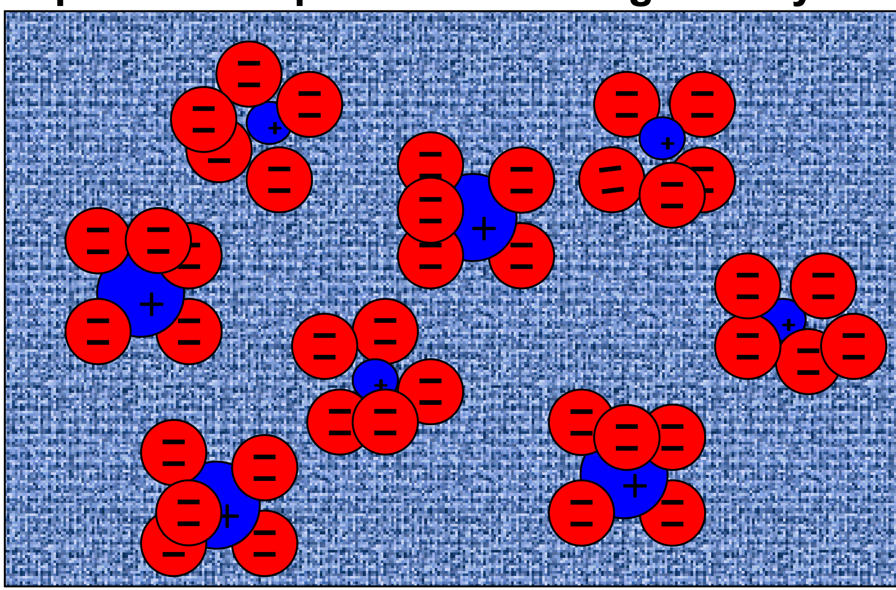
Second step

- Weaker (out of plane) charges bind a ne set of bosons → density of bosons decreases further.

-The size of the bubble increases.

- Bubbles begin to overlap

- Perculation type phase transition prevents supercurrent through the syste



Gorkov, Teitelbaum analysis PRL 97, 247003 (2006) of Hall coefficients, resistivity, ARPES and STM data of the normal phase

$$n_{\mathrm{Hall}}(x,T) = n_0(x) + n_1(x)\exp[-\Delta(x)/T].$$

$$n(x) = n_0(x) + n_1 \exp(E_{bin}(x,M)/T)$$

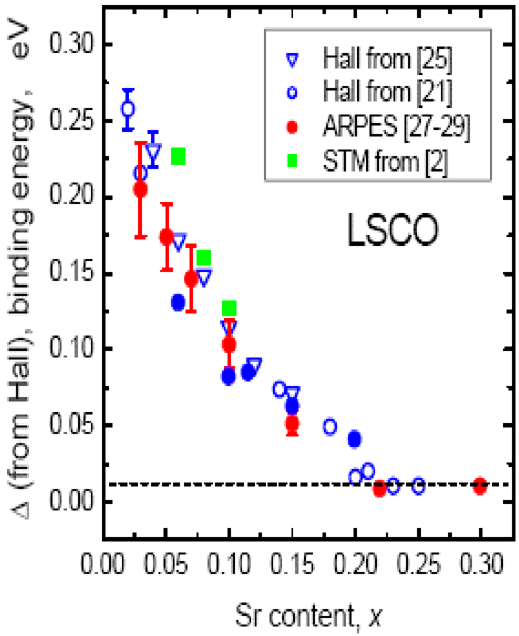
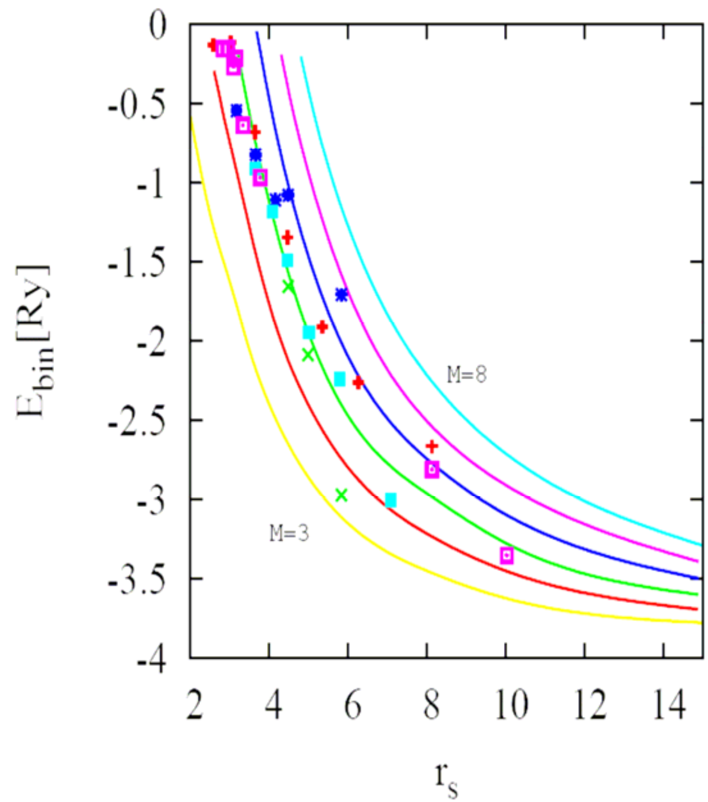


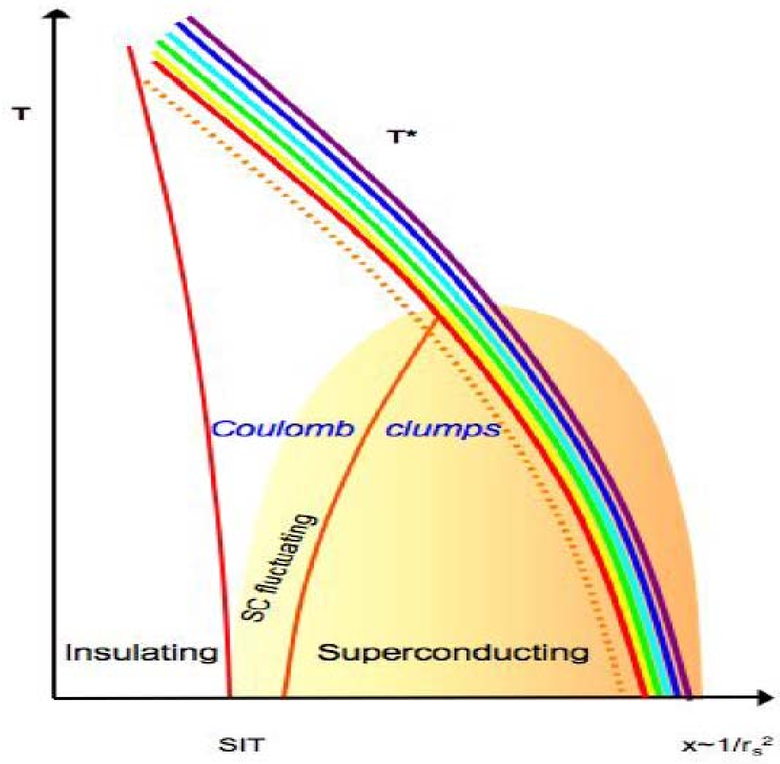
Figure 4. The ARPES binding energy vs the Hall activation energy. (See [1] for the details.)



$$-4Ry = -2me^4/(\epsilon^2\hbar^2) = -0.3eV$$

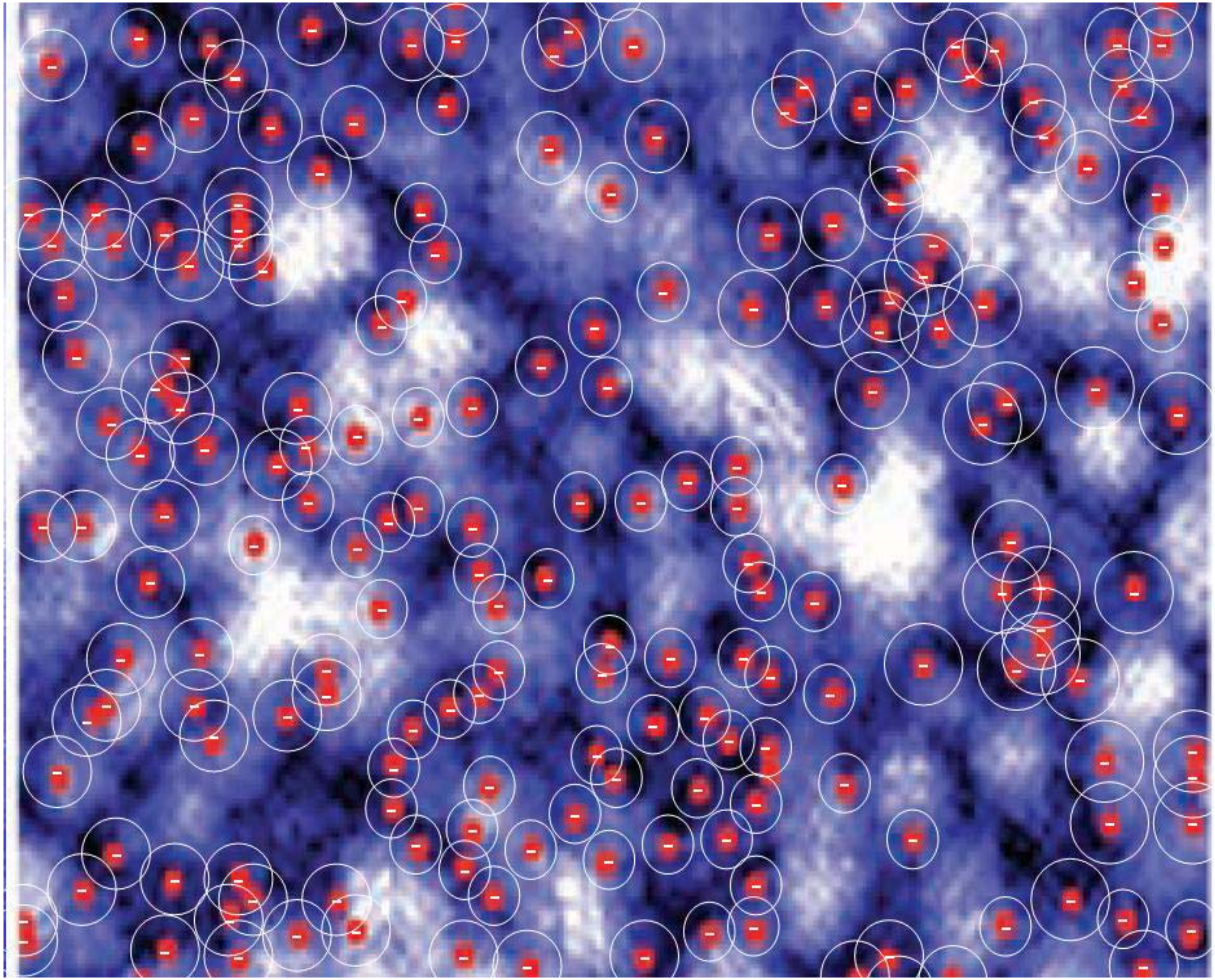
$$x = 1.4/r_s^2$$

Schematic phase diagram of layered superconductors. Paralell color lines mark the pseudogap region.



$$T^*(x) = -E_{bin}/\ln(x)$$

Coulomb bubbles in BSCO comparison with STM data by Davis et al. Science 2005



- LDOS at E~24 meV
- Oxygen impurities
- Modulation, CDW are strong
- Dopants are at minima

Conclusions

- Experimentally charged impurities play the main role in the doping controlled superconducting-insulator transition in quasi two-dimensional layers.
- Charged impurities bind bosons and form Coulomb bubbles. The binding energy determines the pseudogap.
- The superconducting state vanishes with a quantum phase transition when charge carriers are trapped by the Coulomb bubbles in such a way that no coherent phase can percolate through the whole fluid.
- Bubbles are first covered by superfluid liquid due to a proximity effect and invisible.
- With decreasing carrier density, the size of bubbles increases and the superconducting proximity inside bubbles vanishes.
- The insulating state arises via a percolation of insulating islands.

Congratulation SIU

And many happy years to come