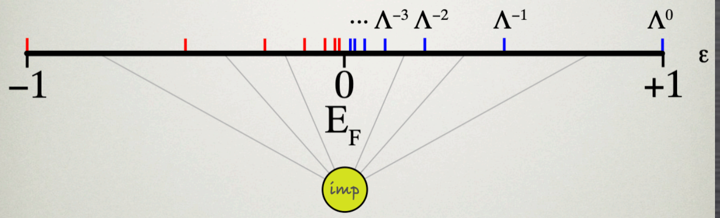
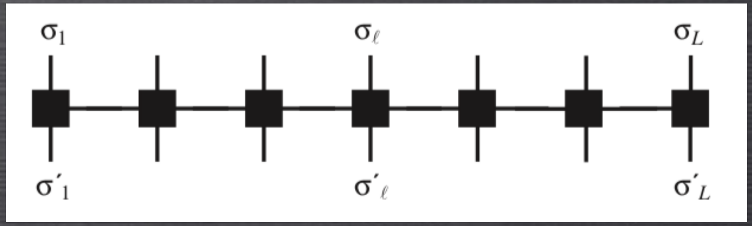
SOLVERS FOR QUANTUM IMPURITY PROBLEMS (WITH SUPERCONDUCTING BATHS)

LECTURE 4: IMPURITIES IN SUPERCONDUCTING BATHS





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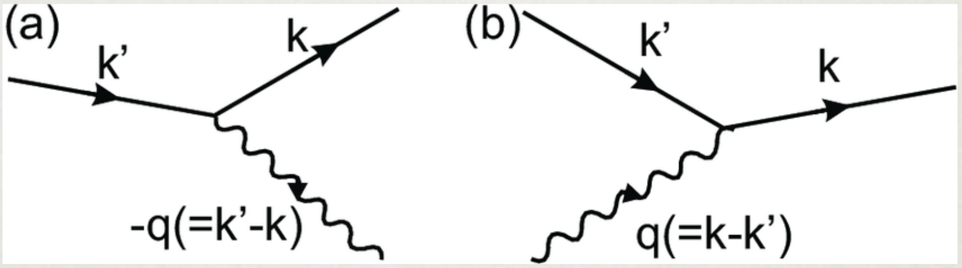
Part 1: models

ELECTRON-PHONON INTERACTION

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_q \omega_q a^\dagger_q a_q + \sum_{k\sigma q} g_{kq} c^\dagger_{k+q,\sigma} c_{k,\sigma} \left(a_q + a^\dagger_{-q} \right)$$

(Fröhlich)



EFFECTIVE E-E INTERACTION

$$H_{\text{pairing}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,q} V_{k,q} c^\dagger_{k+q,\uparrow} c^\dagger_{-k-q,\downarrow} c_{-k,\downarrow} c_{k,\uparrow}$$

$$V_{k,q} \approx \frac{|g_{kq}|^2 \hbar\omega_q}{(\epsilon_{k+q} - \epsilon_k)^2 - (\hbar\omega_q)^2}$$

Attractive for

$\epsilon_k, \epsilon_{k+q} \in [\epsilon_F - \hbar\omega_D : \epsilon_F + \hbar\omega_D]$

$$H_{\text{red}} = \sum_{\mathrm{k}\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,k'} V_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$\Delta_k = \sum_{k'} V_{k,k'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

$$H_{\text{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k} \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

TIME-REVERSAL INVARIANCE

$$\mathbf{k} \leftrightarrow -\mathbf{k}, \quad \uparrow\leftrightarrow\downarrow$$

Preserved in the presence of potential scattering.
Preserved in the presence of spin-orbit coupling.

Broken by spin-dependent scattering.
Broken by magnetic field.
Broken by current flow.

ANDERSON'S THEOREM

Superconductivity in a conventional superconductor is robust with respect to (non-magnetic) disorder. T_c barely depends on material purity (in fact, it increases upon increasing disorder!).

Anderson, P. W. (1959). "Theory of dirty superconductors". J. Phys. Chem. Solids. 11: 26–30.

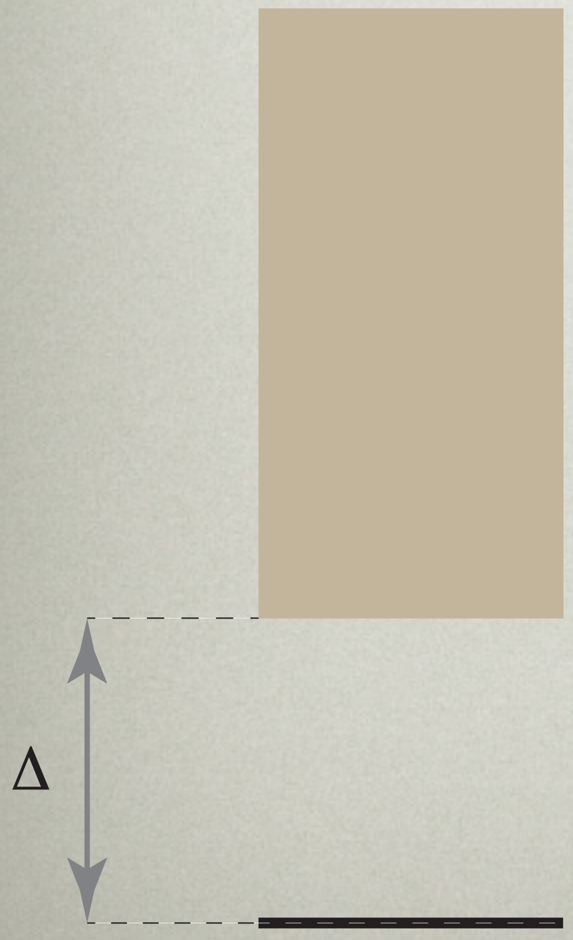
BOGOLIUBOV QUASIPARTICLES

$$H_{\mathrm{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

$$\gamma_{k\uparrow} = u_k c_{k\uparrow} - v_k c^\dagger_{-k\downarrow}$$

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}}\right)$$

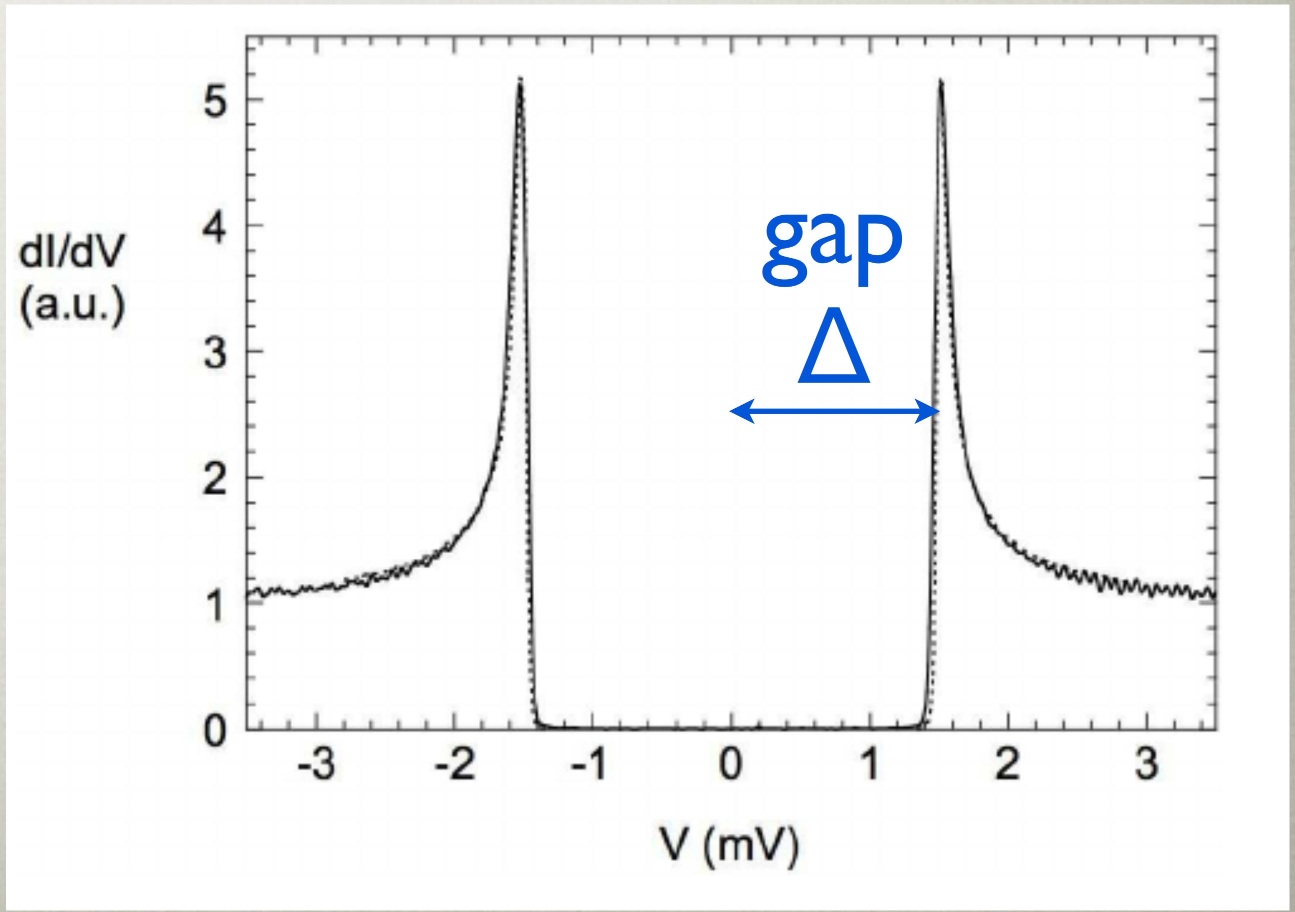
$$v_k^2 = \frac{1}{2}\left(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}}\right)$$



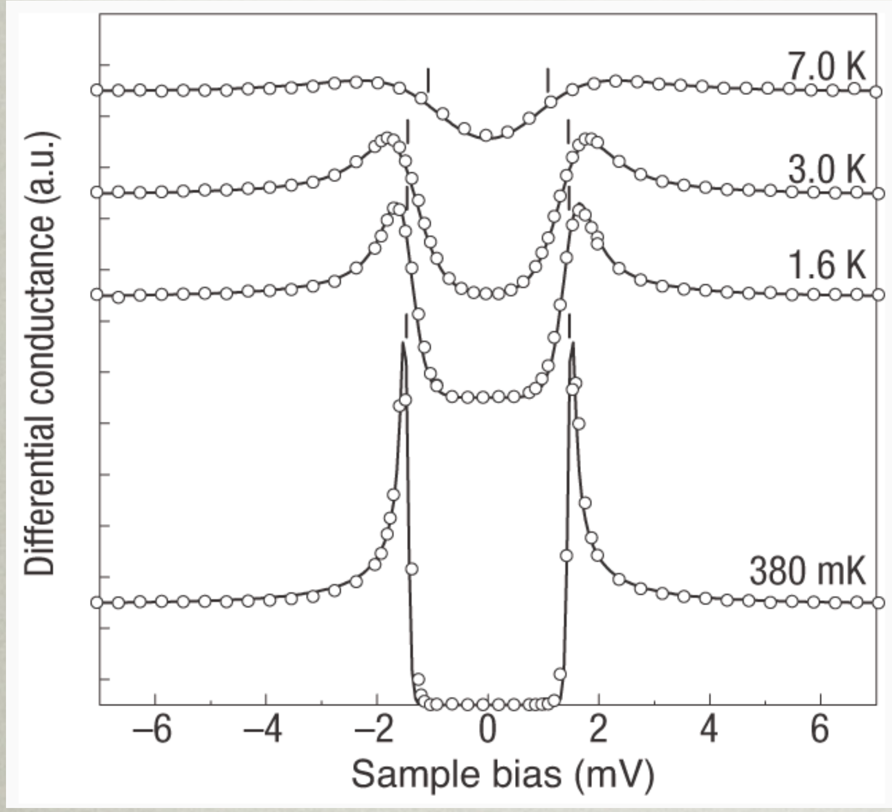
$$E_k = \sqrt{\epsilon_k^2 + \Delta^2}$$

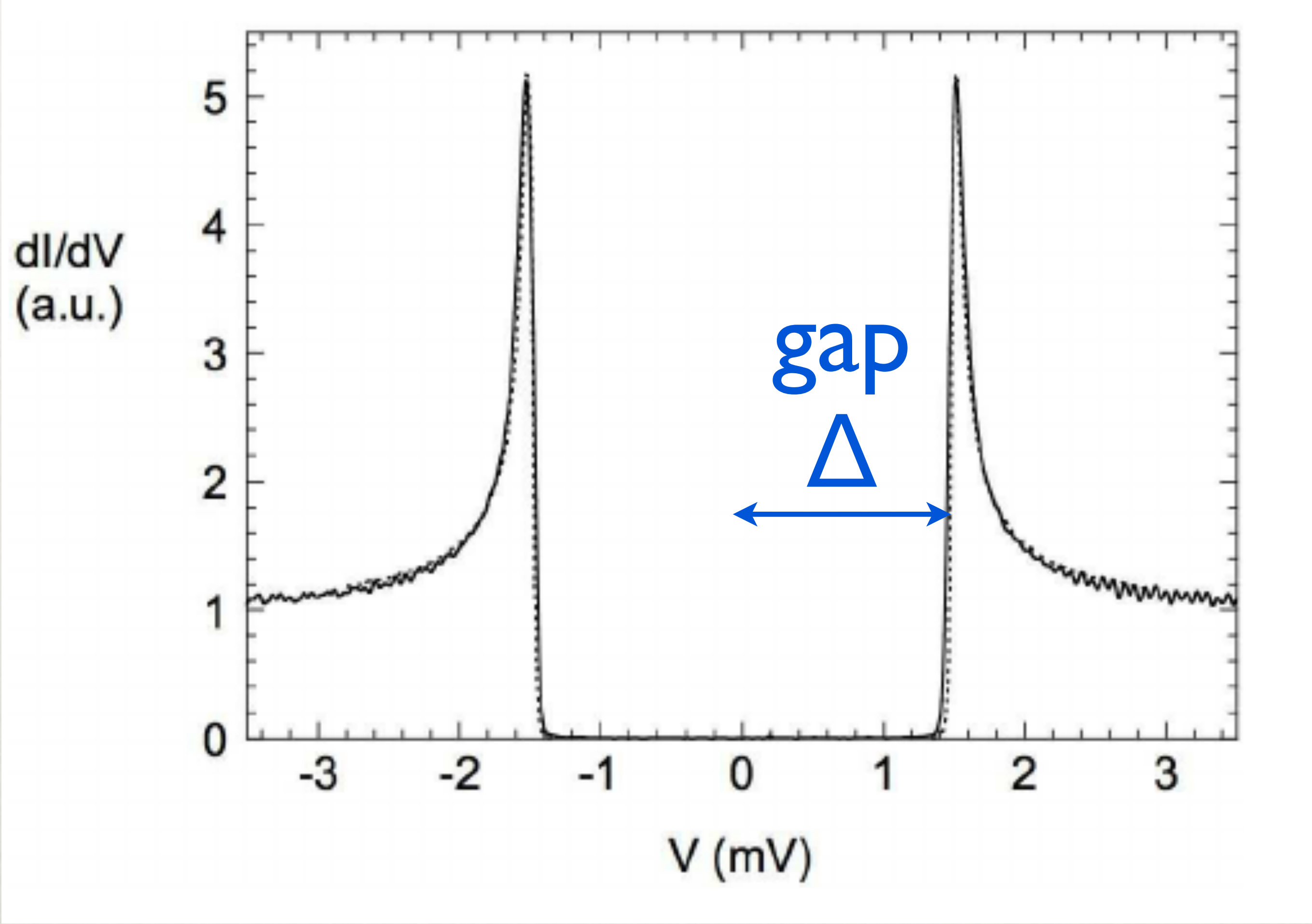
quasiparticle continuum

ground state



SUPERCONDUCTING GAP





Nb, T=170mK, Δ=1.5meV

H. Courtois, Grenoble
PRB (2005)

scanning tunneling microscope (STM) dI/dV spectra

(proportional to the local density of states)

NAMBU NOTATION

dim=2 for B=0 and B along z-axis,
dim=4 for general direction of B

$$\psi_k^\dagger = \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow} \end{pmatrix} \qquad \psi_k^\dagger = \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{k\downarrow}^\dagger \\ c_{-k\uparrow} \\ c_{-k\downarrow} \end{pmatrix}$$

Hamiltonian expressed in terms of 2x2 or 4x4 matrices.

Richardson model

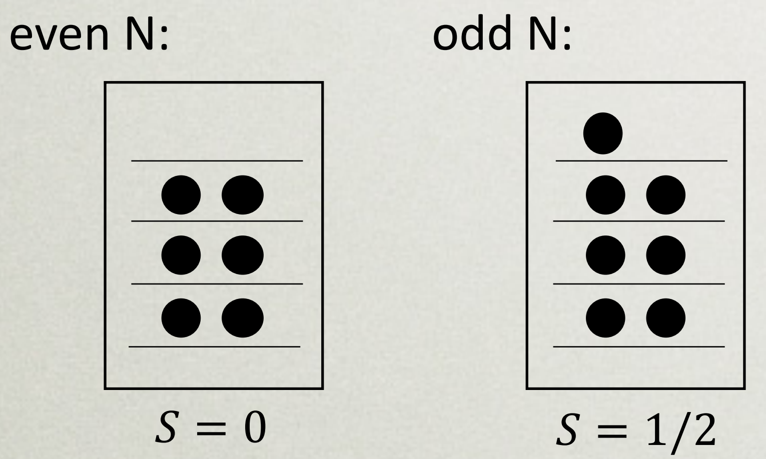
charge-conserving Hamiltonian for superconducting grains

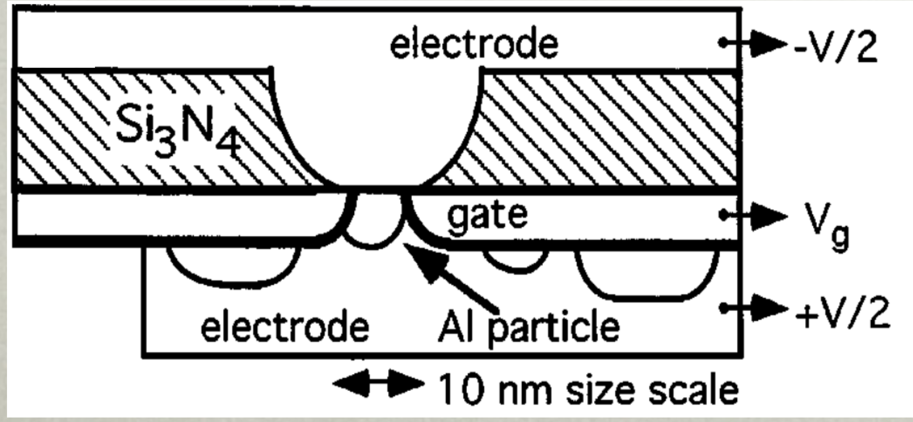
$$H = \sum_i \epsilon_i c^\dagger_{i\sigma} c_{i\sigma} - \alpha d \sum_{i,j} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow}$$

coupling strength

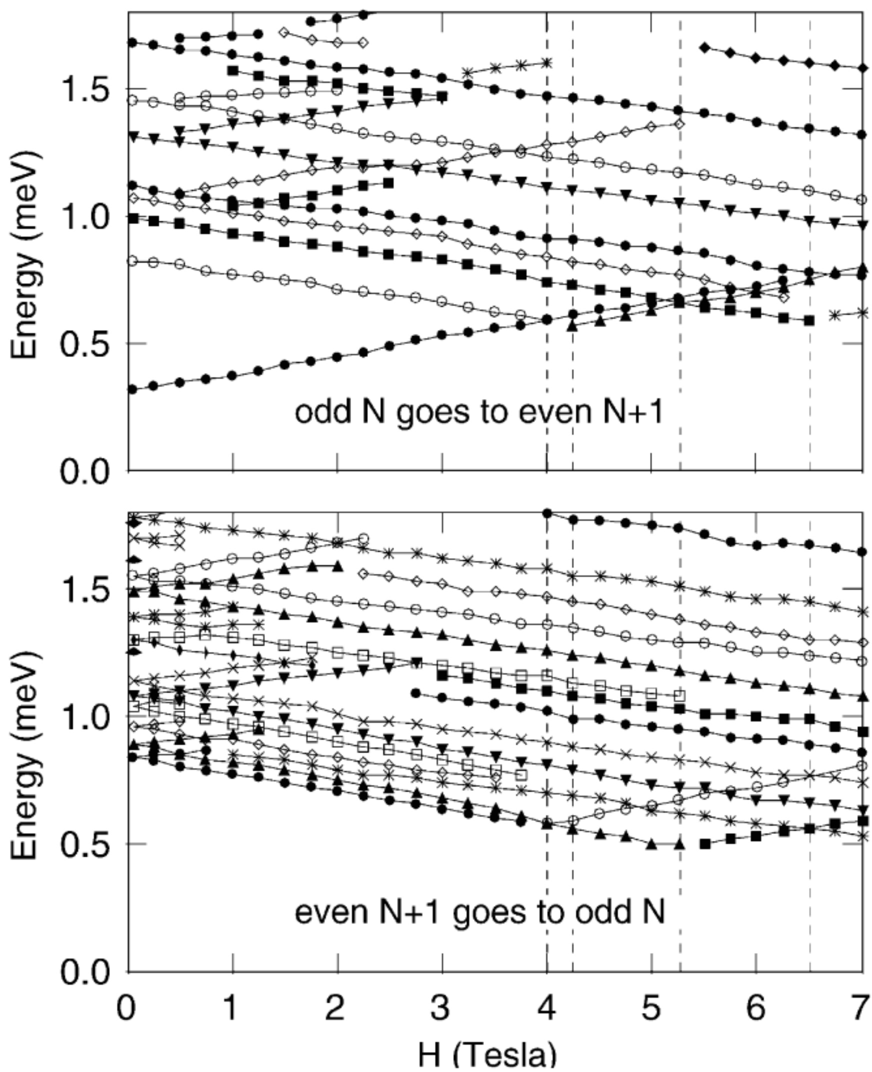
interlevel spacing

coupling between
the time-reversal conjugate pairs!





Ralph, Black, Tinkham, 1996, 1997



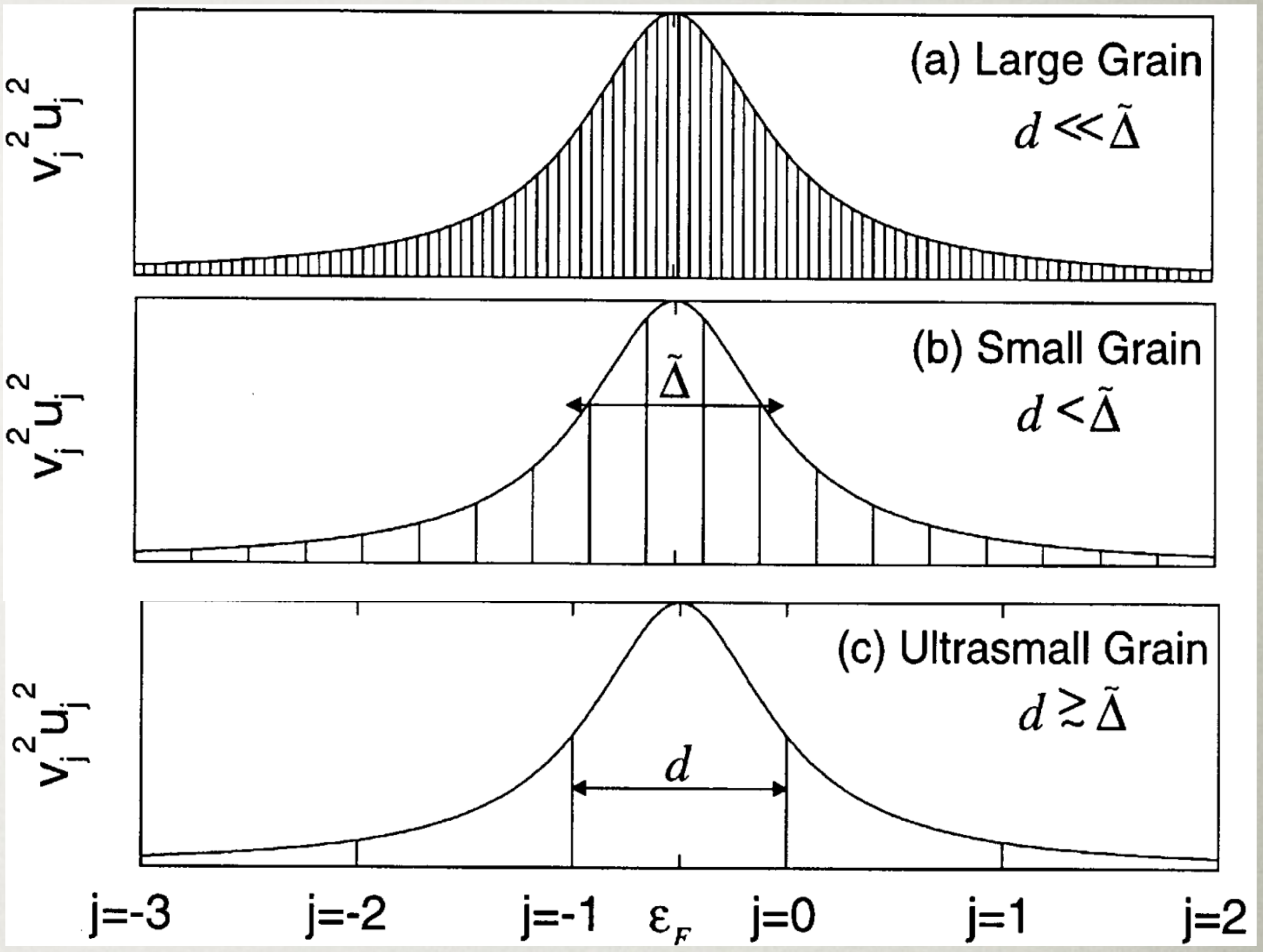
What is the smallest system size at which the superconductivity persists?

interlevel spacing $d \propto \dfrac{1}{V}$

number of Cooper pairs = d/Δ

$$\frac{d}{\Delta} \approx 1$$

Anderson (1959)



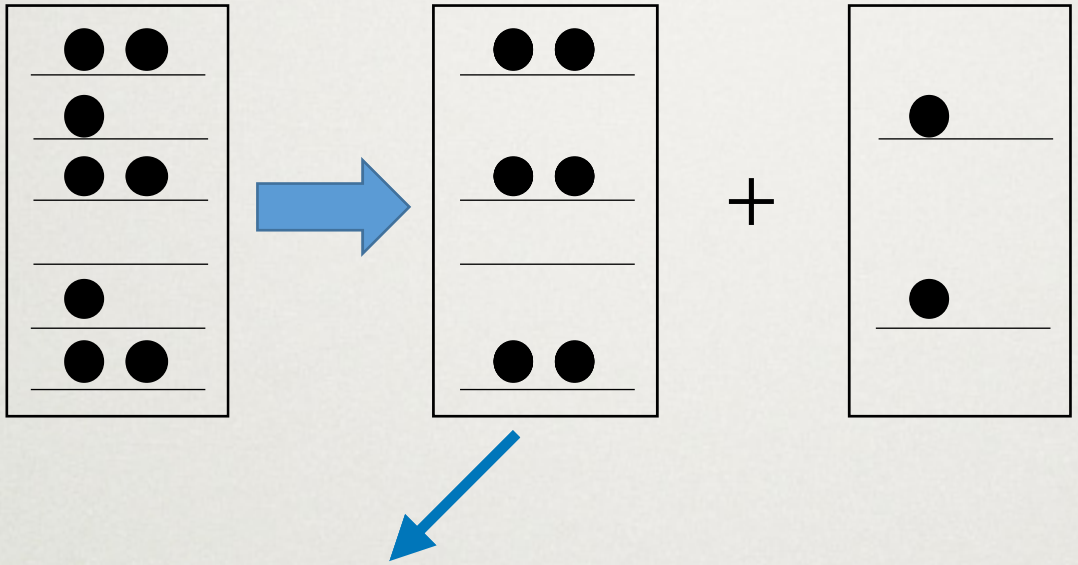
von Delft, Ralph, 2001

Averin, Nazarov (1992)
Jankó, Smith, Ambegaokar (1994)
Golubev, Zaikin (1996)

von Delft, Zaikin, Golubev, Tichy (1996)
Mastellone, Falci, Fazio (1998)
Braun, von Delft (1998,1999)
Dukelsky, Sierra (1999,2000)

Tuominen, Hergenrother, Tighe, Tinkham (1992)
Lafarge, Joyez, Esteve, Urbina, Devoret (1993)
Eiles, Martinis, Devoret (1993)

EXACT SOLUTION OF RICHARDSON MODEL



single-occupied levels are inert
(blocking effect!)

$$H = \sum_{ij} (2\epsilon_i \delta_{ij} - \alpha d) b_i^\dagger b_j$$

$$b_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$$

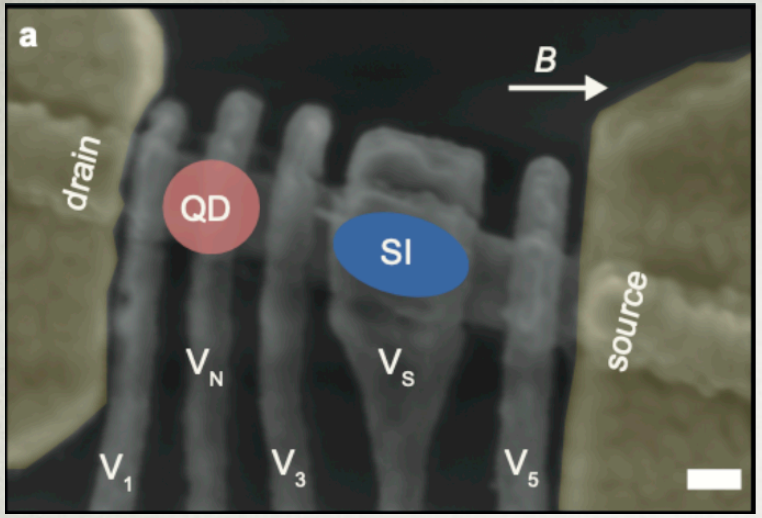
hard-core bosons

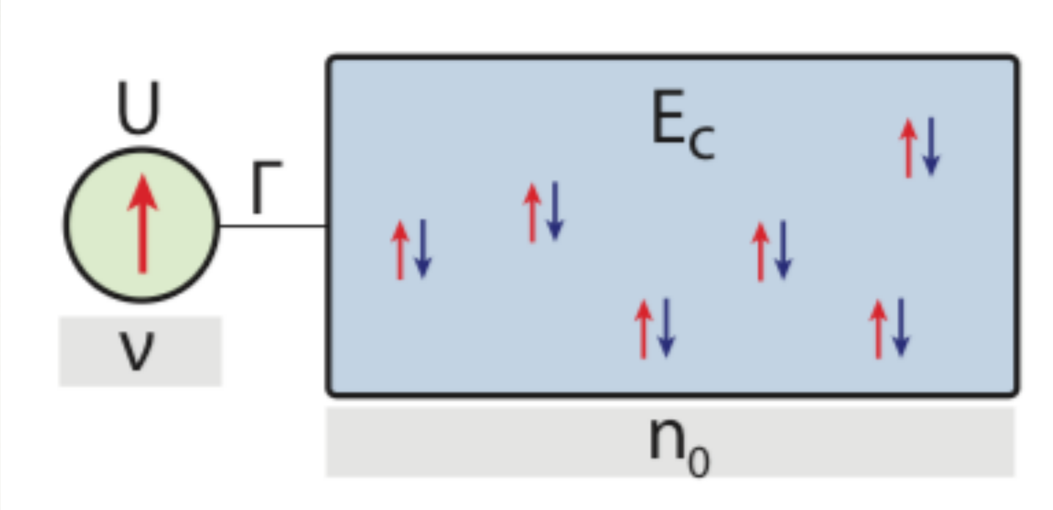
$$|\psi\rangle = \prod_\alpha \left(\sum_{i=1}^{N} \frac{b_i^\dagger}{2\epsilon_i - E_\alpha} \right) |0\rangle$$

eigenvalue equation: $$\frac{1}{\alpha d} - \sum_j \frac{1}{2\epsilon_j - E_\nu} + \sum_{\mu \neq \nu} \frac{2}{E_\mu - E_\nu} = 0$$

Fully equivalent to BCS in the large-N, small-α limit

Richardson, 1963

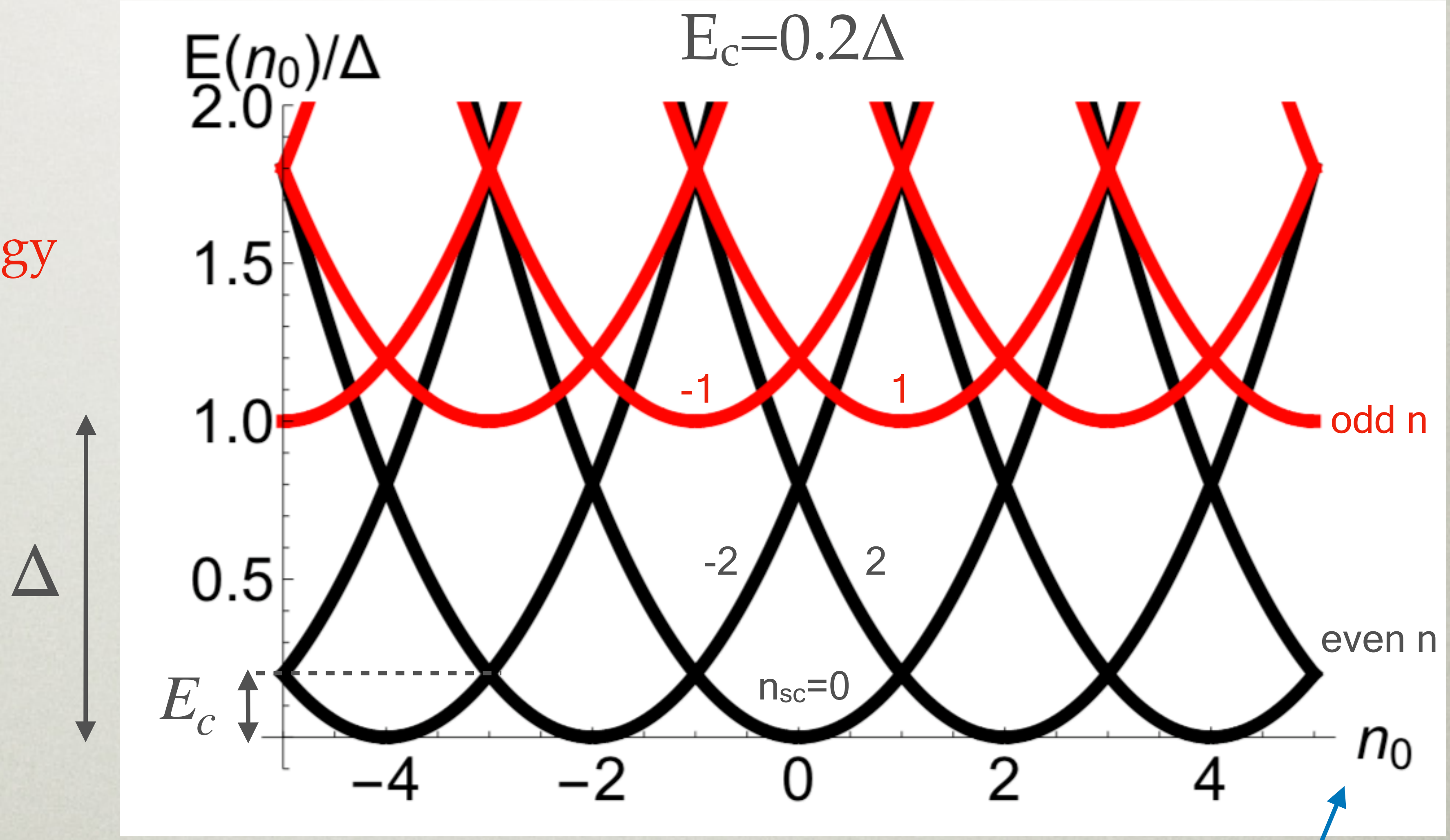




$$E_c(\hat{n}_{\mathrm{sc}} - n_0)^2$$

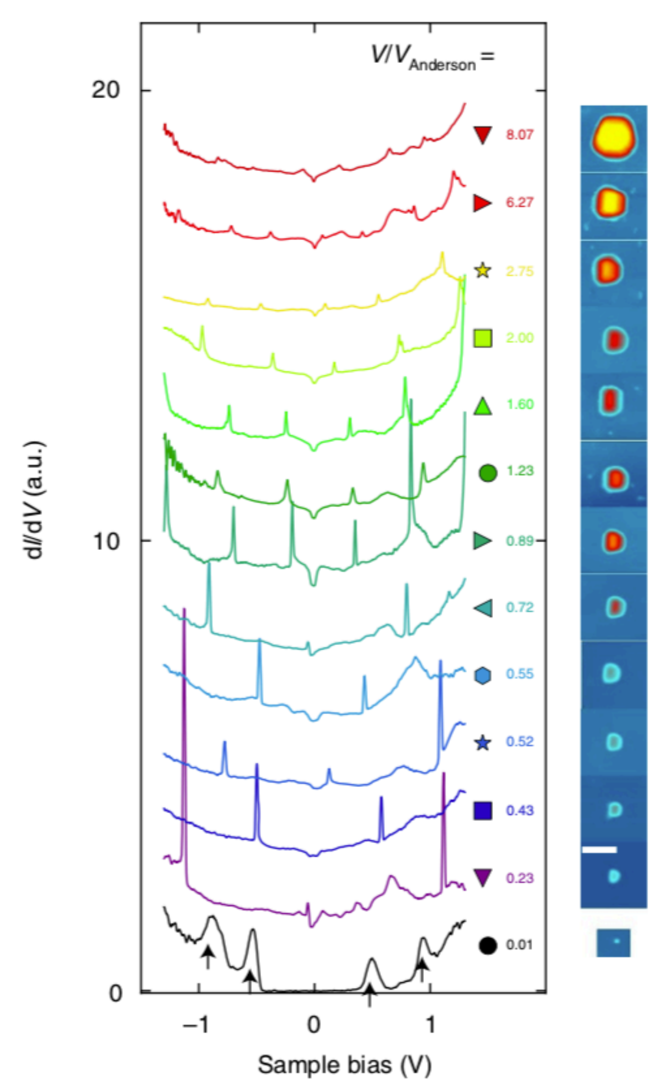
$$E_c = \frac{e_0^2}{2C}$$

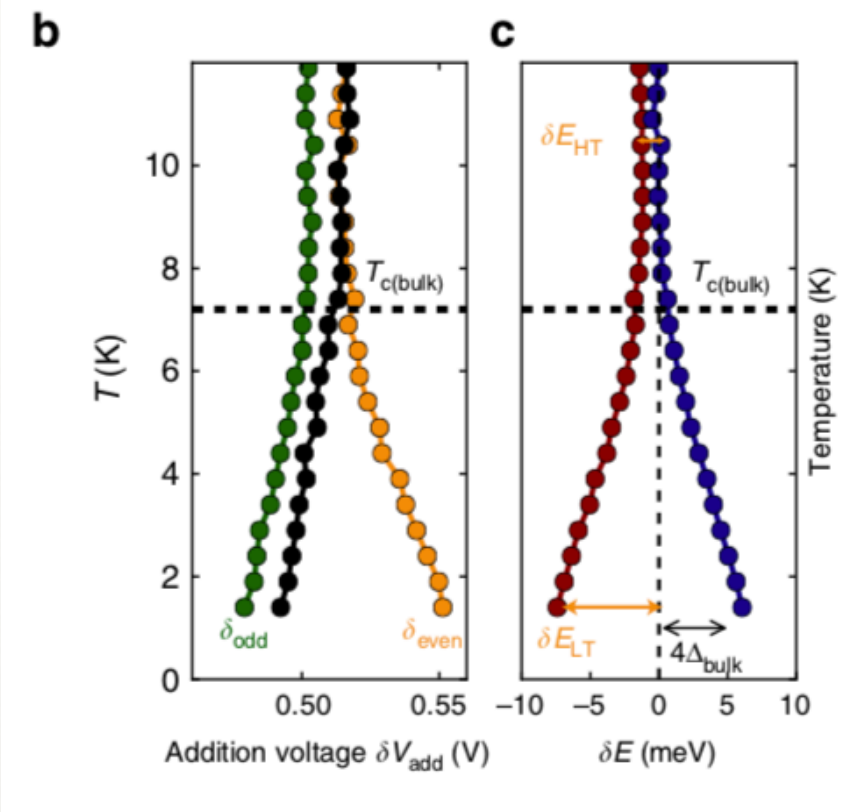
charging energy

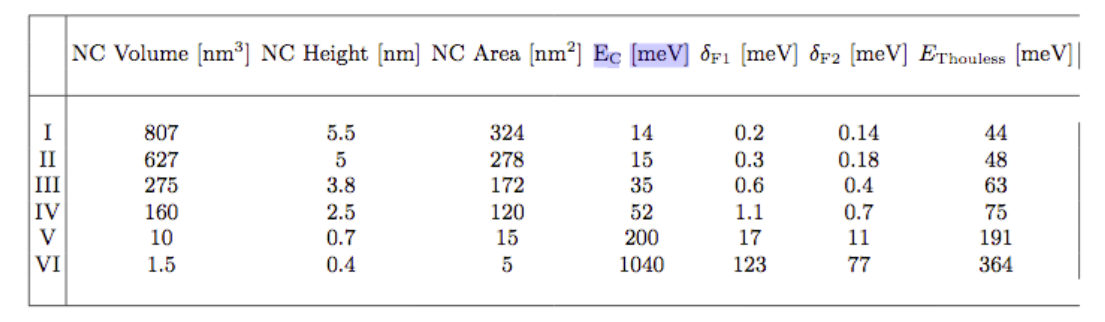


energy-level / gate-voltage expressed in units of electron number

PB ISLANDS ON INAS(110)







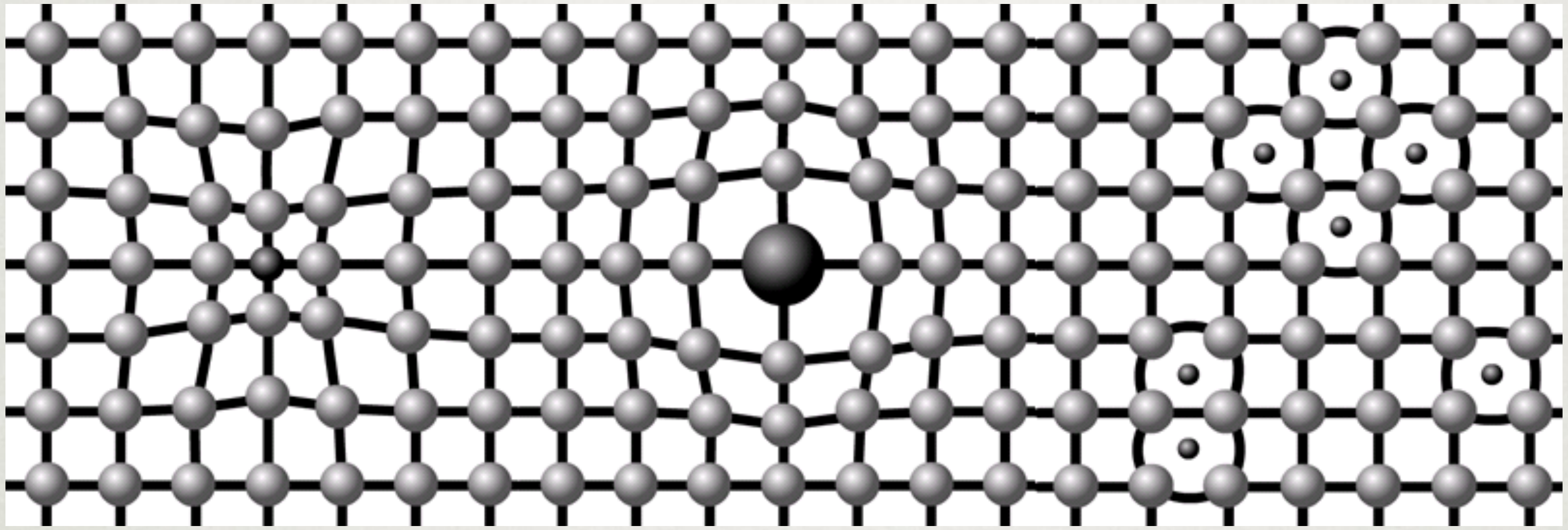
	NC Volume [nm^3]	NC Height [nm]	NC Area [nm^2]	E_C [meV]	δ_{F1} [meV]	δ_{F2} [meV]	E_{Thouless} [meV]
I	807	5.5	324	14	0.2	0.14	44
II	627	5	278	15	0.3	0.18	48
III	275	3.8	172	35	0.6	0.4	63
IV	160	2.5	120	52	1.1	0.7	75
V	10	0.7	15	200	17	11	191
VI	1.5	0.4	5	1040	123	77	364

Vlaic et al. (2017), Hervé Aubin group

CHARGE-PHASE DUALITY

$$\Delta\phi \cdot \Delta N \gtrsim 1$$

DEFECTS IN SUPERCONDUCTORS



<u>Non-magnetic</u>: hardly any effect (Anderson's theorem)

Clean superconductor: pairing between k↑ and -k↓ Bloch states

Dirty superconductor: pairing between time-reversal partners

<u>Magnetic</u>: broken time-reversal symmetry, pair-breaking effect

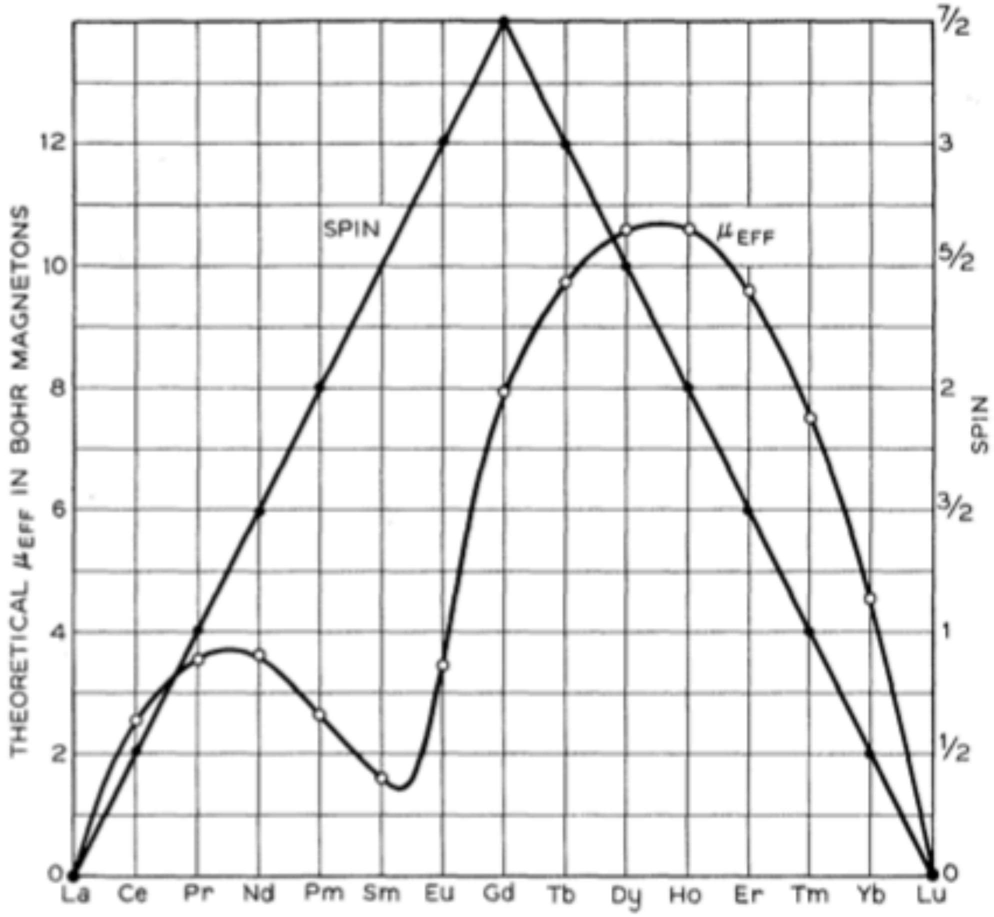


FIG. 1. Effective magnetic moments and spins of the rare earth elements (see reference 2).

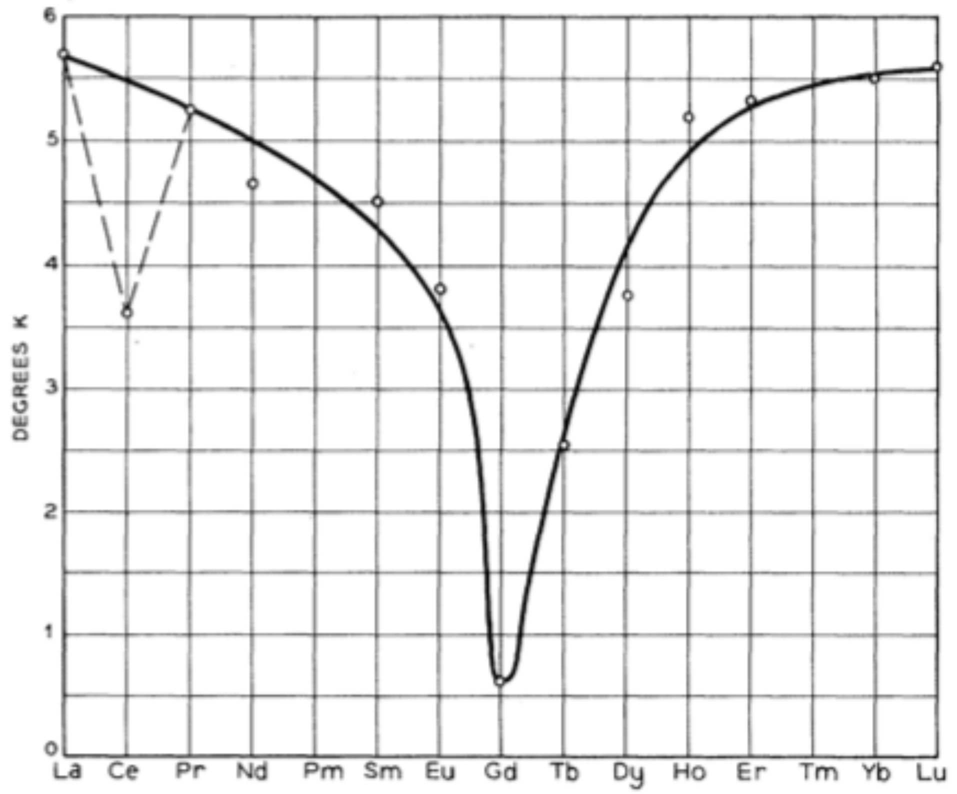


FIG. 2. Superconducting transition temperatures of 1 at % rare earth solid solutions in lanthanum.

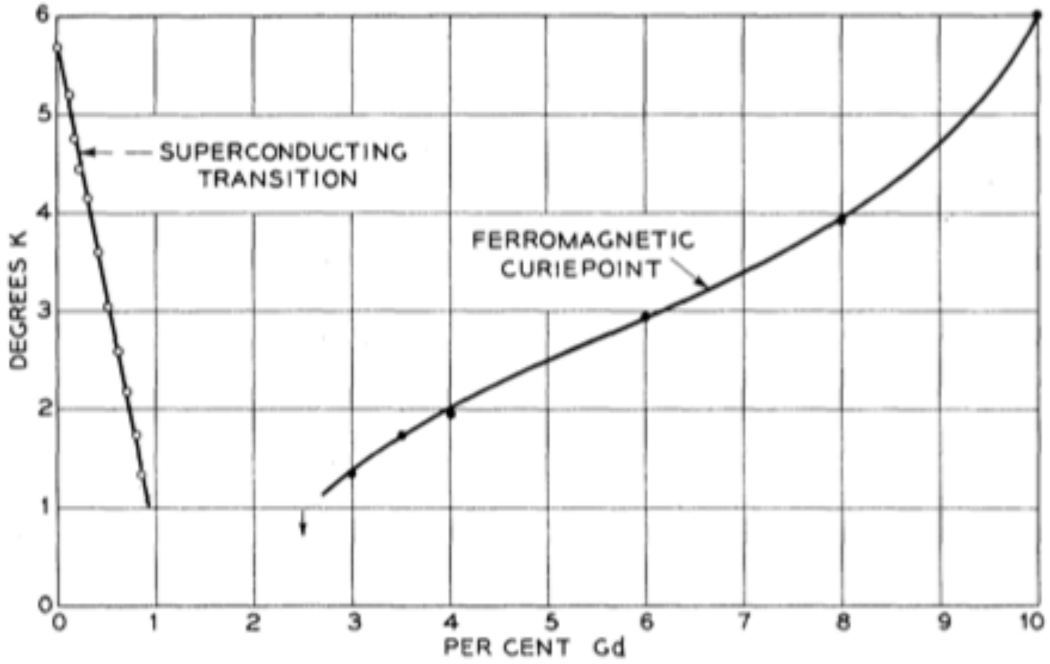


FIG. 3. Ferromagnetic and superconducting transition temperatures of solid solutions of gadolinium in lanthanum.

- individual impurities involved
- exchange scattering (spin d.o.f.)
- coupling to itinerant bulk states

Matthias, Suhl, Corenzwit (1958)

$$H_{\mathrm{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

$$H_{\mathrm{imp}} = J \mathbf{S} \cdot \mathbf{s}(\mathbf{r} = 0)$$

with $\mathbf{s} = \frac{1}{N} \sum_{kk'} c^\dagger_k \left(\frac{1}{2} \boldsymbol{\sigma} \right) c_{k'} = f^\dagger_0 \left(\frac{1}{2} \boldsymbol{\sigma} \right) f_0$

This is Kondo model with superconducting bath.
Difficult non-perturbative many-body problem!

Classical limit: $S \to \infty, JS = \mathrm{const}$

$J\langle i|S^+|j\rangle \propto \dfrac{1}{\sqrt{S}} \to 0 \quad \Longrightarrow$ effectively a static local magnetic field of strength B$_{\mathrm{eff}}$=JS

How do quasiparticles scatter on a static point-like magnetic moment?

$$\gamma_{k\uparrow} = u_k c_{k\uparrow} - v_k c^\dagger_{-k\downarrow}$$

Spin-dependent potential scattering:
attractive for one spin orientation, repulsive for the other.

Attractive potential for s-wave Bogoliubov wavefunctions
has a bound state for any J!

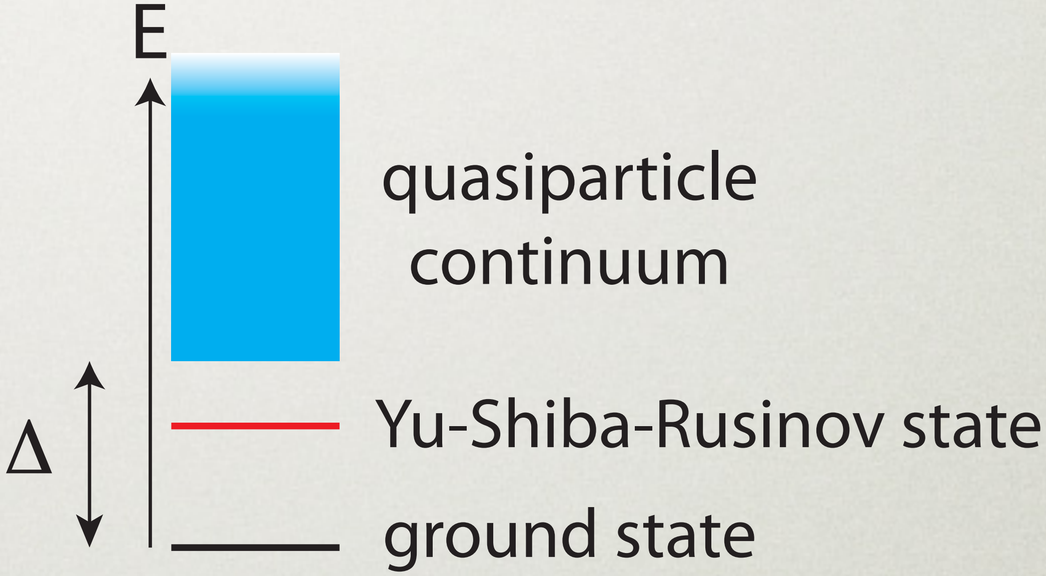
YU-SHIBA-RUSINOV STATES

Magnetic impurity creates a bound state inside the superconducting gap (= subgap state).

$$E_{\mathrm{YSR}} = \Delta \frac{1-\alpha^2}{1+\alpha^2}$$

$$\alpha = JS\pi\rho/2$$

Yu Lu, Acta Physica Sinica (1965)
H. Shiba, Prog. Theor. Phys. (1968)
A. I. Rusinov, ZhETF Pis. Red (1969)



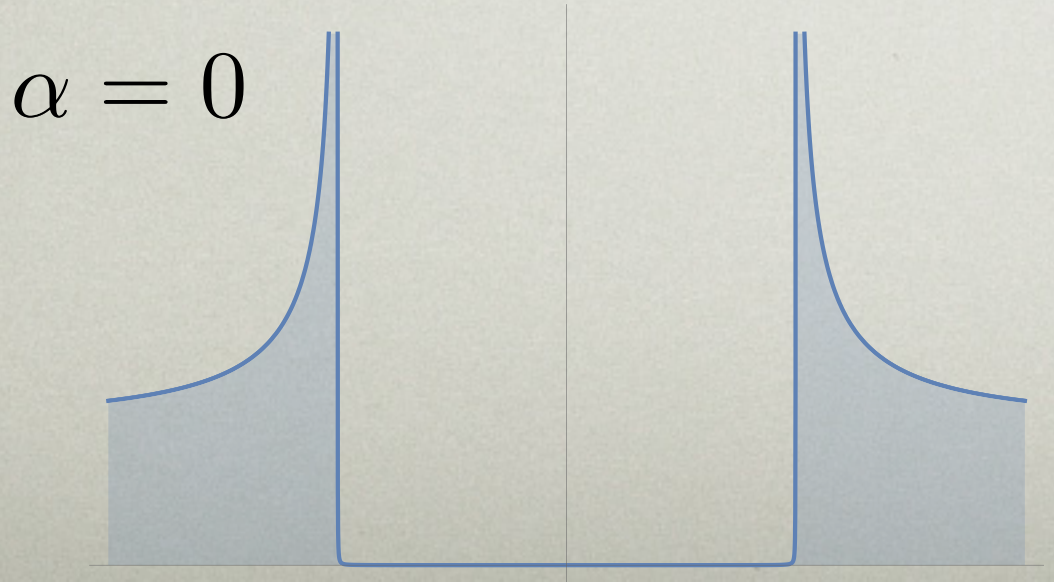
E

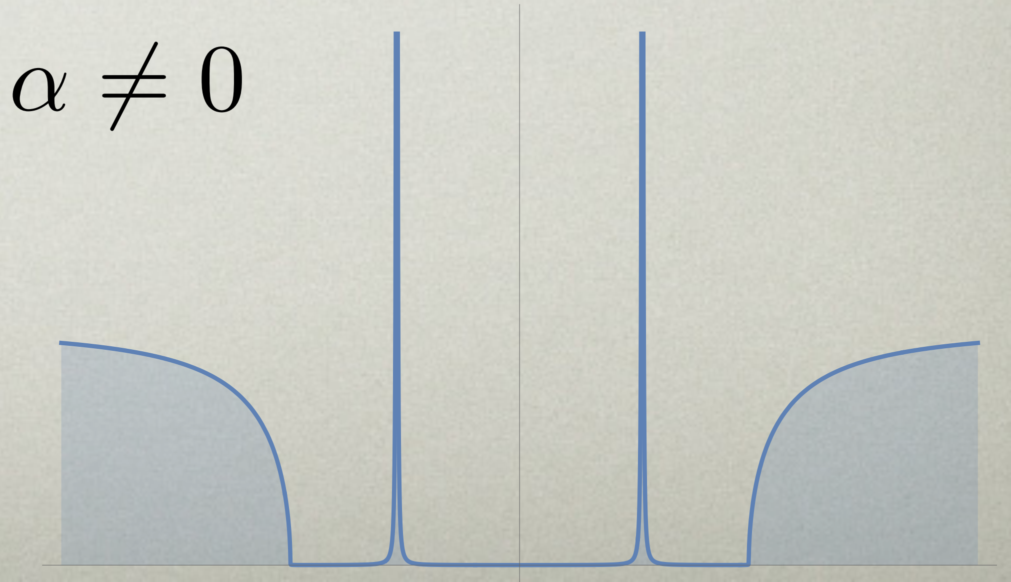
quasiparticle continuum

Yu-Shiba-Rusinov state

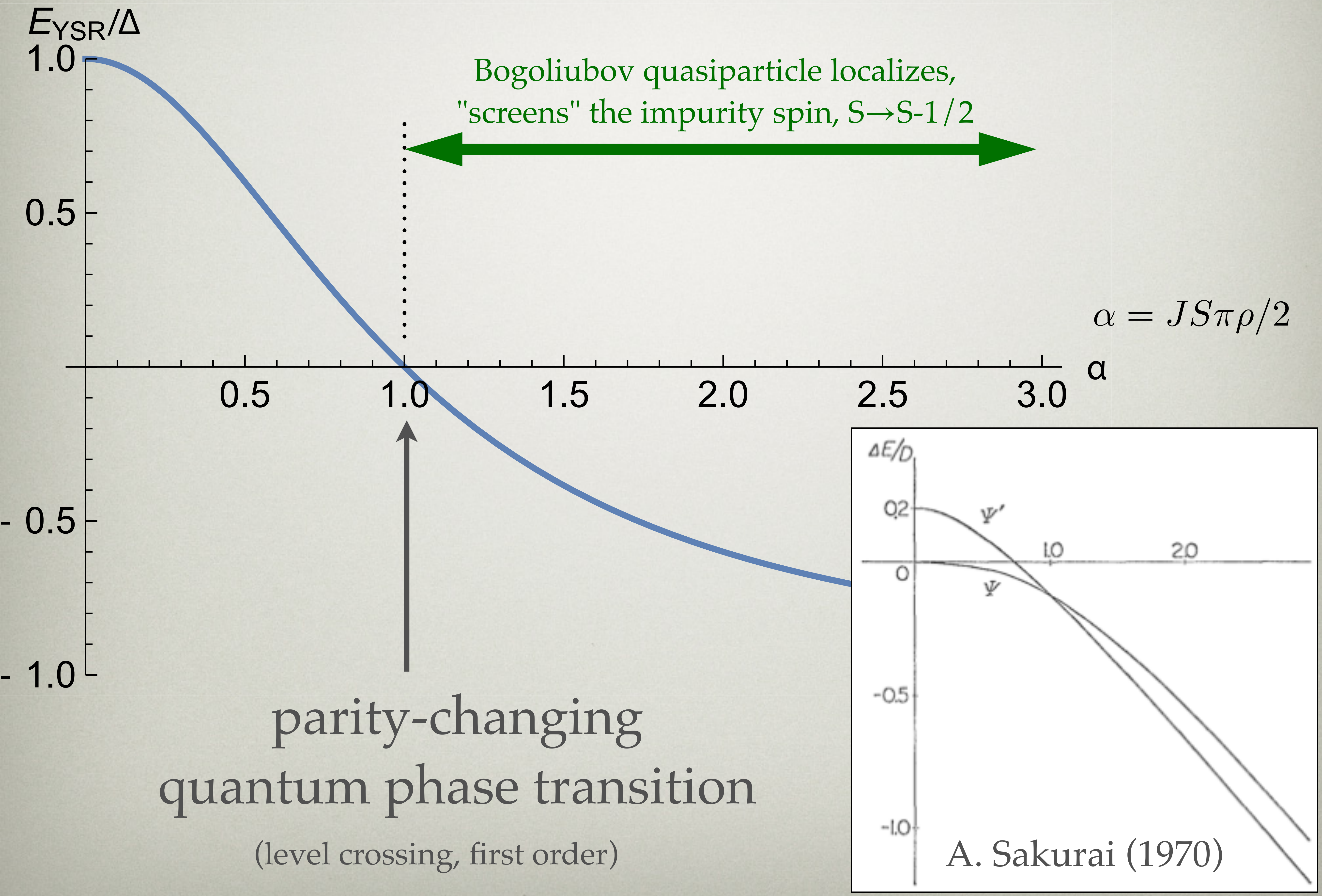
Δ

ground state





$S \to \infty$



Bogoliubov quasiparticle localizes, "screens" the impurity spin, S→S-1/2

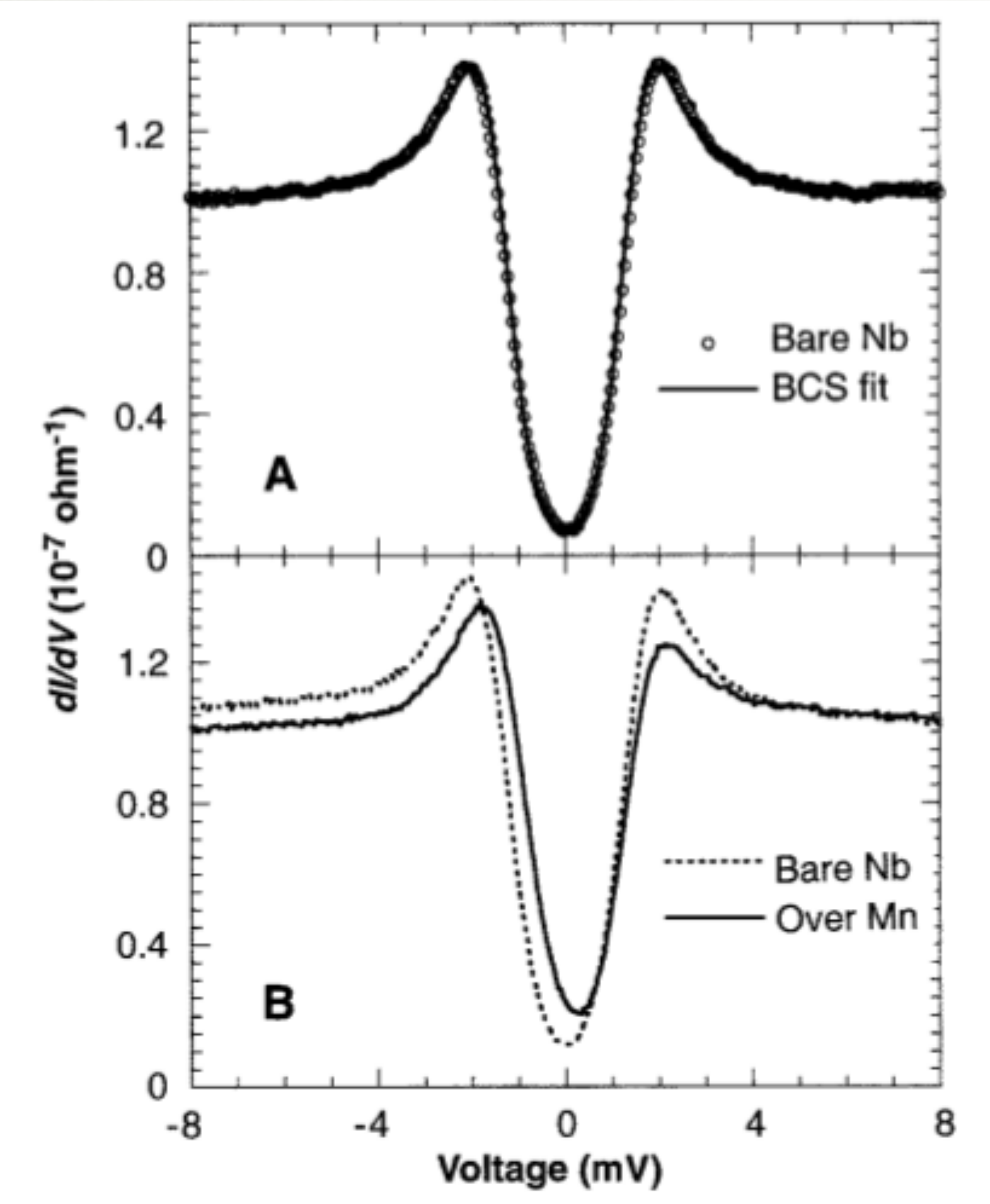
$\alpha = JS\pi\rho/2$

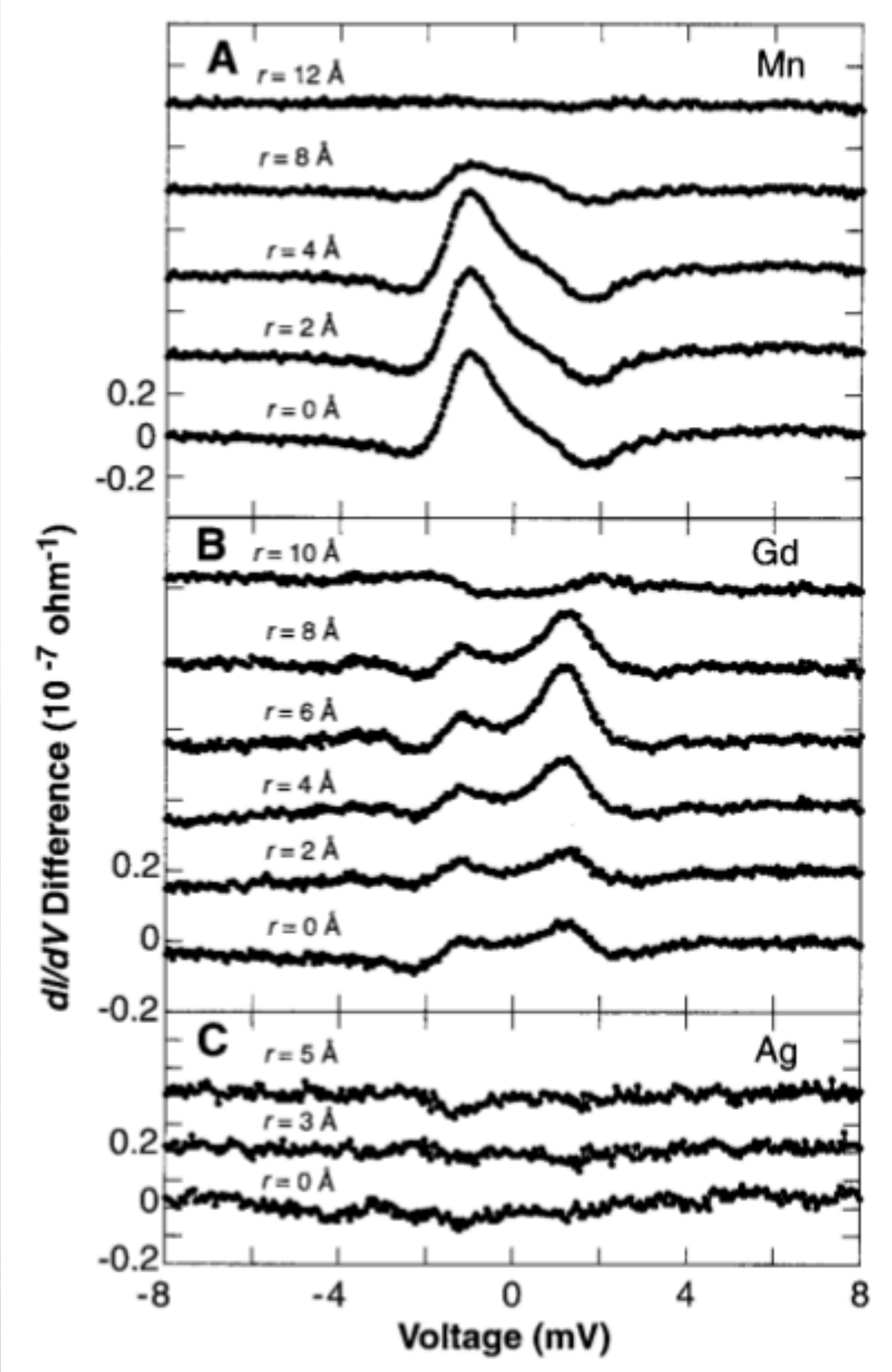
parity-changing quantum phase transition

(level crossing, first order)

A. Sakurai (1970)

Single magnetic atoms adsorbed on Nb surface



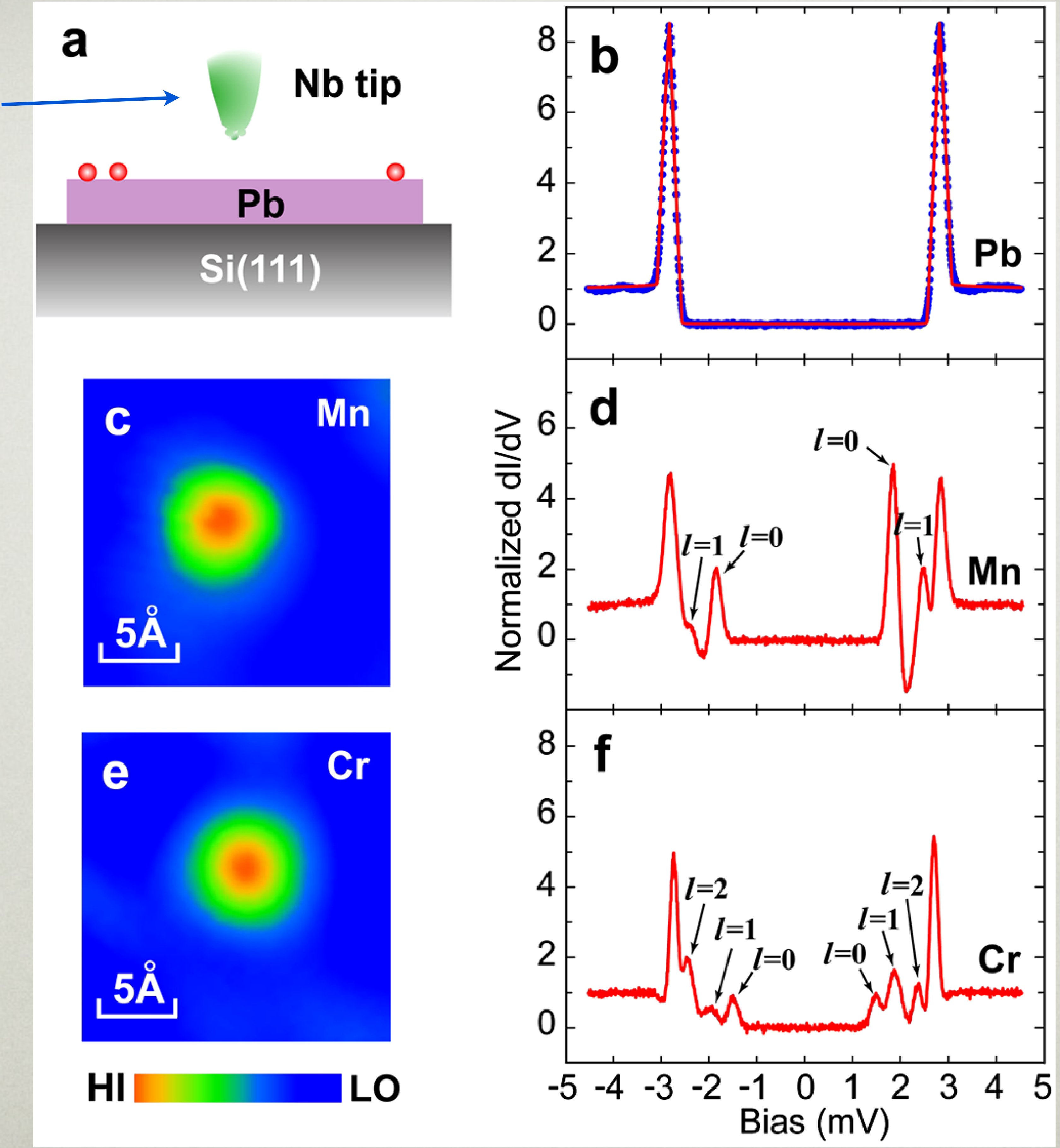


$T=3.8K$

T_c(Nb)~9.2K

A. Yazdani et al., Science 275, 1767 (1997)

TRICK:
superconducting
STM tip

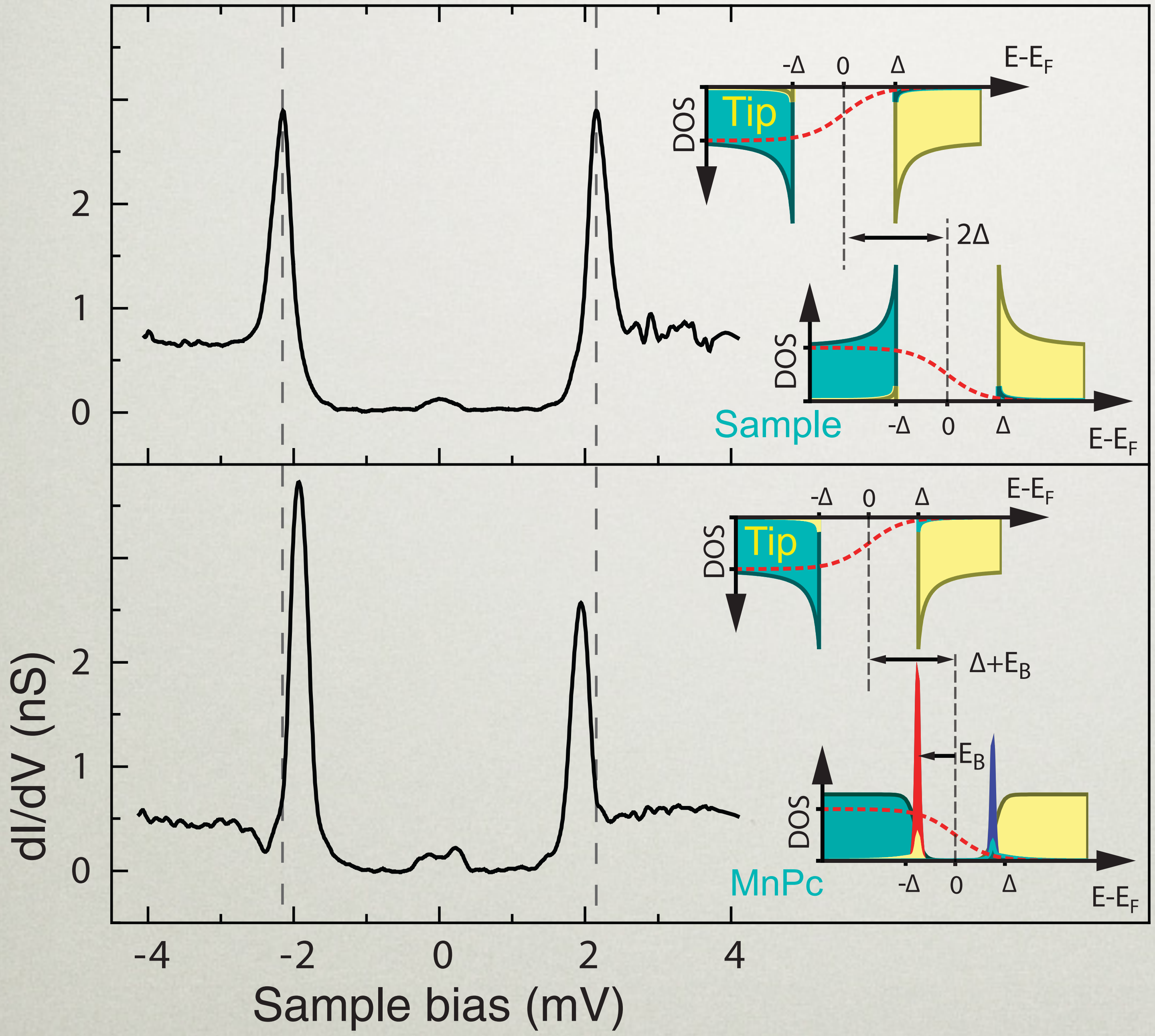


T=400mK

T_c(Pb)~7.2K

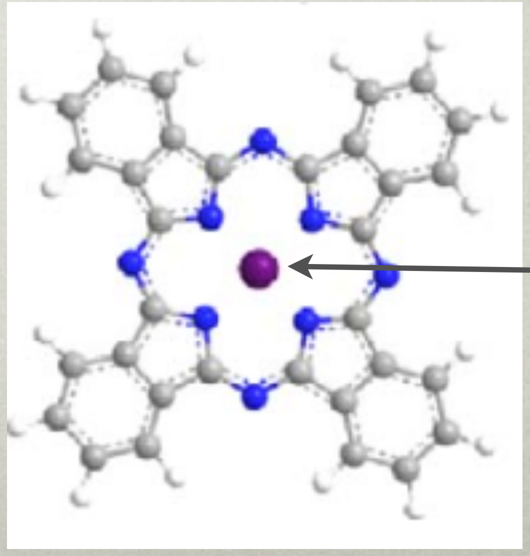
Shuai-Hua Ji et al., Phys. Rev. Lett. 100, 226801 (2008)

MAGNETIC MOLECULES ON SURFACES OF SUPERCONDUCTORS



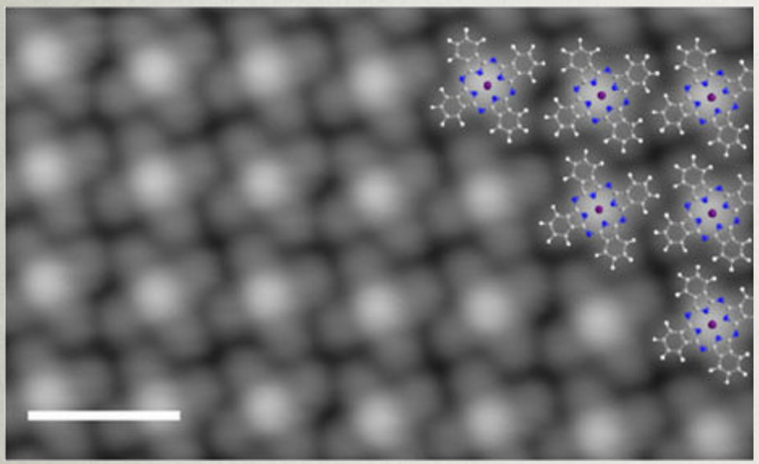
clean Pb(111)

MnPC/Pb(111)

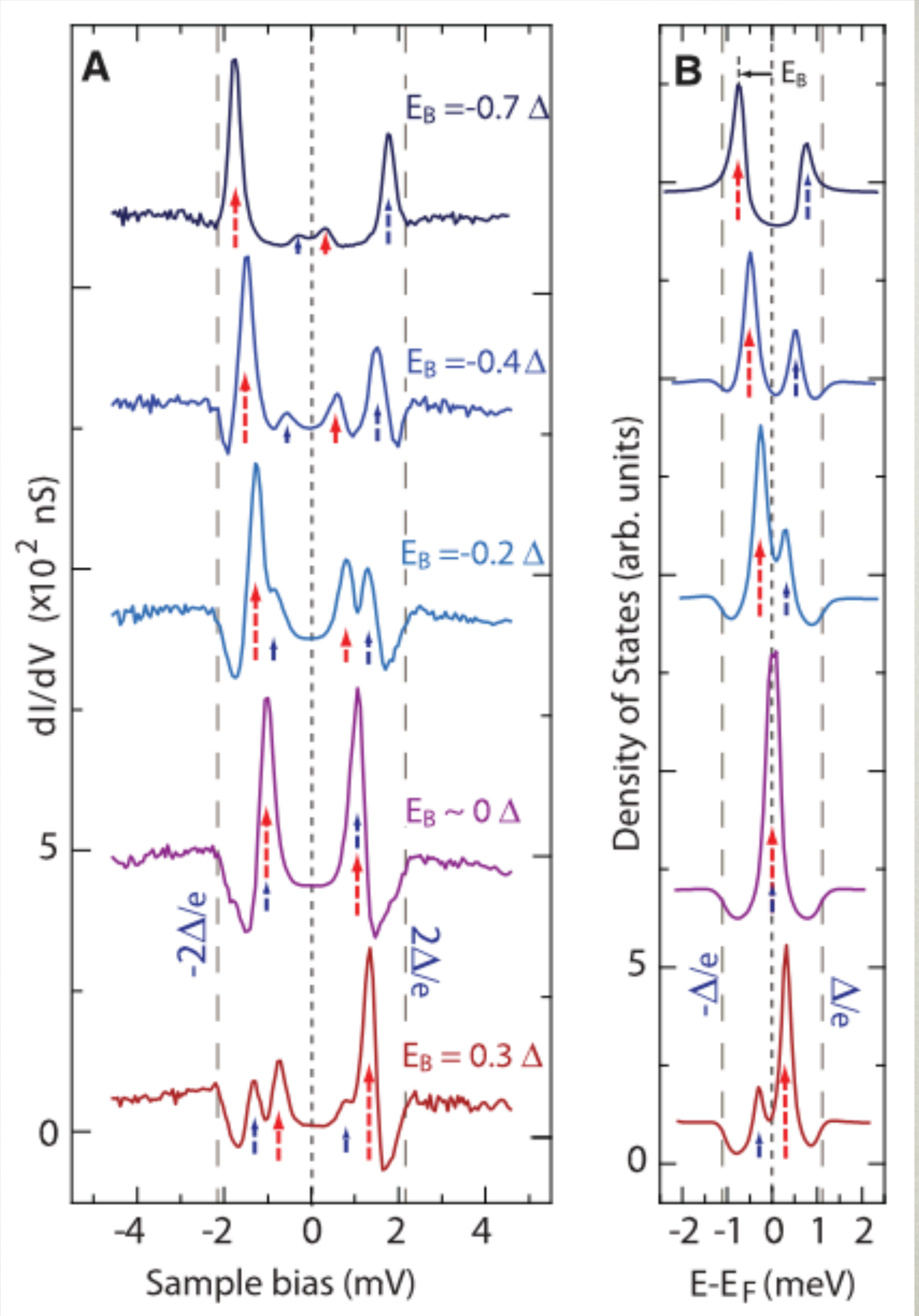


spin center

Franke, Schulze, Pascual, Science 332, 940 (2011)



Moiré-like structure:
molecules have different
binding strengths
to the substrate



Franke, Schulze, Pascual, Science 332, 940 (2011)

T=4.5K

QUANTUM IMPURITY

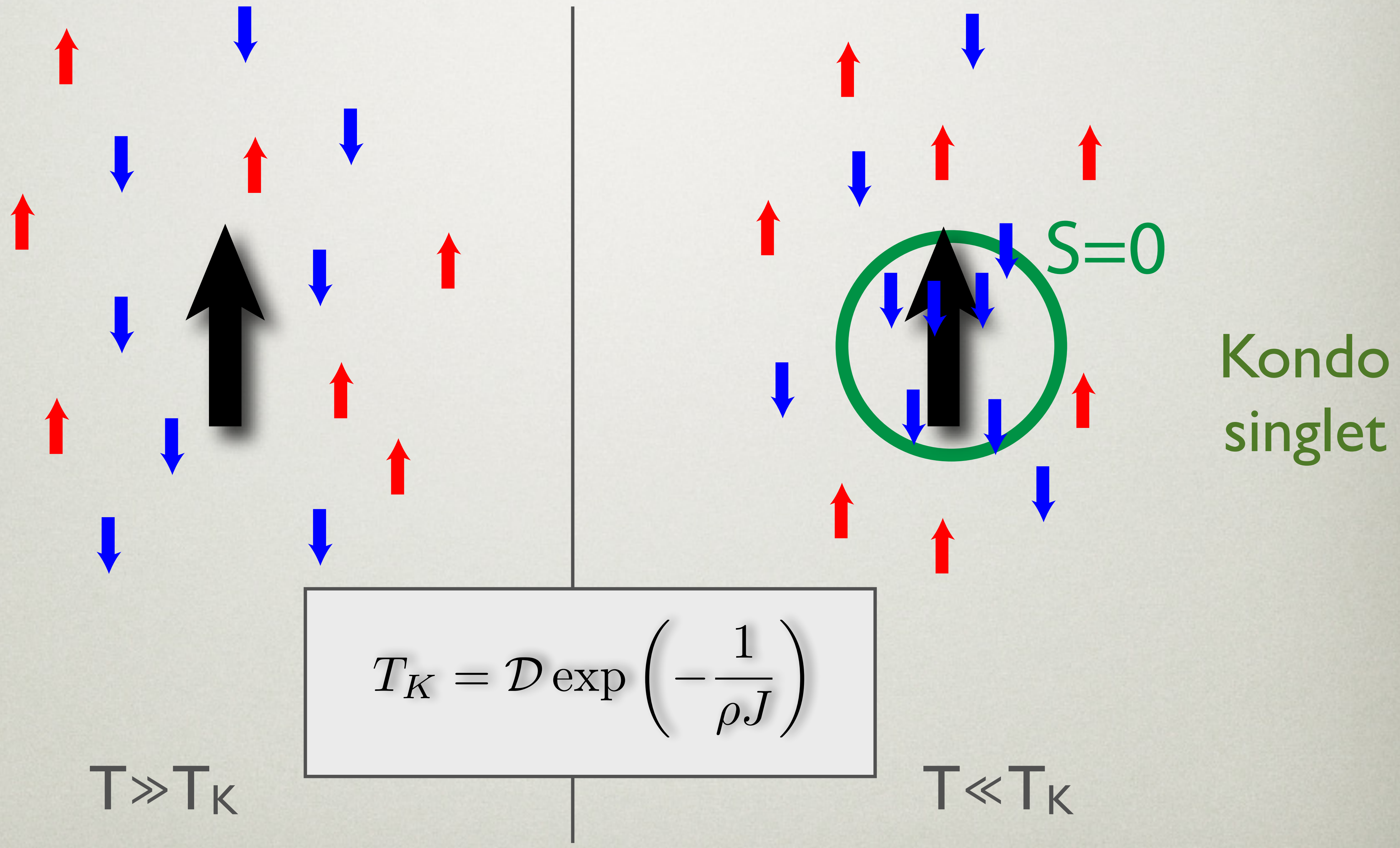
$$H_{\mathrm{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

$$H_{\mathrm{imp}} = J\mathbf{S} \cdot \mathbf{s}(\mathbf{r} = 0)$$

$$\mathbf{s} = \frac{1}{N} \sum_{kk'} c^\dagger_k \left(\frac{1}{2} \boldsymbol{\sigma} \right) c_{k'} = f^\dagger_0 \left(\frac{1}{2} \boldsymbol{\sigma} \right) f_0$$

Quantum impurities have internal dynamics: spin can flip!

QUANTUM IMPURITY IN A NORMAL METAL: THE KONDO EFFECT



$$T_K = \mathcal{D} \exp\left(-\frac{1}{\rho J}\right)$$

T≫T$_K$

free local moments

T≪T$_K$

screened local moments

Part II: methods

NRG FOR BCS MEAN-FIELD BATH

HYBRIDISATION FUNCTION FOR SUPERCONDUCTING BATHS

$$\Delta(z) = \frac{V^2}{z^2 - [(\epsilon - \mu)^2 + \Delta^2]} \begin{pmatrix} z + (\epsilon - \mu) & -\Delta \\ -\Delta & z - (\epsilon - \mu) \end{pmatrix}$$

Generalization of ODE discretization scheme to (Nambu) matrix case

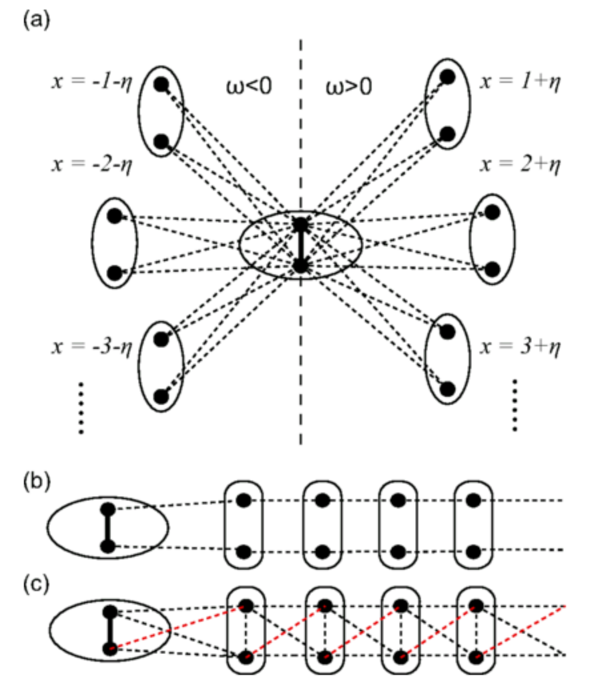
Normal state: $\Delta(z) = \sum_k |V_k|^2 g_k(z) \qquad g_k(z) = \frac{1}{z - \epsilon_k}$

SC state: $\mathbf{\Delta} = \sum_k |V_k|^2 \mathbf{g}_k(z) \qquad \mathbf{g}_k^{-1}(z) = z\mathbf{1} - \begin{pmatrix} \epsilon_k & -\Delta_k \\ -\Delta_k & -\epsilon_k \end{pmatrix}$

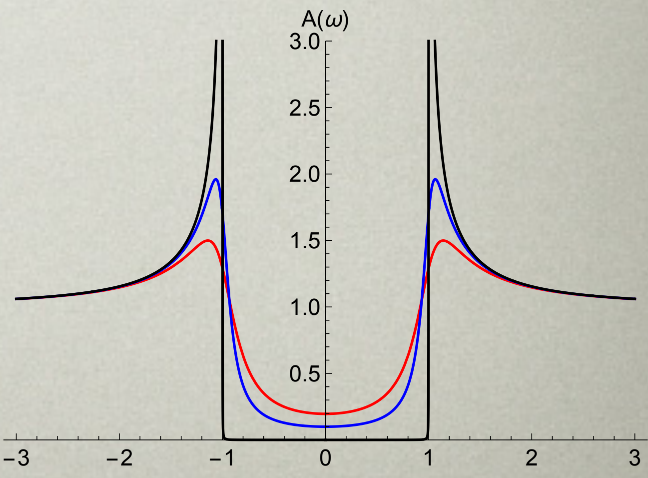
Additive quantity in presence of multiple (either N or SC) channels: $\mathbf{\Delta} = \sum_\alpha \mathbf{\Delta}_\alpha$

Quantum impurities in channel mixing baths
Jin-Guo Liu, Da Wang, Qiang-Hua Wang
Phys. Rev. B 93, 035102 (2016)

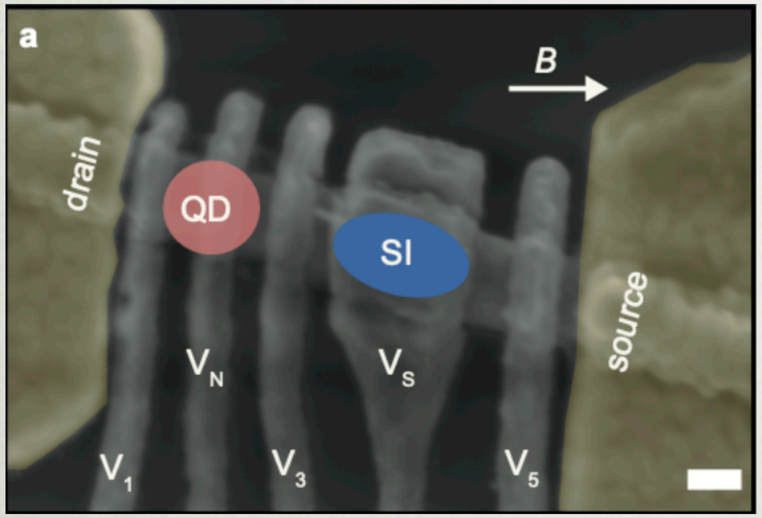
https://github.com/GiggleLiu/nrg_mapping

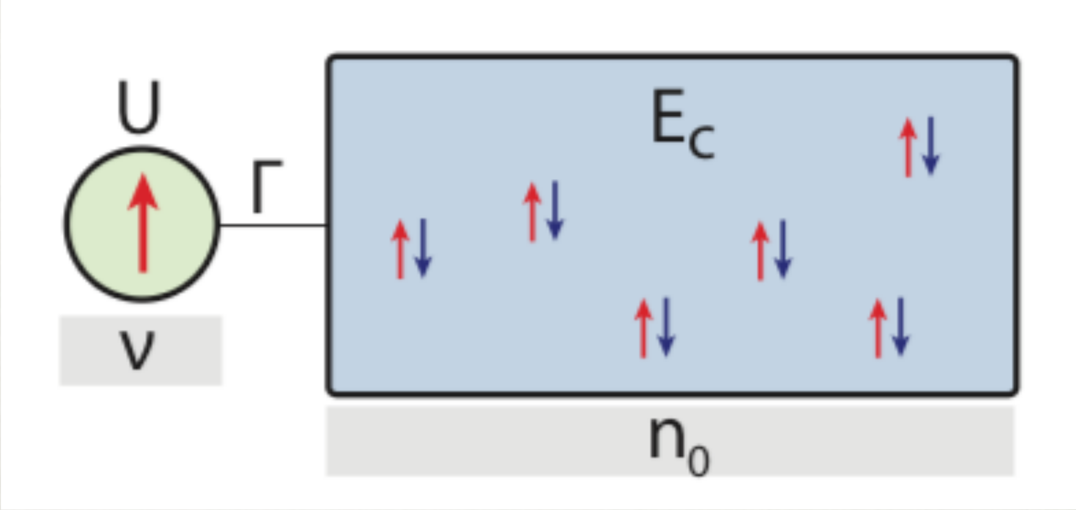


Soft gaps, too!



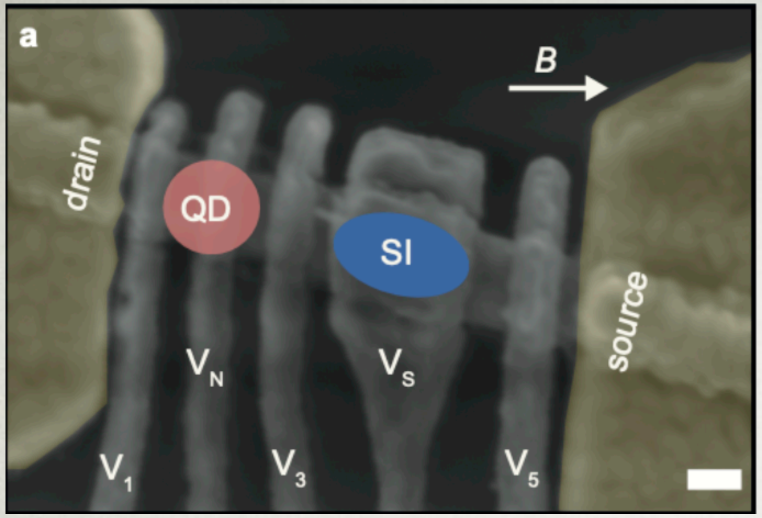
COULOMB INTERACTION AND CHARGING TERMS

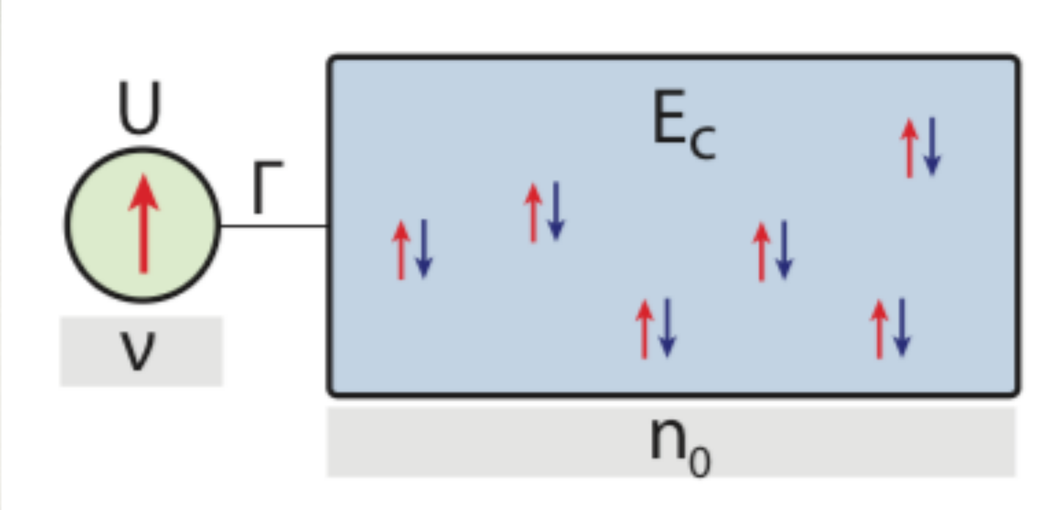




QD (Anderson impurity) + SI (Richardson model)

J. C. Estrada Saldaña et al., arxiv:2101.10794

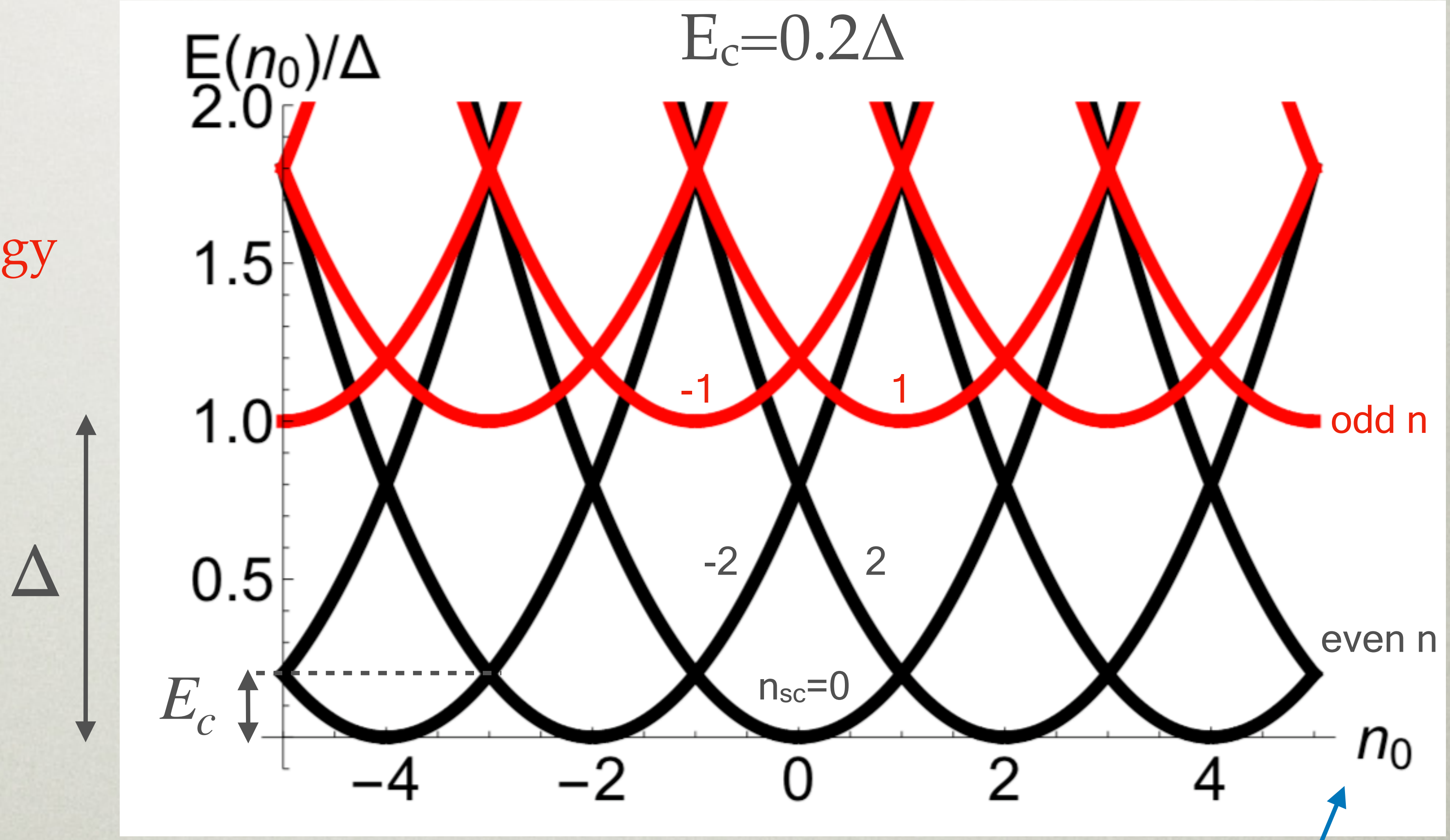




$$E_c(\hat{n}_{\rm sc} - n_0)^2$$

$$E_c = \frac{e_0^2}{2C}$$

charging energy



energy-level / gate-voltage expressed in units of electron number

QD

$$H_{\text{imp}} = \epsilon\hat{n} + U\hat{n}_\uparrow\hat{n}_\downarrow = \frac{U}{2}(\hat{n}-\nu)^2 + \text{const.}$$

$\hat{n} = \sum_\sigma \hat{n}_\sigma$ $\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$ $\sigma = \uparrow,\downarrow$

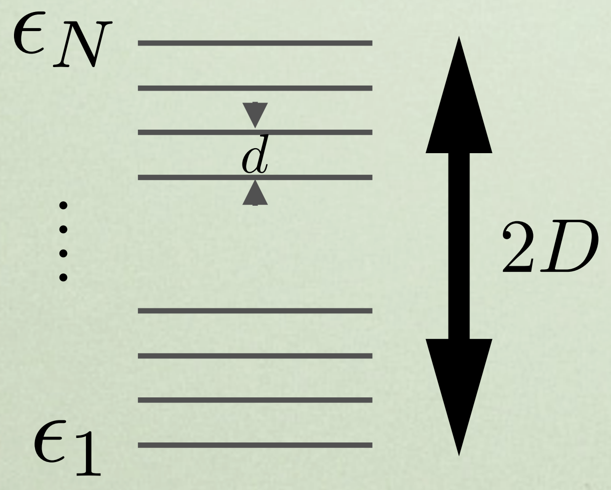
energy-level / gate-voltage expressed in units of electron number

$\nu = 1/2 - \epsilon/U = 1 - \delta/U$

SC

$$H_{\text{SC}} = \sum_{i,\sigma} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma} - \alpha d \sum_{i,j} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow} + E_c(\hat{n}_{\text{sc}} - n_0)^2$$

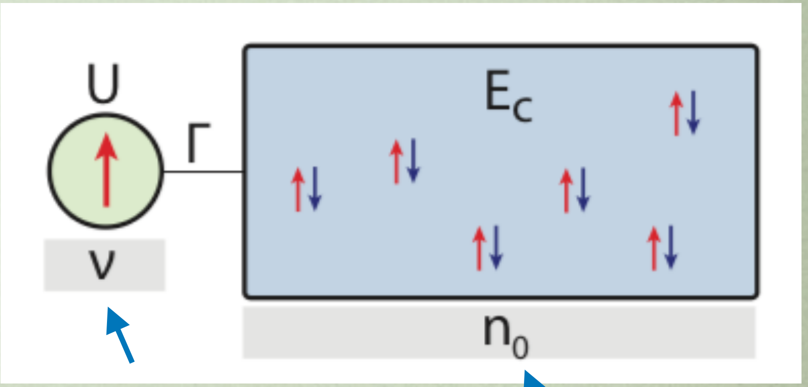
$i = 1, \dots, N$



$\hat{n}_{\text{sc}} = \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma}$

$$d = \frac{2D}{N}$$

$$\rho = \frac{1}{2D}$$



coupling

$$H_{\text{hyb}} = (v/\sqrt{N}) \sum_{i\sigma} \left(c^\dagger_{i\sigma} d_\sigma + \text{H.c.} \right)$$

$$\Gamma = \pi\rho v^2$$

matrix product operator (MPO) representation of H

$$W_0 = \begin{pmatrix} I & \epsilon_{\mathrm{imp}}\hat{n}_{\mathrm{imp}} + U\hat{n}_{\mathrm{imp},\uparrow}\hat{n}_{\mathrm{imp},\downarrow} & -d_\uparrow F & -d_\downarrow F & +d^\dagger_\uparrow F & +d^\dagger_\downarrow F & 0 & 0 & 0 \end{pmatrix}$$

$$W_i = \begin{pmatrix}
1 & [\epsilon_i + E_c(1-2n_0)]\hat{n}_i + (g+2E_c)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} & 0 & 0 & 0 & 0 & g c_{i\downarrow}c_{i\uparrow} & g c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} & 2E_c\hat{n}_i \\
0 & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & Vc^\dagger_{i\uparrow} & F & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & Vc^\dagger_{i\downarrow} & 0 & F & 0 & 0 & 0 & 0 & 0 \\
0 & Vc_{i\uparrow} & 0 & 0 & F & 0 & 0 & 0 & 0 \\
0 & Vc_{i\downarrow} & 0 & 0 & 0 & F & 0 & 0 & 0 \\
0 & c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} & 0 & 0 & 0 & 0 & I & 0 & 0 \\
0 & c_{i\downarrow}c_{i\uparrow} & 0 & 0 & 0 & 0 & 0 & I & 0 \\
0 & \hat{n}_i & 0 & 0 & 0 & 0 & 0 & 0 & I
\end{pmatrix}$$

$$W_N = \begin{pmatrix}
[\epsilon_N + E_c(1-2n_0)]\hat{n}_N + (g+2E_c)\hat{n}_{N\uparrow}\hat{n}_{N\downarrow} \\
I \\
Vc^\dagger_{N\uparrow} \\
Vc^\dagger_{N\downarrow} \\
Vc_{N\uparrow} \\
Vc_{N\downarrow} \\
c^\dagger_{N\uparrow}c^\dagger_{N\downarrow} \\
c_{N\downarrow}c_{N\uparrow} \\
\hat{n}_N
\end{pmatrix}$$

F is fermion-parity operator

$$g = \alpha d$$

$$H = \prod_{i=0}^{N} W_i$$

$$\mathrm{dim} = 9$$

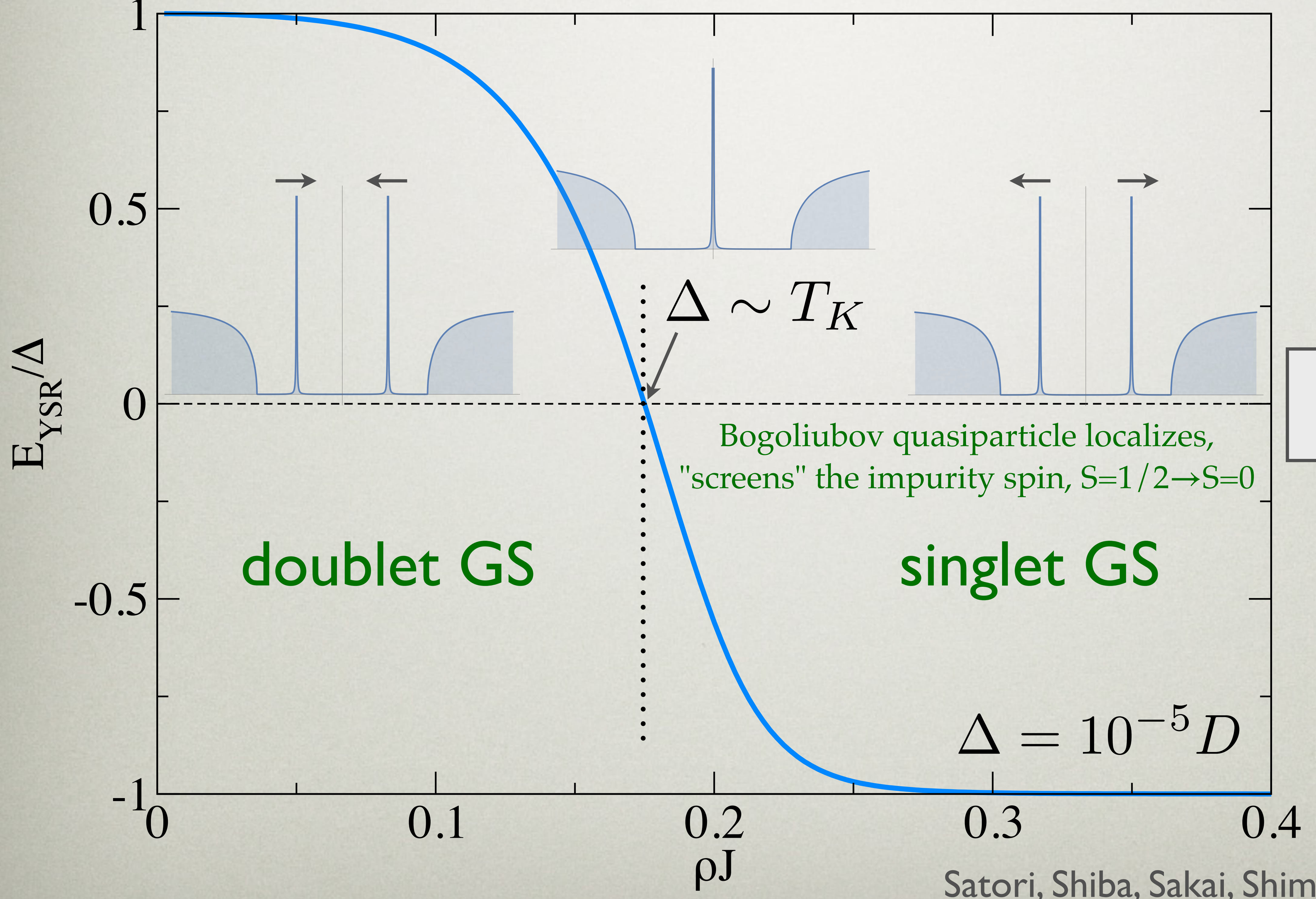
Pavešić, Bauernfeind, Žitko, arxiv:2101.10168

Part III: basic properties

S=1/2

QUANTUM IMPURITY IN A SUPERCONDUCTOR:

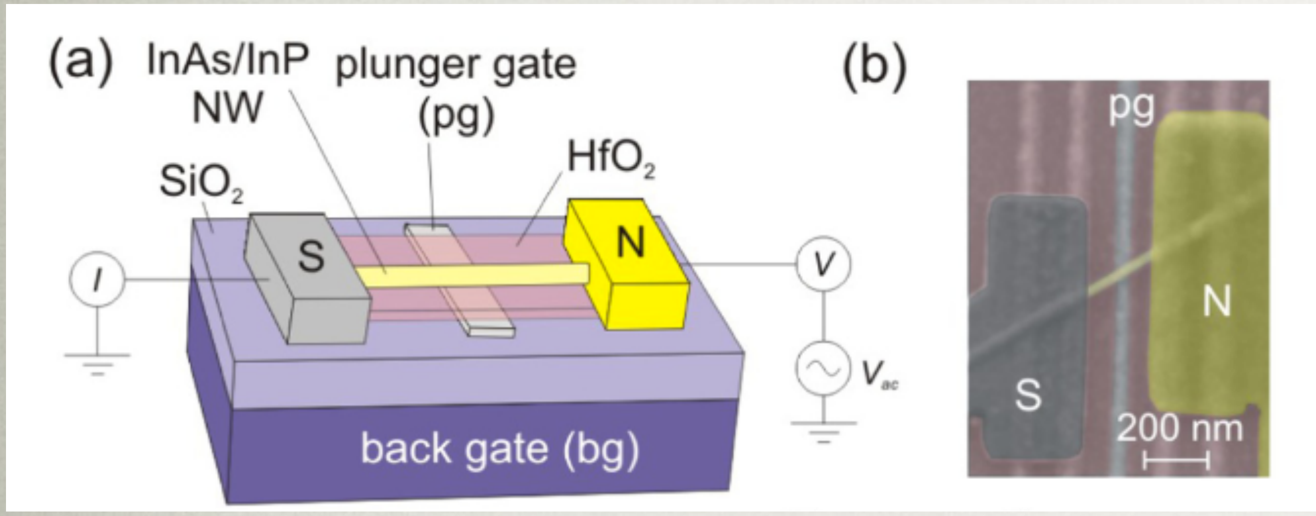
DOUBLET-SINGLET TRANSITION

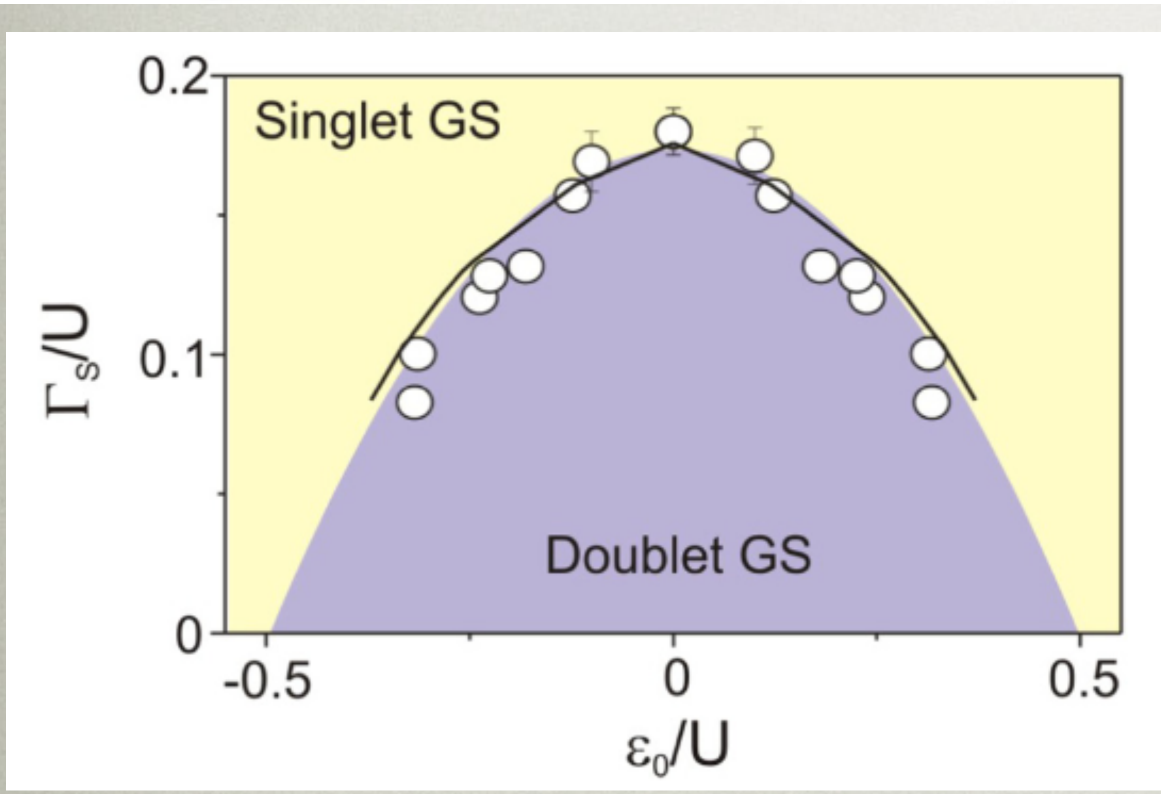


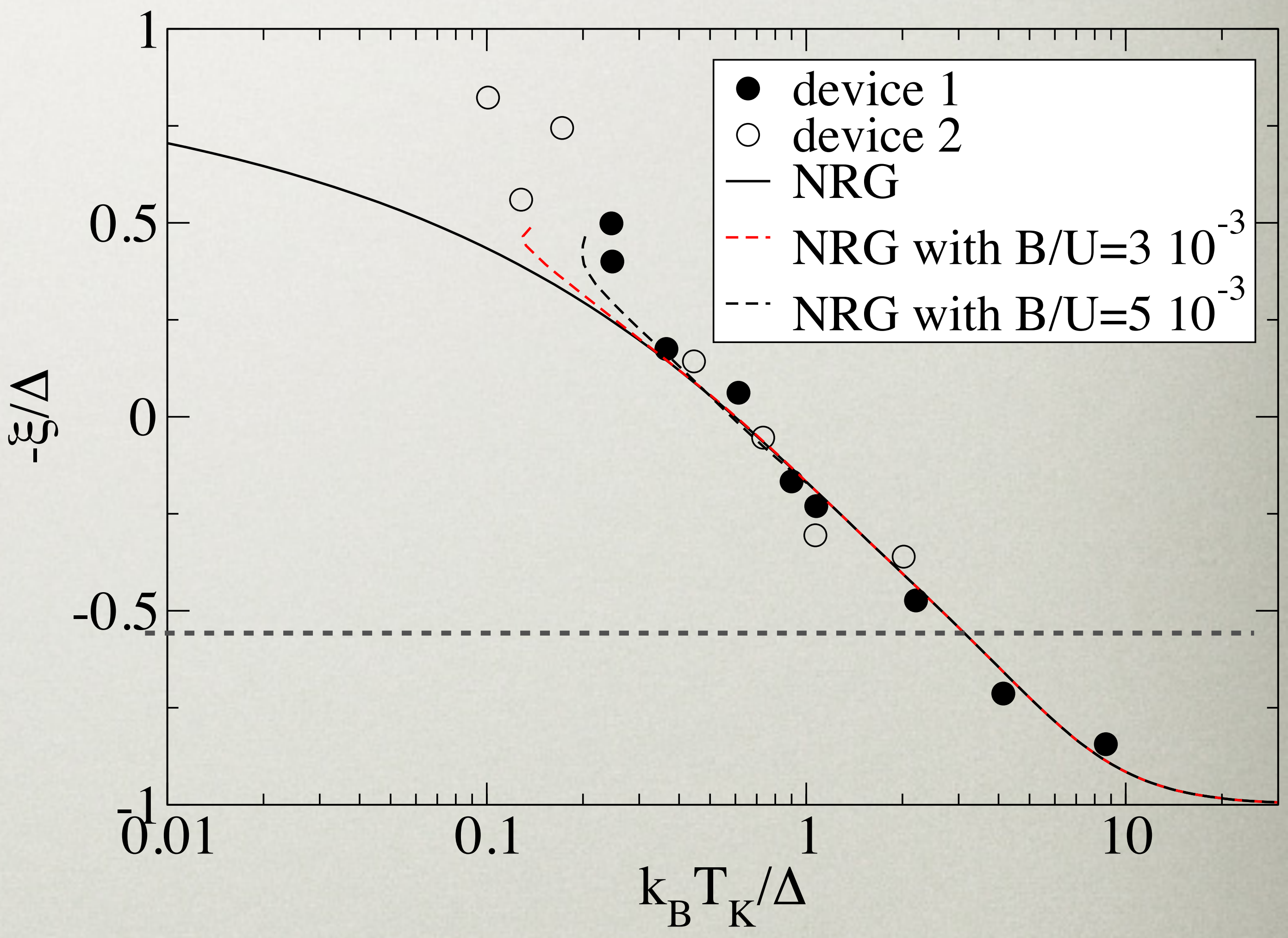
$$T_K = \mathcal{D} \exp\left(-\frac{1}{\rho J}\right)$$

Satori, Shiba, Sakai, Shimizu JPSJ (1992);
Yoshioka, Ohashi JPSJ (1998, 2000)

SCALING OF SUB-GAP EXCITATIONS



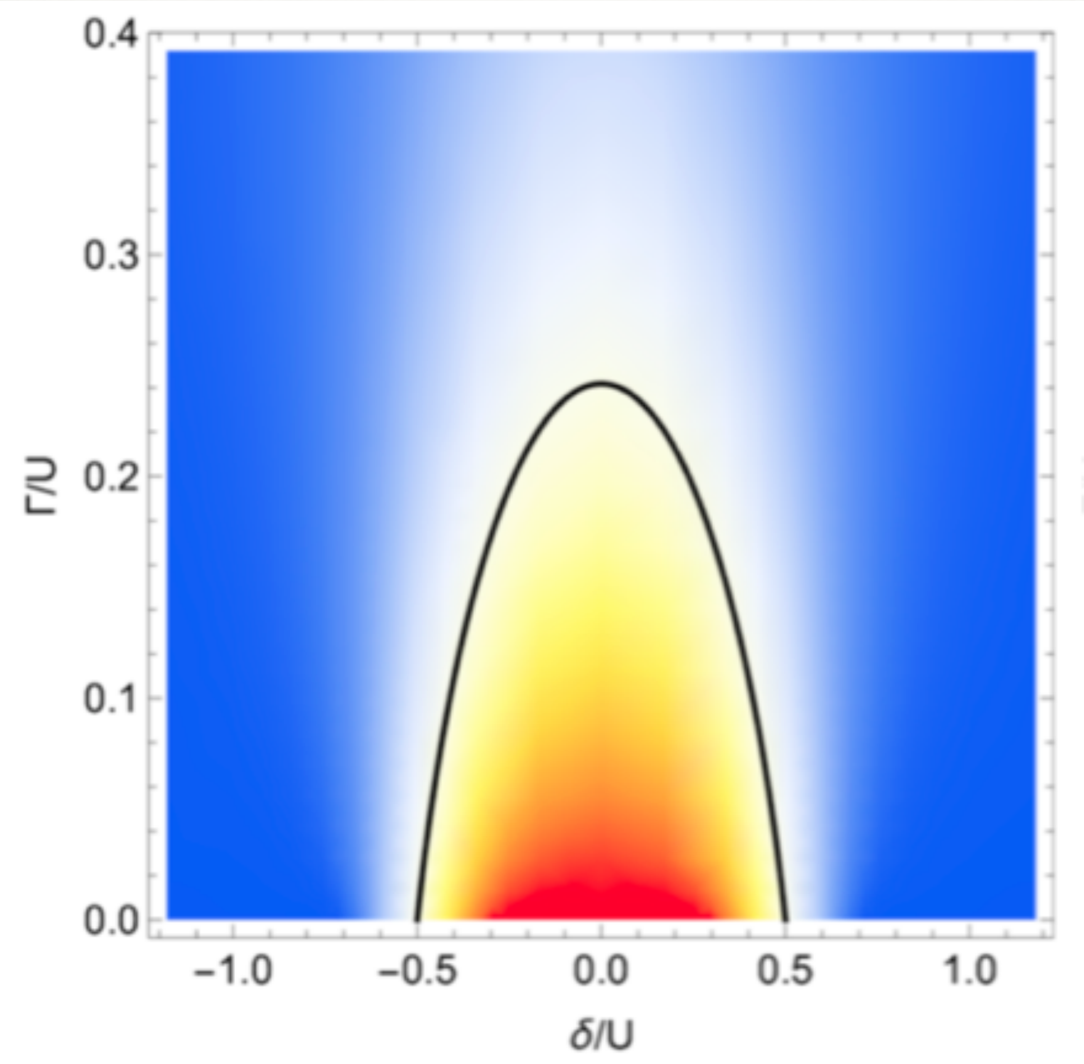




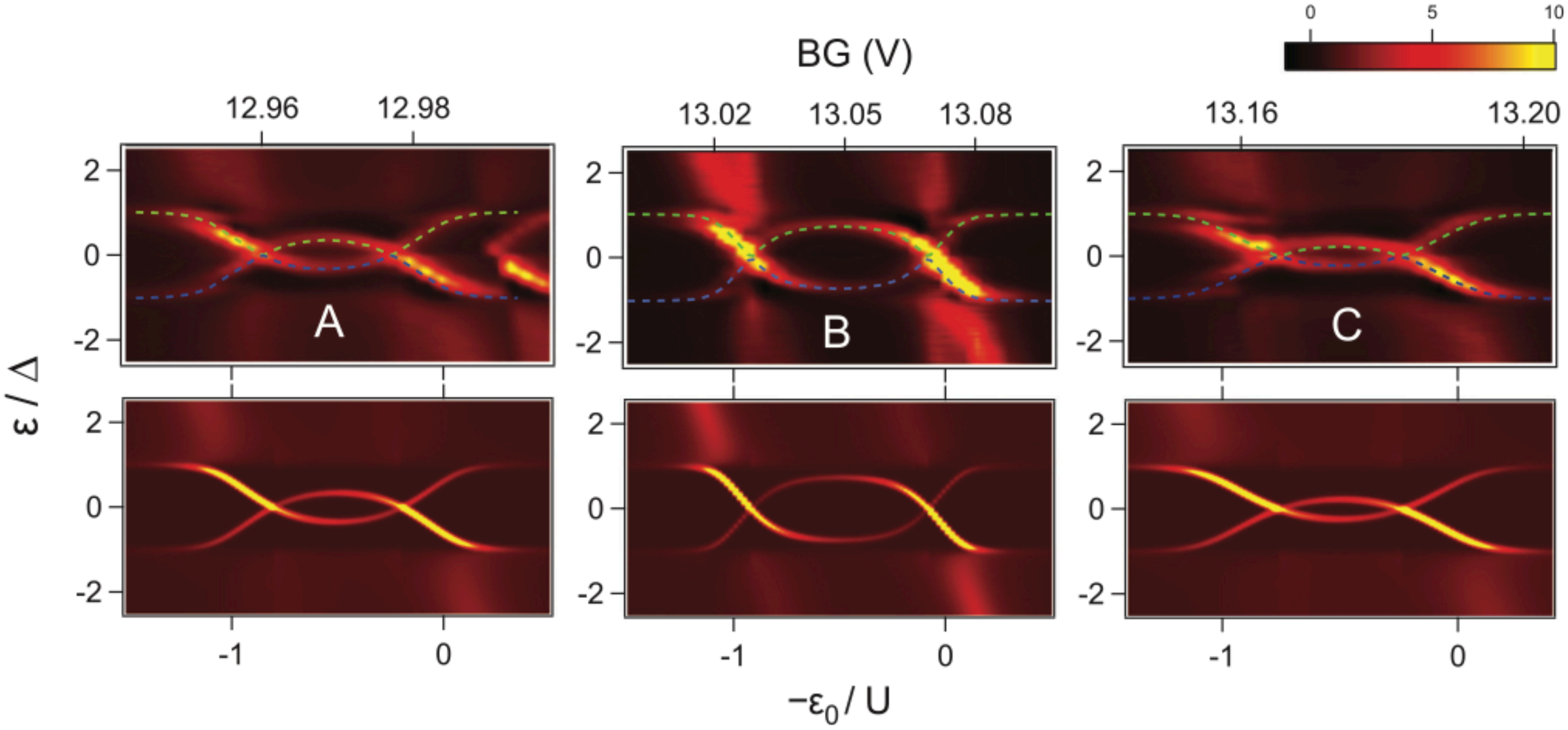
Lee, Jiang, Žitko, Aguado, Lieber, de Francesci, PRB (2017)

see also Luitz, Assaad, Novotný, Karrasch, Meden, PRL 108, 227001 (2012)

GATE DEPENDENCE



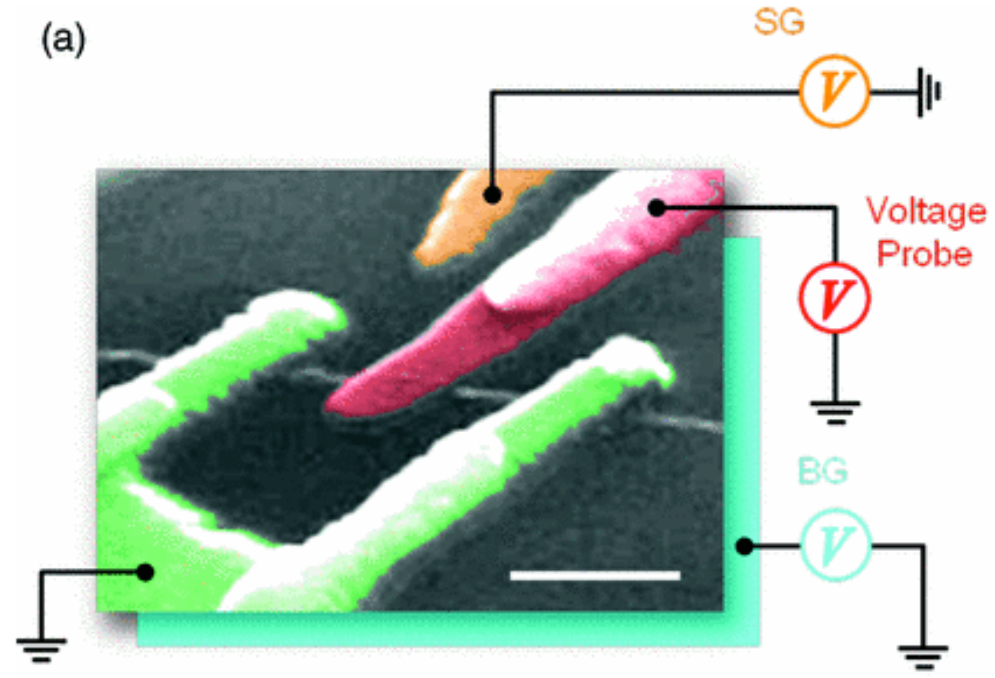
CARBON NANOTUBE QUANTUM DOT

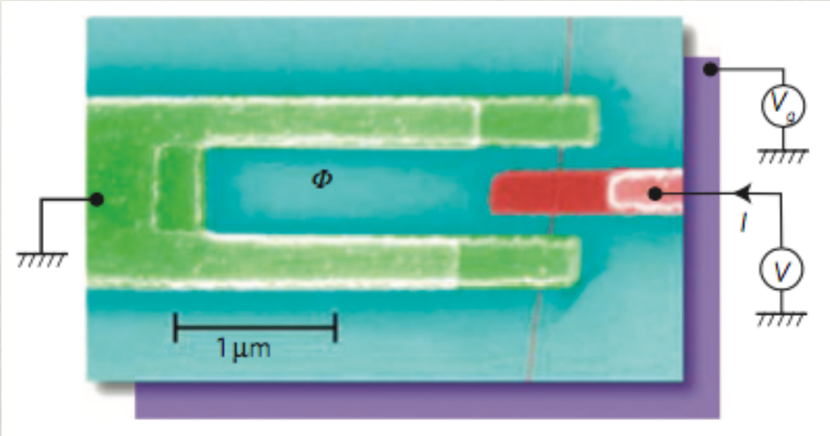


experiment

theory

(NRG calculation)





JD Pillet, P Joyez, R Žitko, MF Goffman, PRB 88, 045101 (2013)

ANDREEV BOUND STATES, U=0 LIMIT

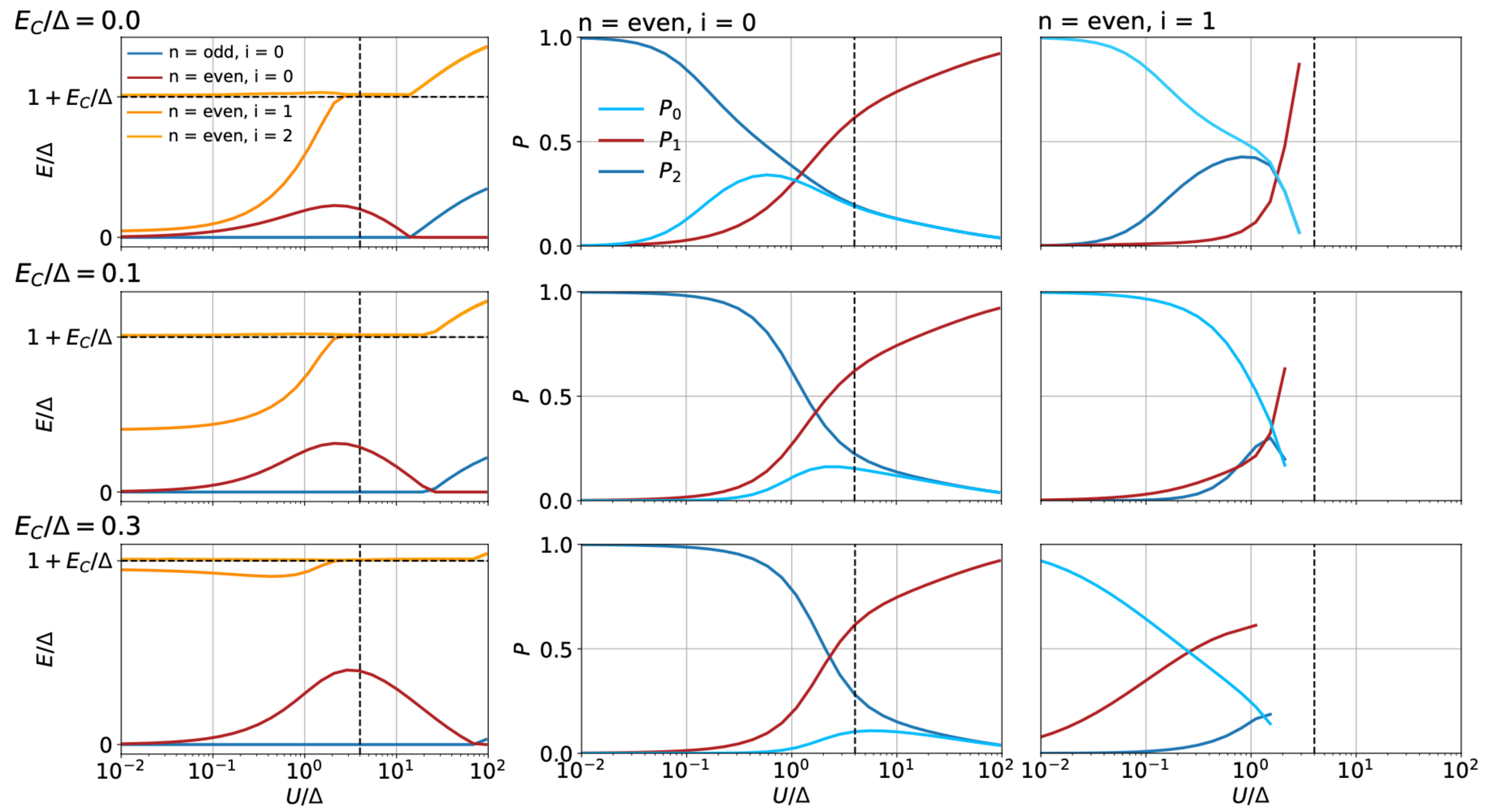
$$H = \sum_{\sigma} \epsilon d_{\sigma}^{\dagger} d_{\sigma} + \Gamma d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} + \text{H.c.}$$

large Δ limit

$$\epsilon = 0$$

$$\psi = \frac{1}{\sqrt{2}} \left(|0\rangle \pm |2\rangle \right)$$

YSR VS ABS: ROLE OF U/Δ

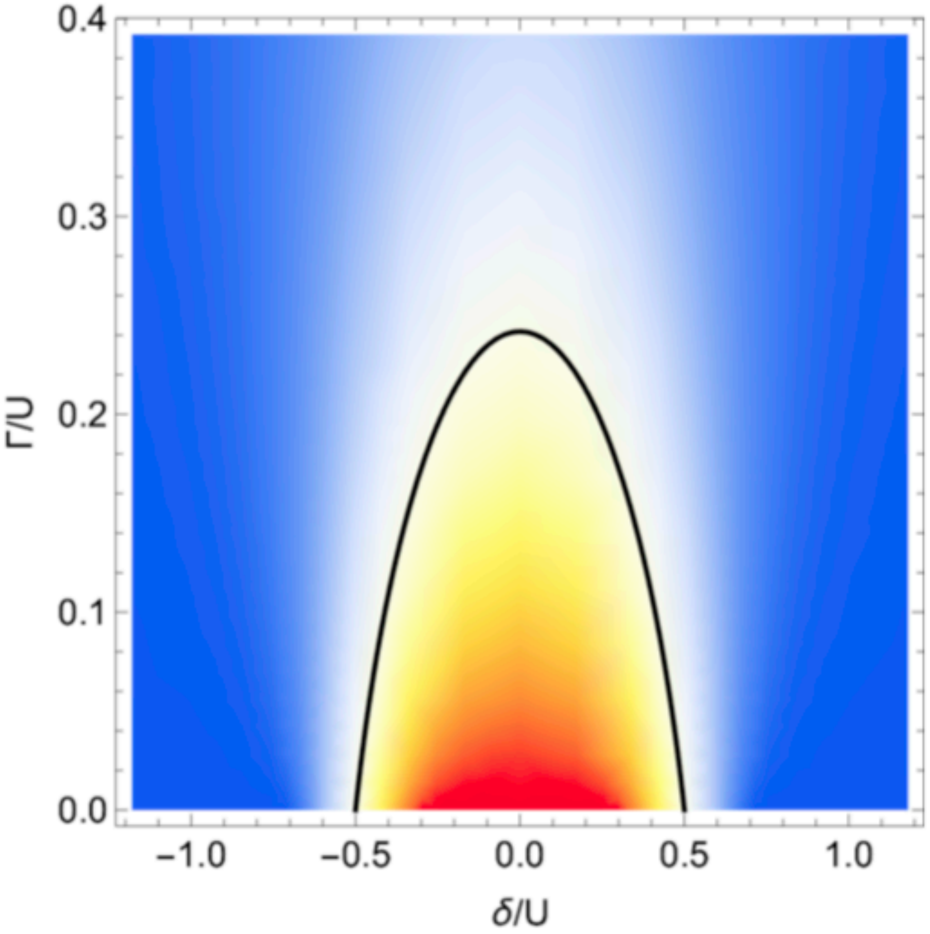


IMPURITY IN A JOSEPHSON'S JUNCTION

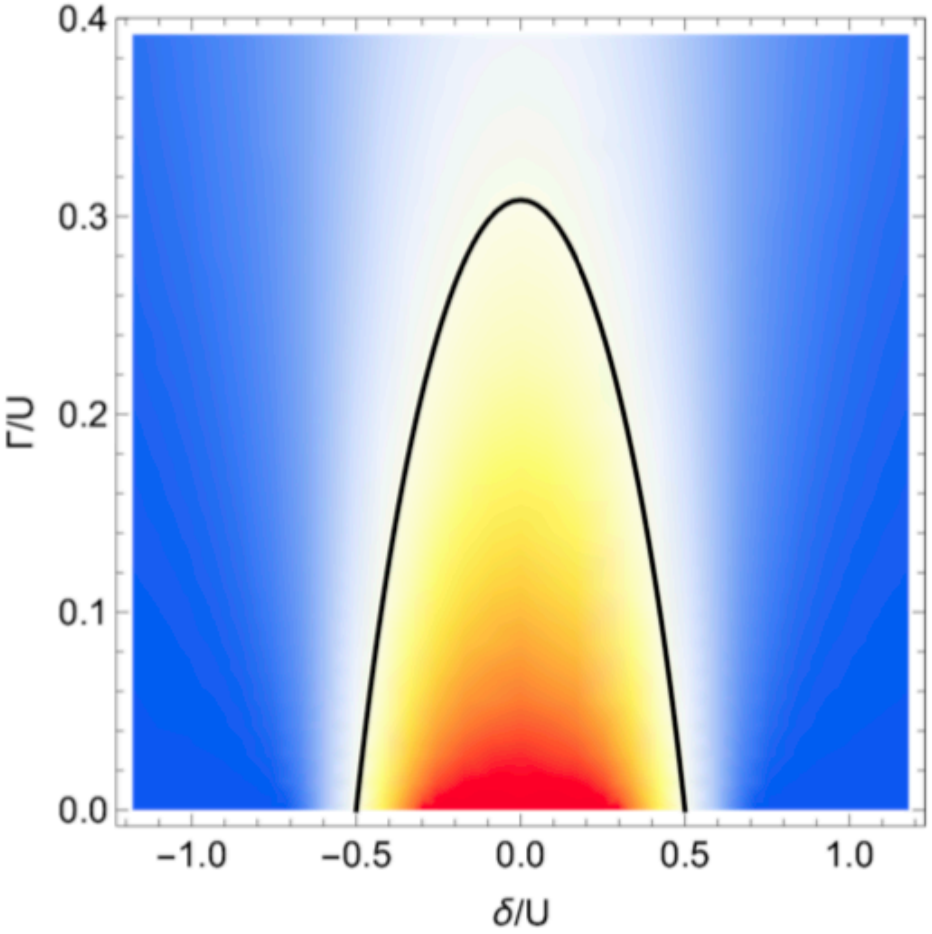
$$H = \epsilon n + U n_\uparrow n_\downarrow + \sum_{k,i} \epsilon_k n_{k,i} + \sum_{k,i} \left(\Delta_i c^\dagger_{ki\uparrow} c^\dagger_{ki\downarrow} + \text{H.c.} \right) + \sum_{k,i,\sigma} \left(V_i c^\dagger_{ki\sigma} d_\sigma + \text{H.c.} \right)$$

$$\Delta_1 = \Delta e^{i\phi/2} \text{ and } \Delta_2 = \Delta e^{-i\phi/2}$$

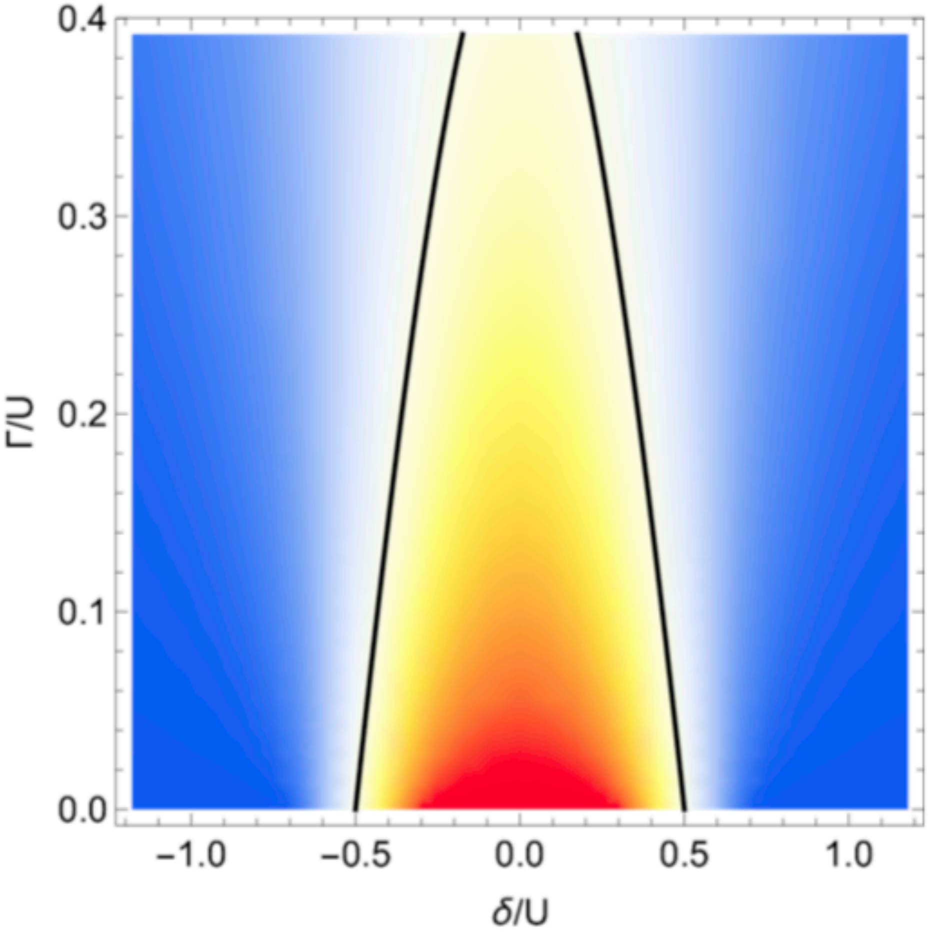
SINGLET-DOUBLET PHASE DIAGRAMS



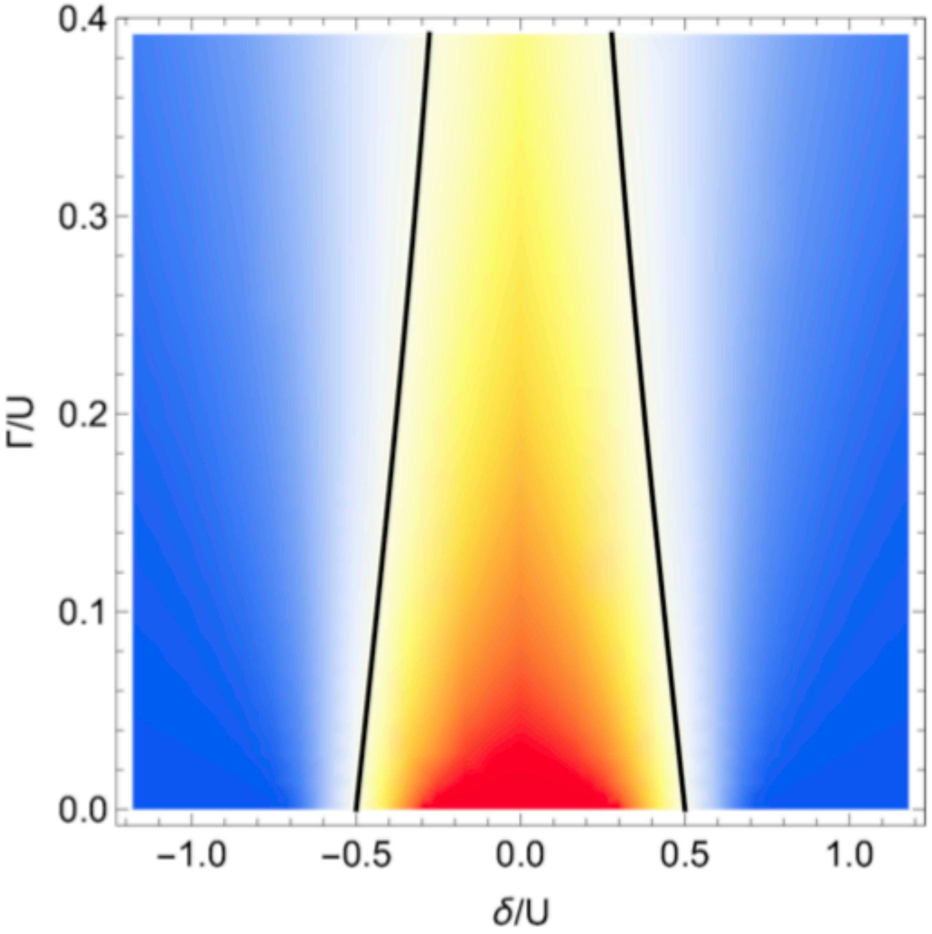
(a) $\phi = 0$



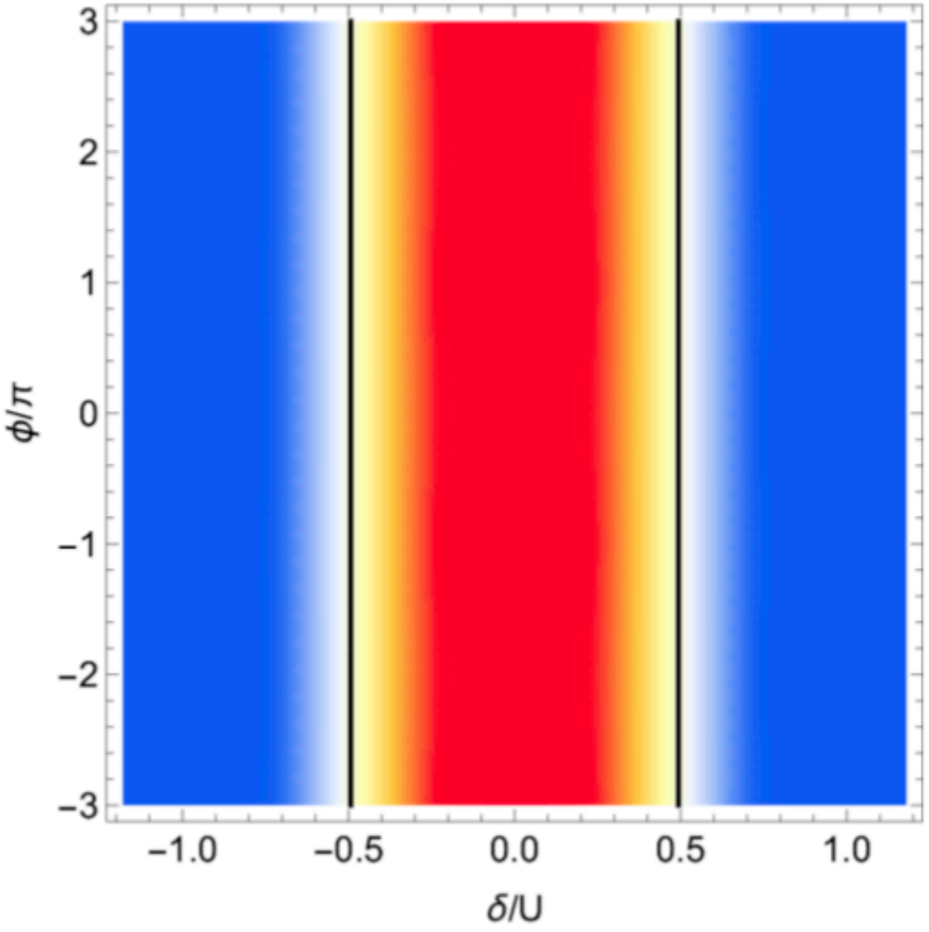
(b) $\phi = \pi/2$



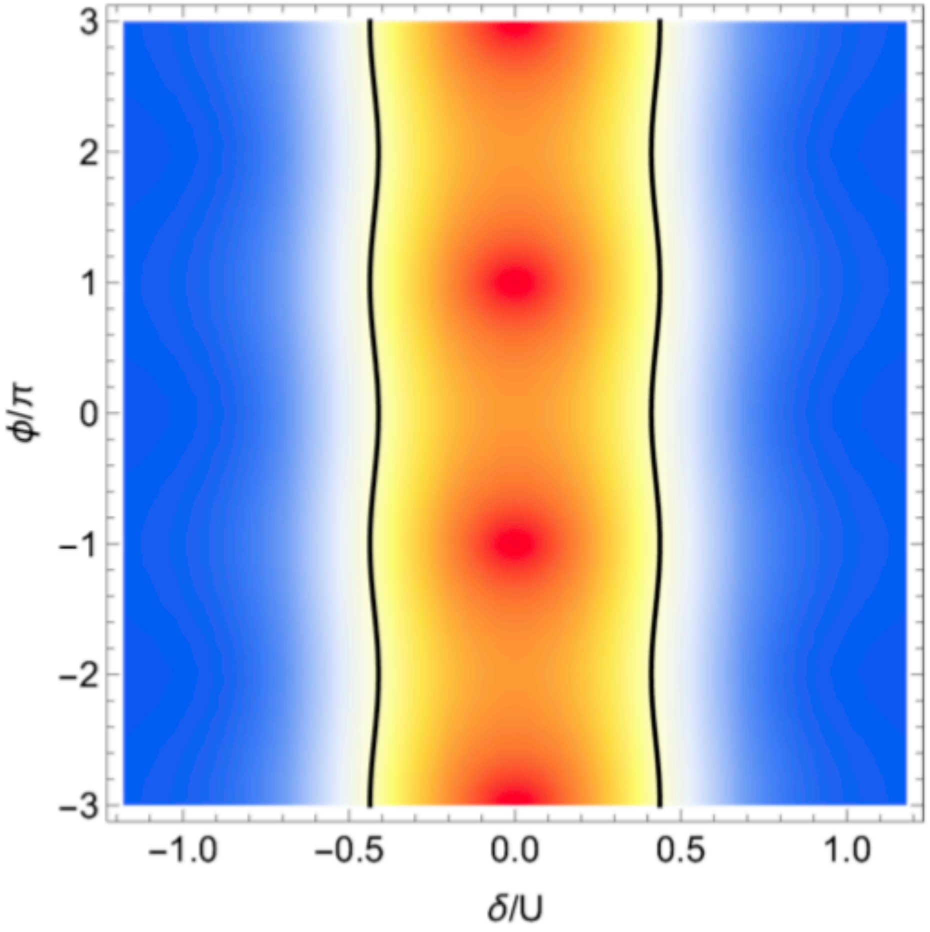
(c) $\phi = 3\pi/4$



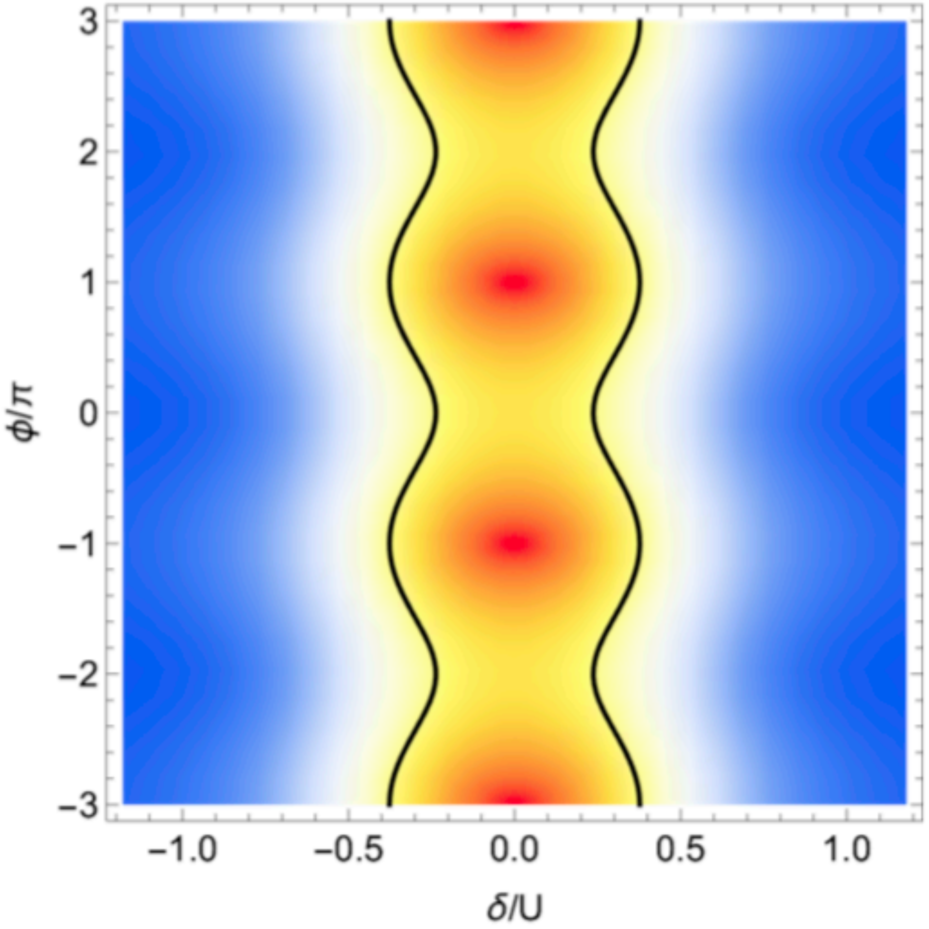
(d) $\phi = \pi$



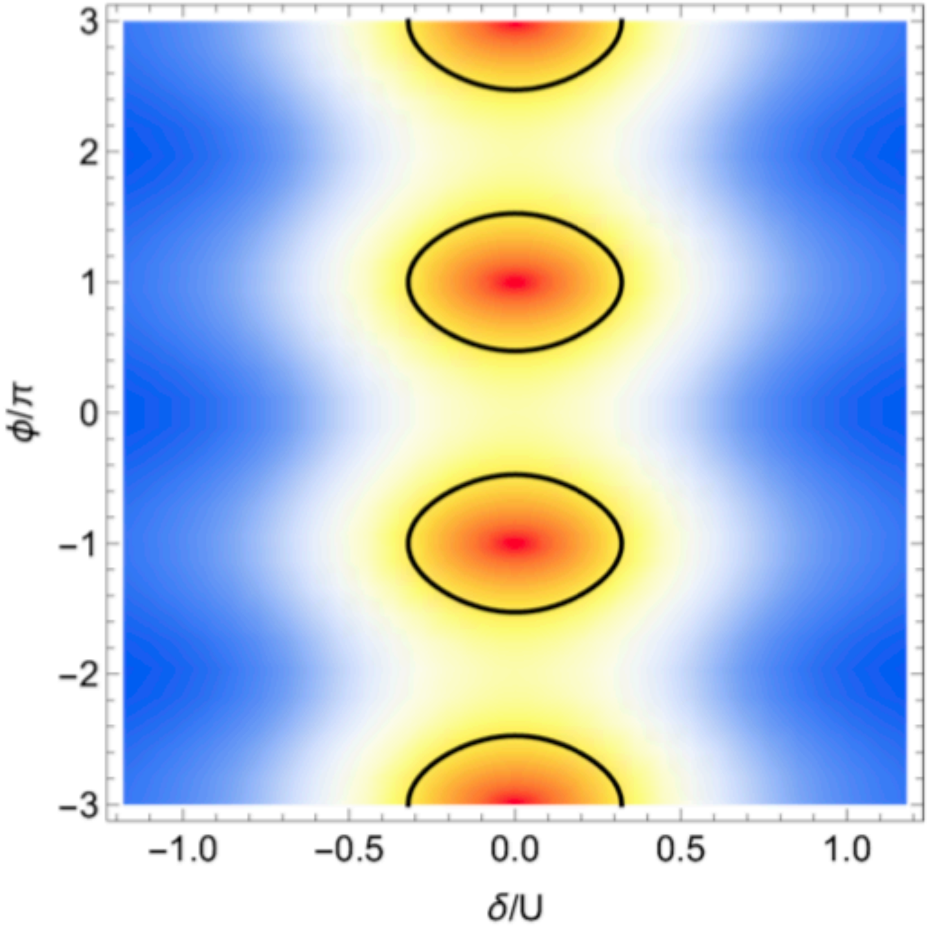
(a) $\Gamma/U = 0.01$



(b) $\Gamma/U = 0.1$

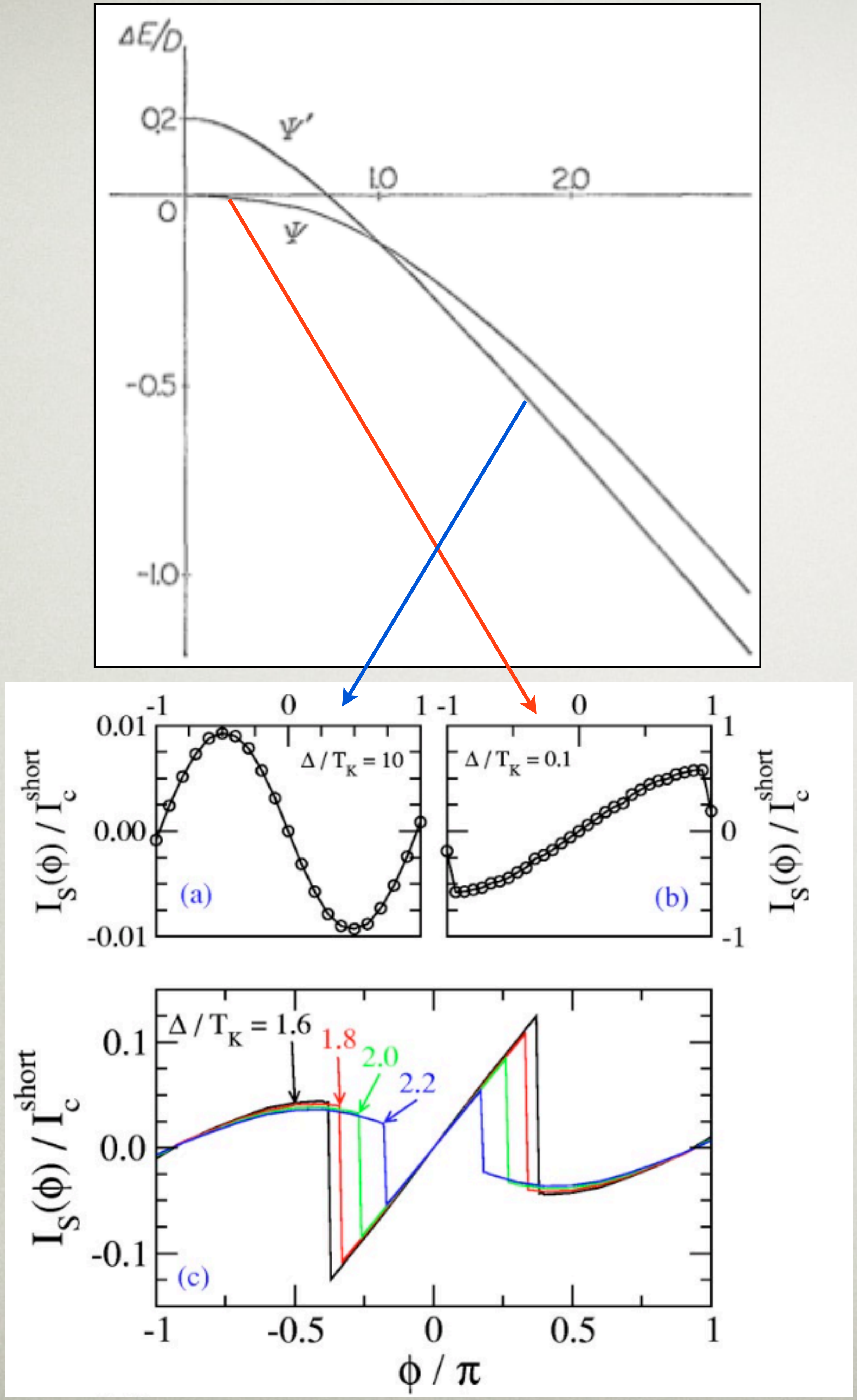


(c) $\Gamma/U = 0.2$



(d) $\Gamma/U = 0.3$

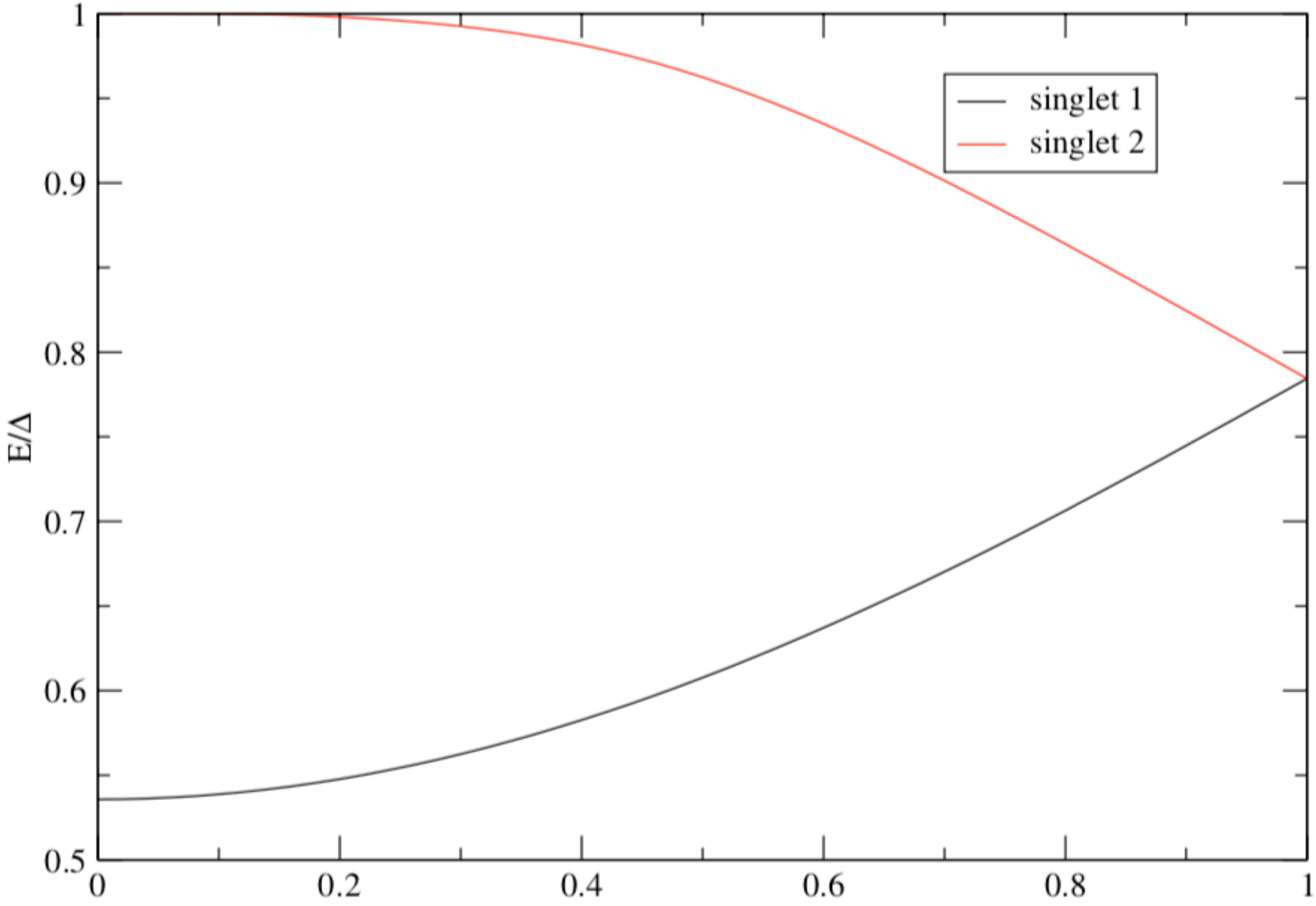
JOSEPHSON CURRENT



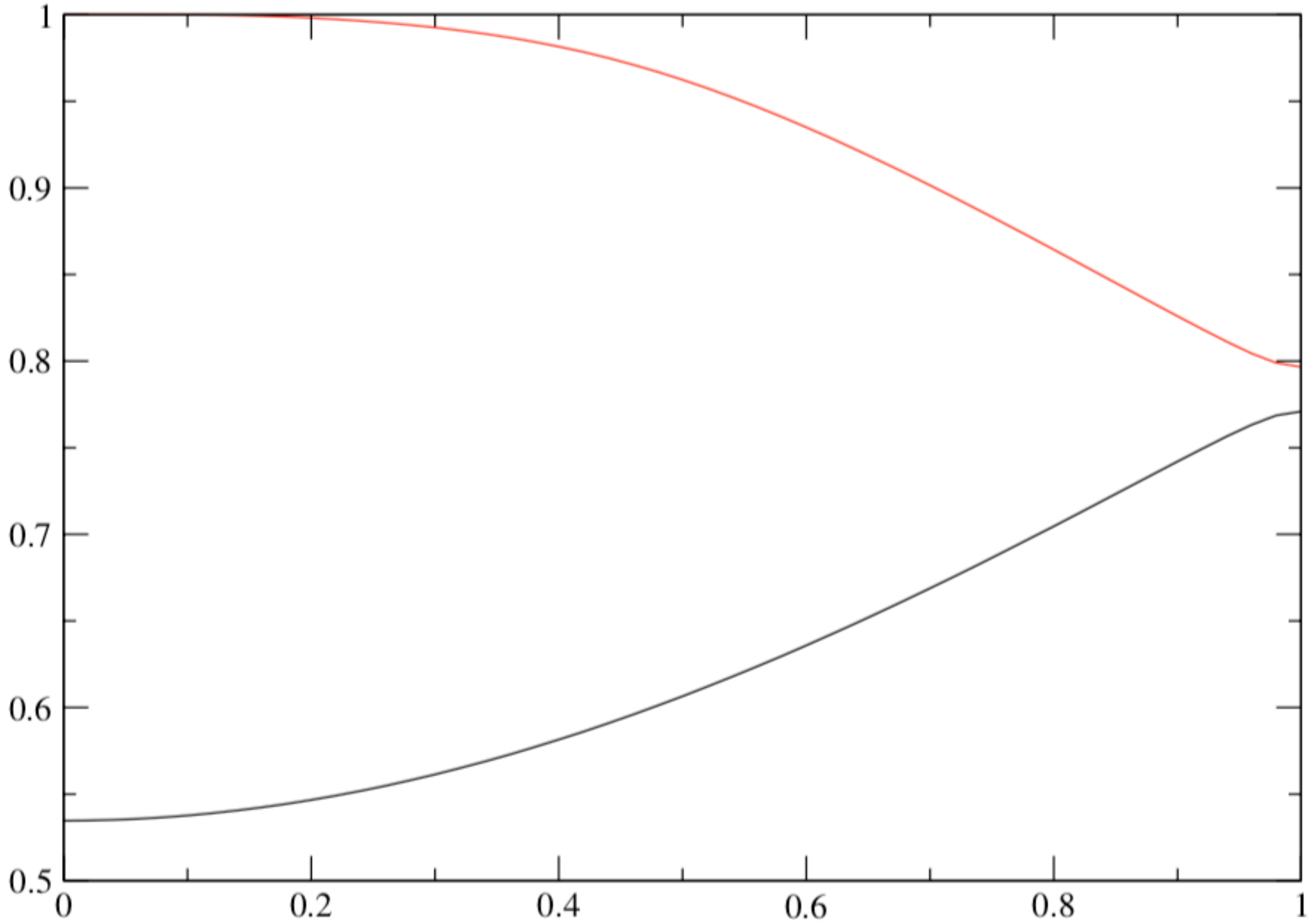
$$j = \frac{\partial E}{\partial \phi}$$

Choi et al. PRB 70, 020502 (2004)

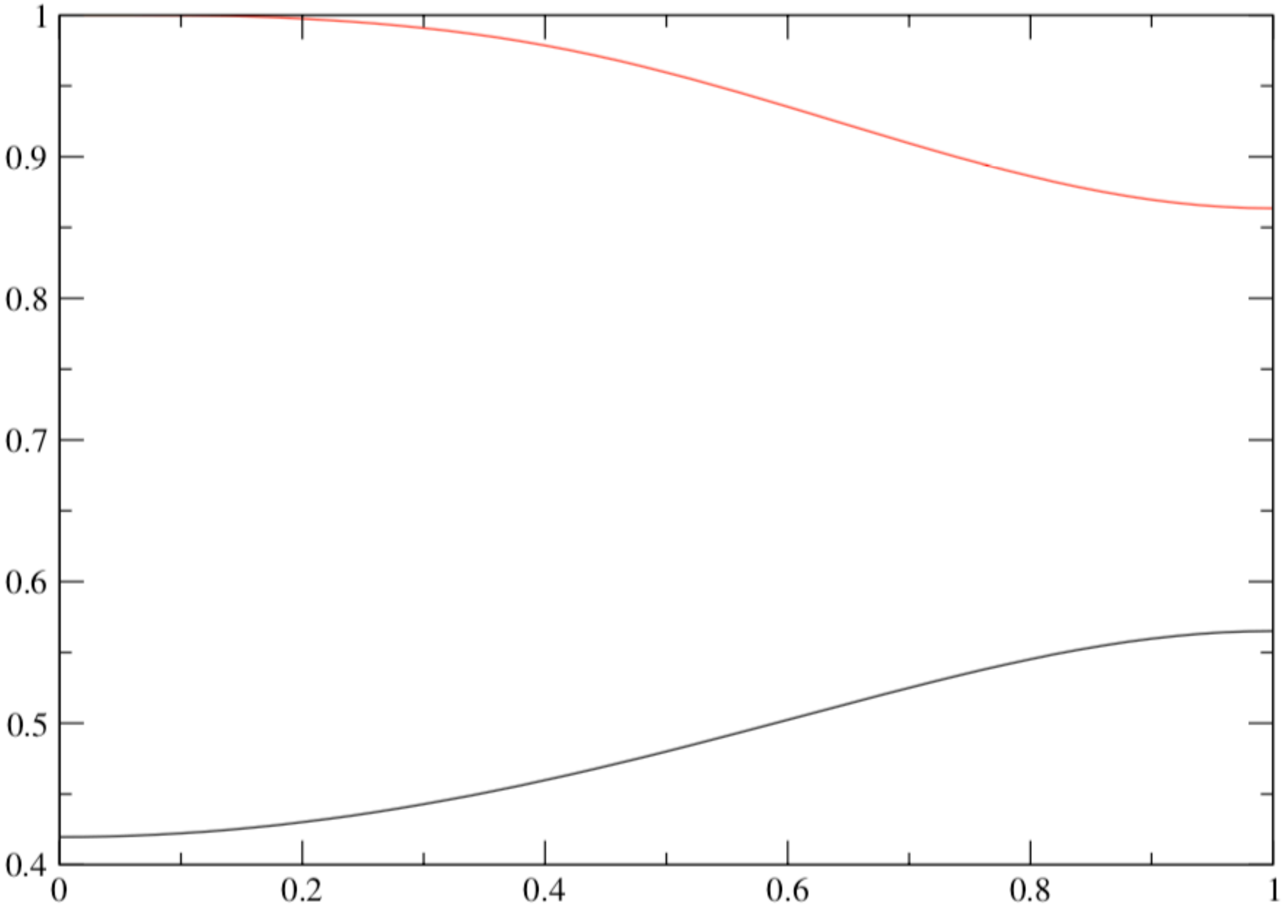
PHASE BIAS DEPENDENCE



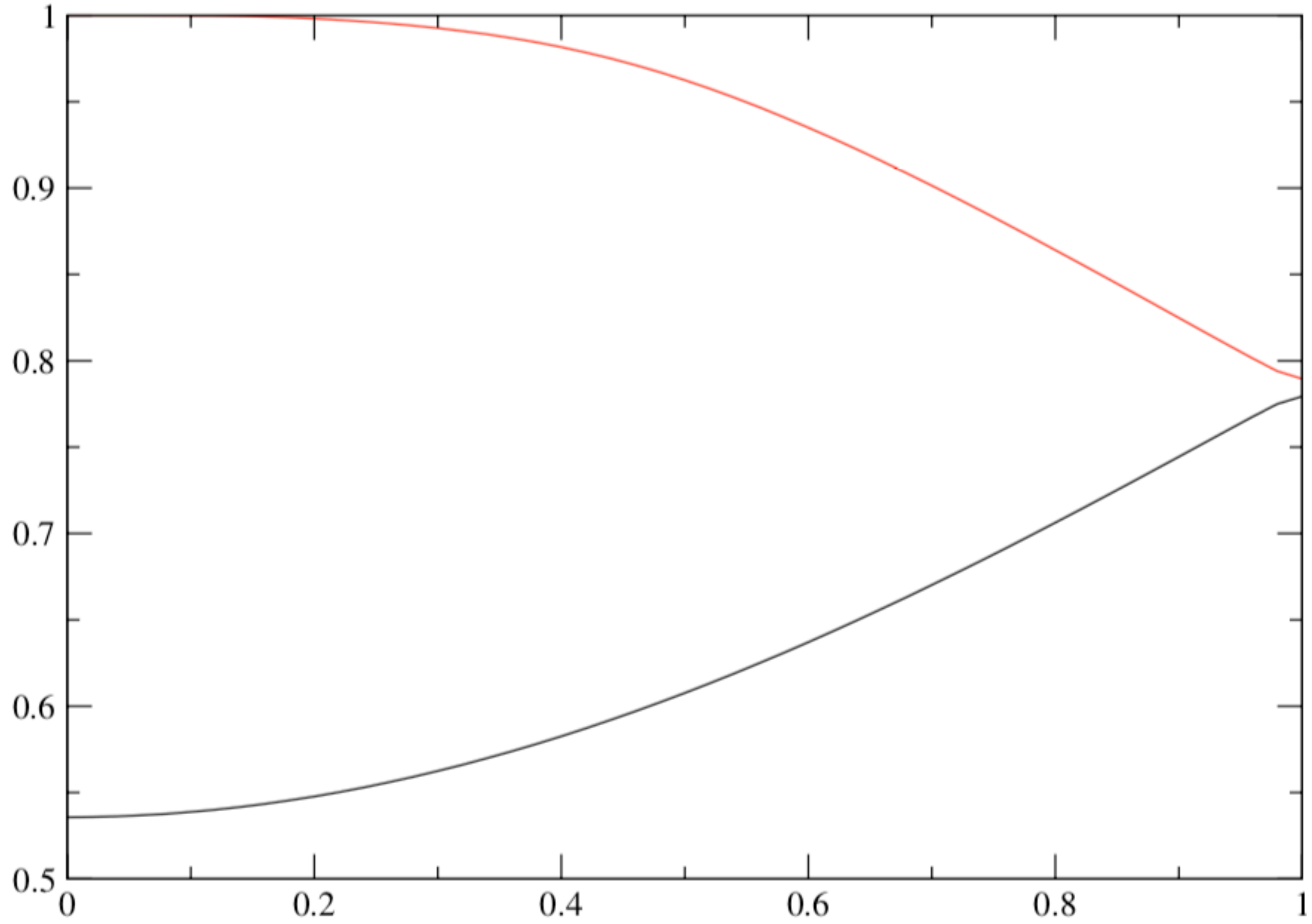
(a) $\delta = 0, \Gamma_1 = \Gamma_2 = 0.1U$



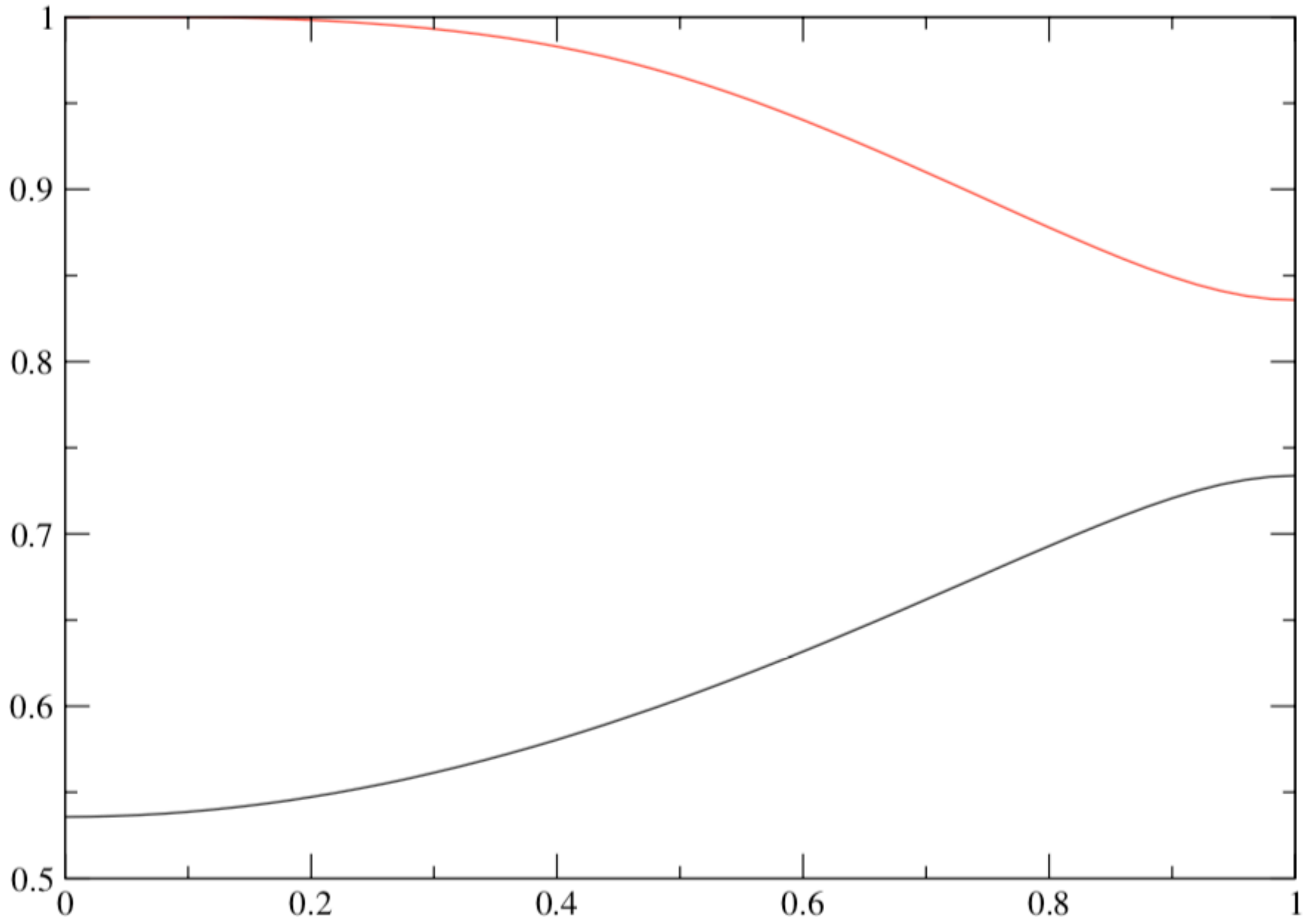
(b) $\delta = 0.01, \Gamma_1 = \Gamma_2 = 0.1U$



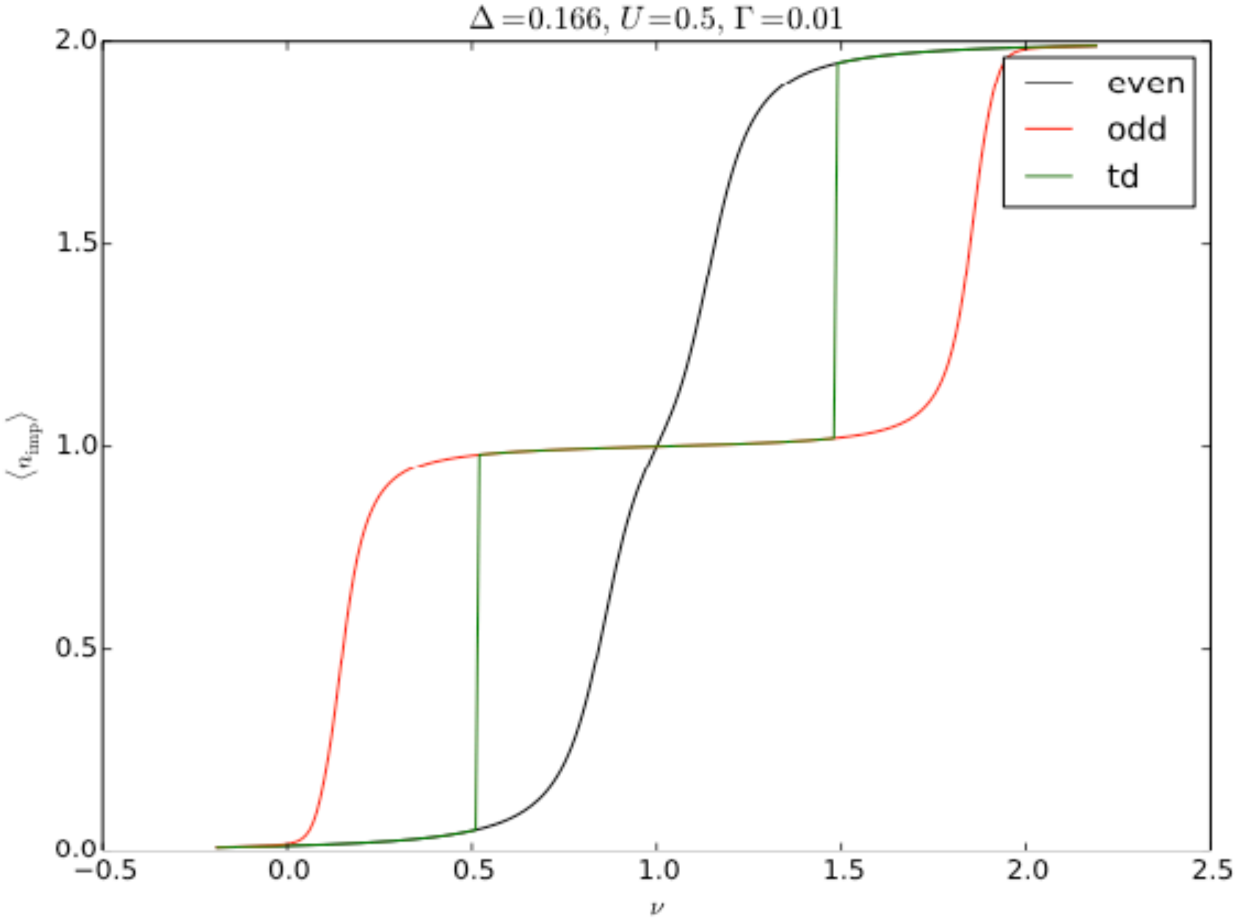
(c) $\delta = 0.1, \Gamma_1 = \Gamma_2 = 0.1U$

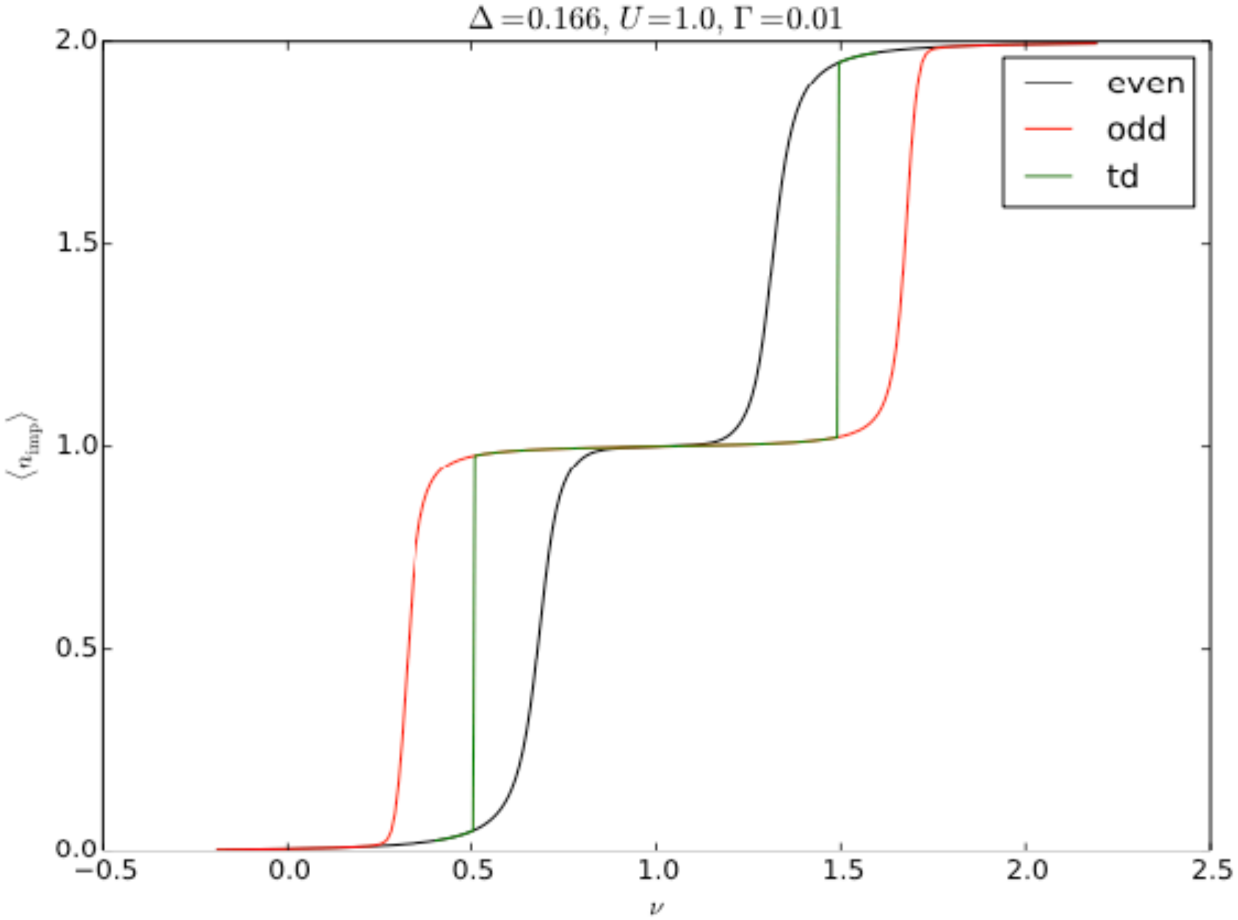


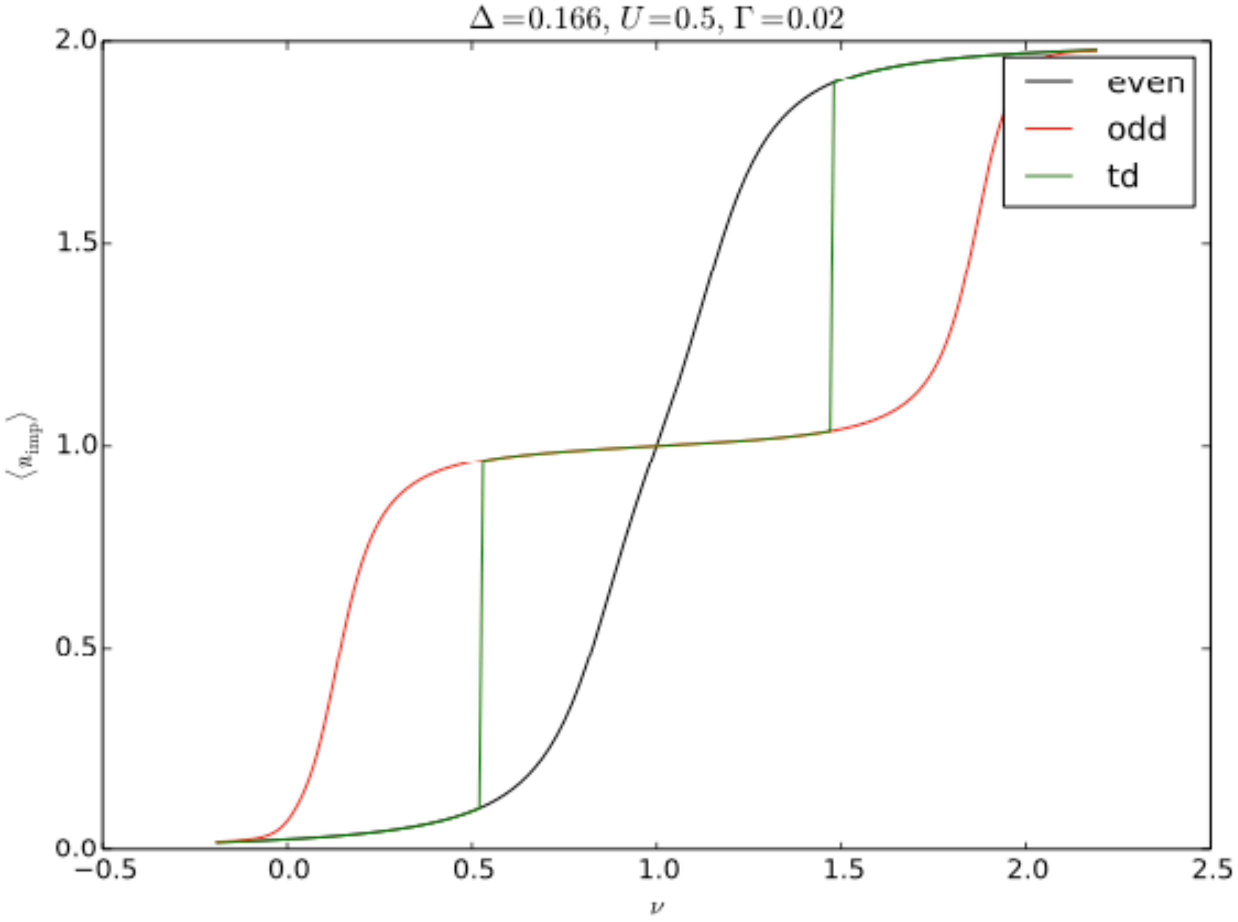
(d) $\delta = 0, \Gamma_{1,2} = 0.1(1 \pm 0.02)U$

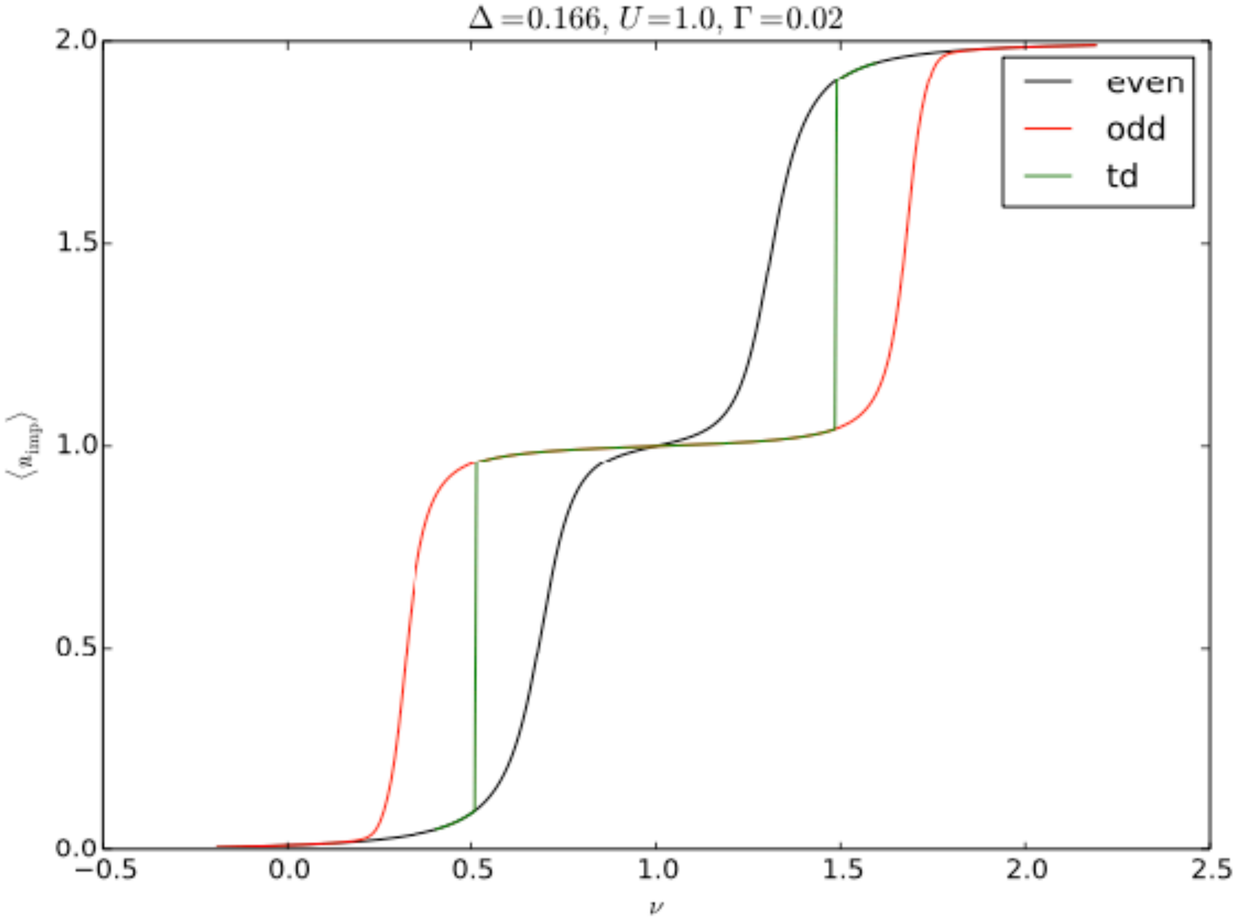


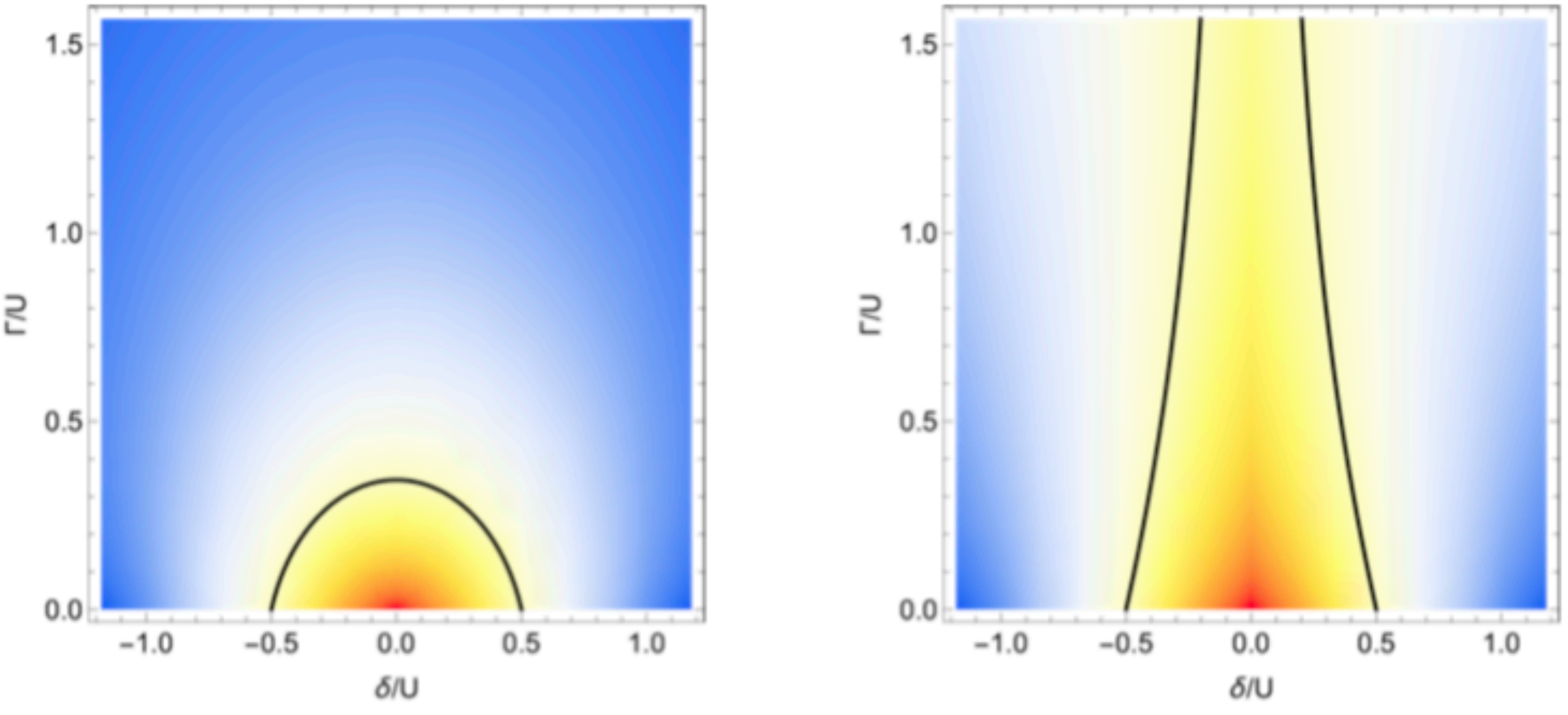
(e) $\delta = 0, \Gamma_{1,2} = 0.1(1 \pm 0.2)U$


$\Delta=0.166$, $U=0.5$, $\Gamma=0.01$
even
odd
td
$\langle n_{\mathrm{imp}}\rangle$
0.0
0.5
1.0
1.5
2.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
ν

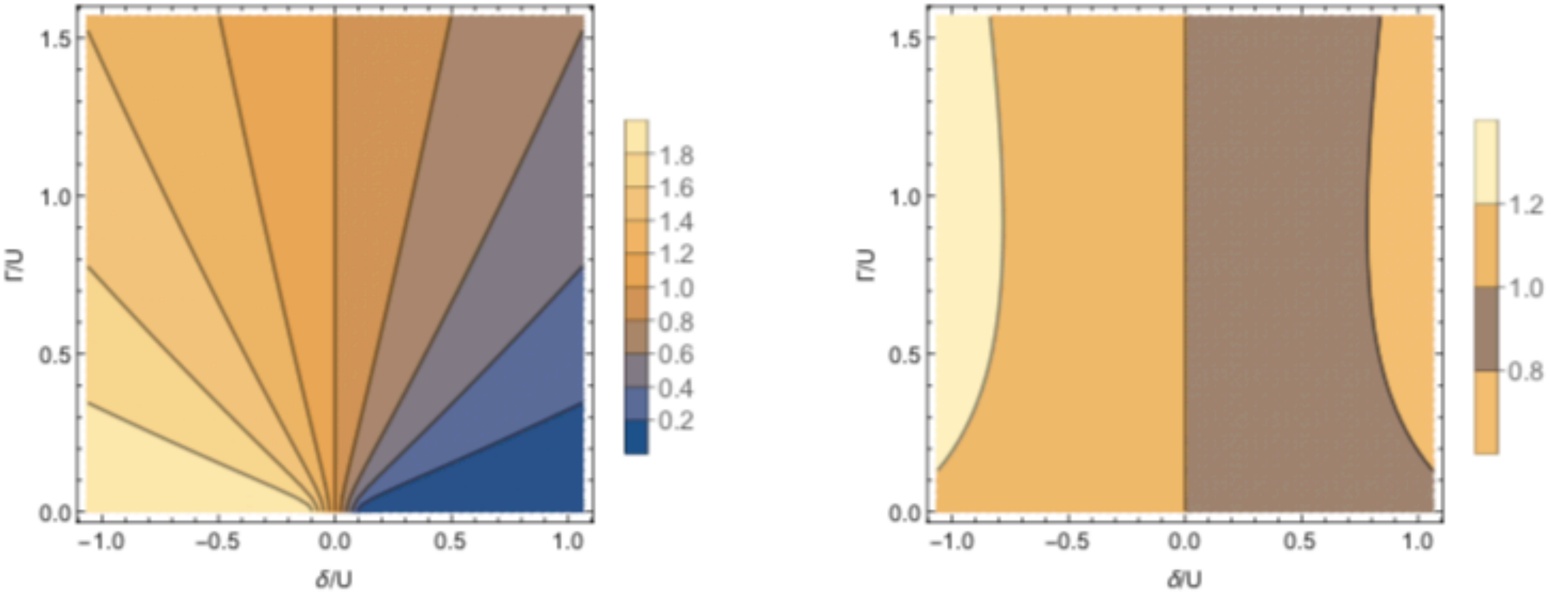

$\Delta=0.166$, $U=1.0$, $\Gamma=0.01$
even
odd
td
$\langle n_{\mathrm{imp}}\rangle$
0.0
0.5
1.0
1.5
2.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
ν


$\Delta=0.166$, $U=0.5$, $\Gamma=0.02$
even
odd
td
$\langle n_{\mathrm{imp}}\rangle$
0.0
0.5
1.0
1.5
2.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
ν


$\Delta=0.166$, $U=1.0$, $\Gamma=0.02$
even
odd
td
$\langle n_{\mathrm{imp}}\rangle$
0.0
0.5
1.0
1.5
2.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
ν

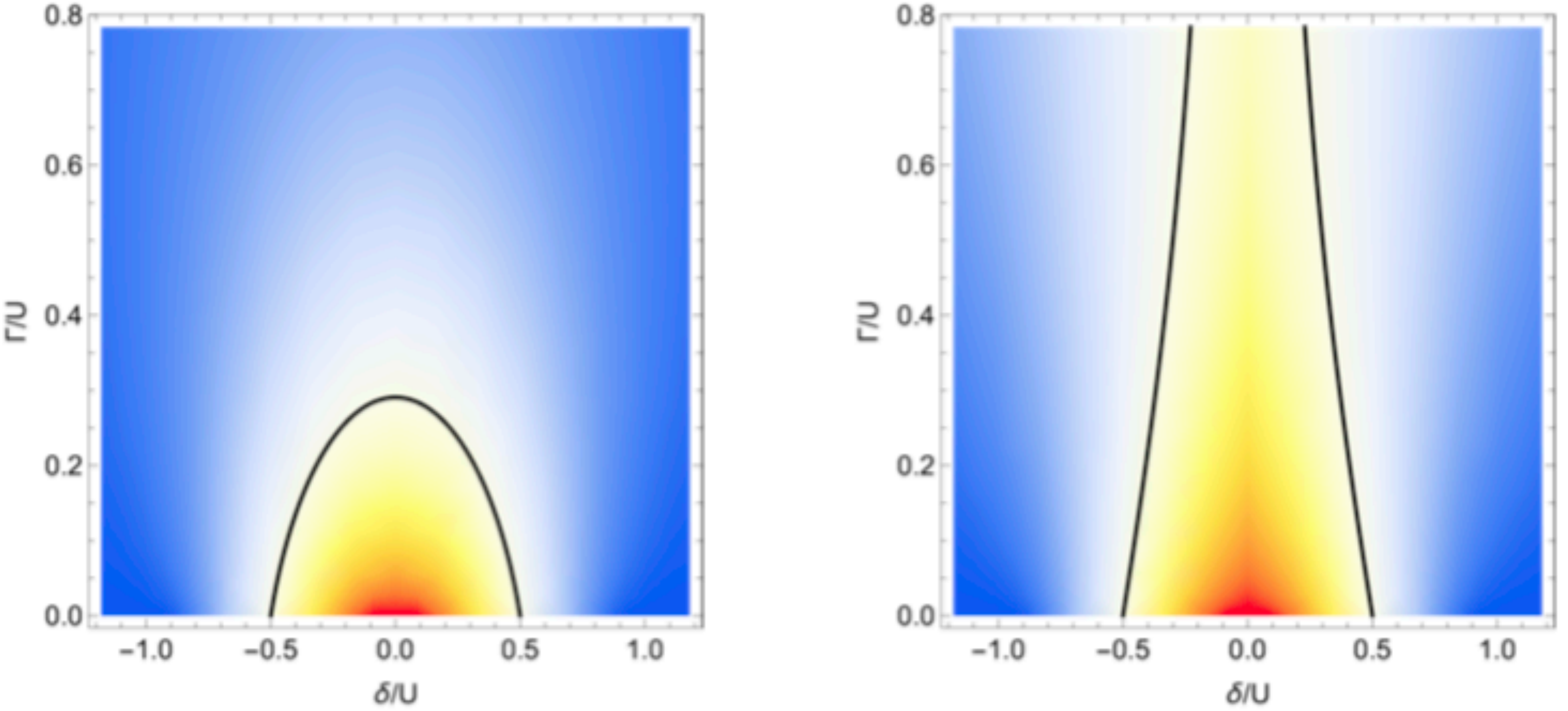


(a) Phase diagram at $\phi = 0$ (b) Phase diagram at $\phi = \pi$

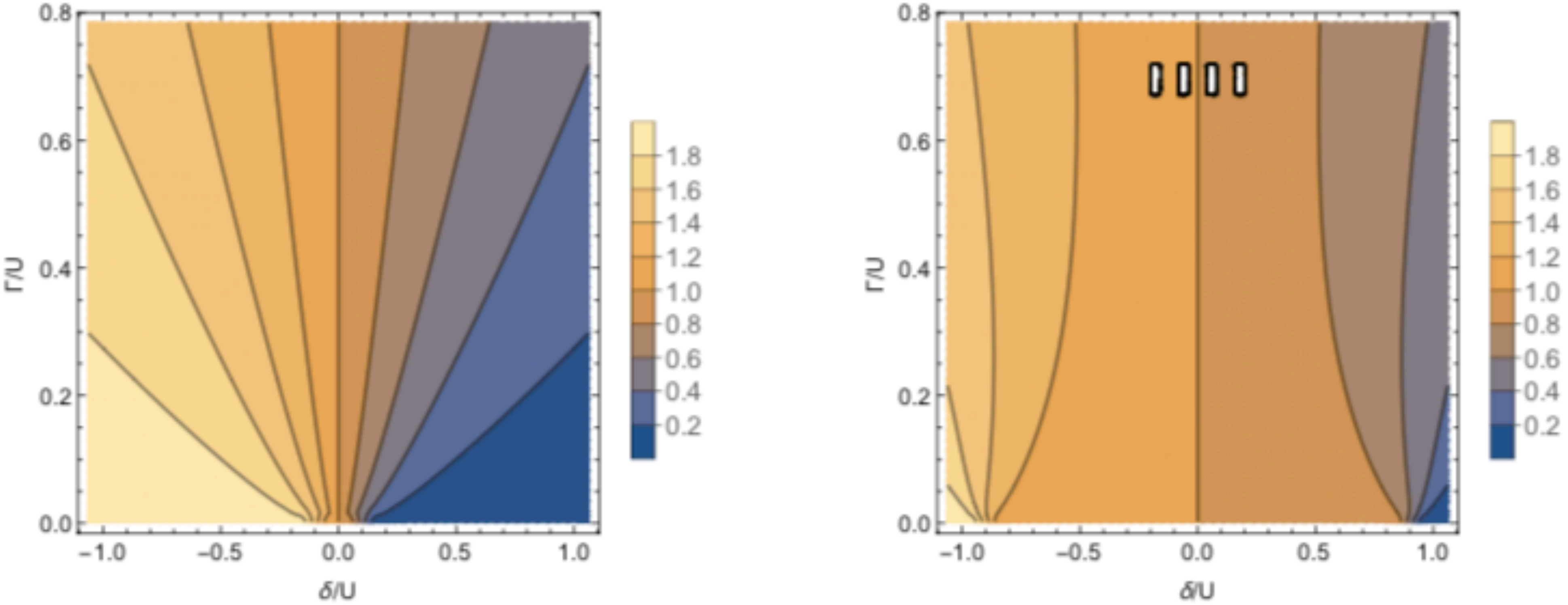


(g) $n_{\rm imp}$ for $S = 0$ (h) $n_{\rm imp}$ for $S = 1/2$

Figure 9: Results for $U/\Delta = 1.25$.

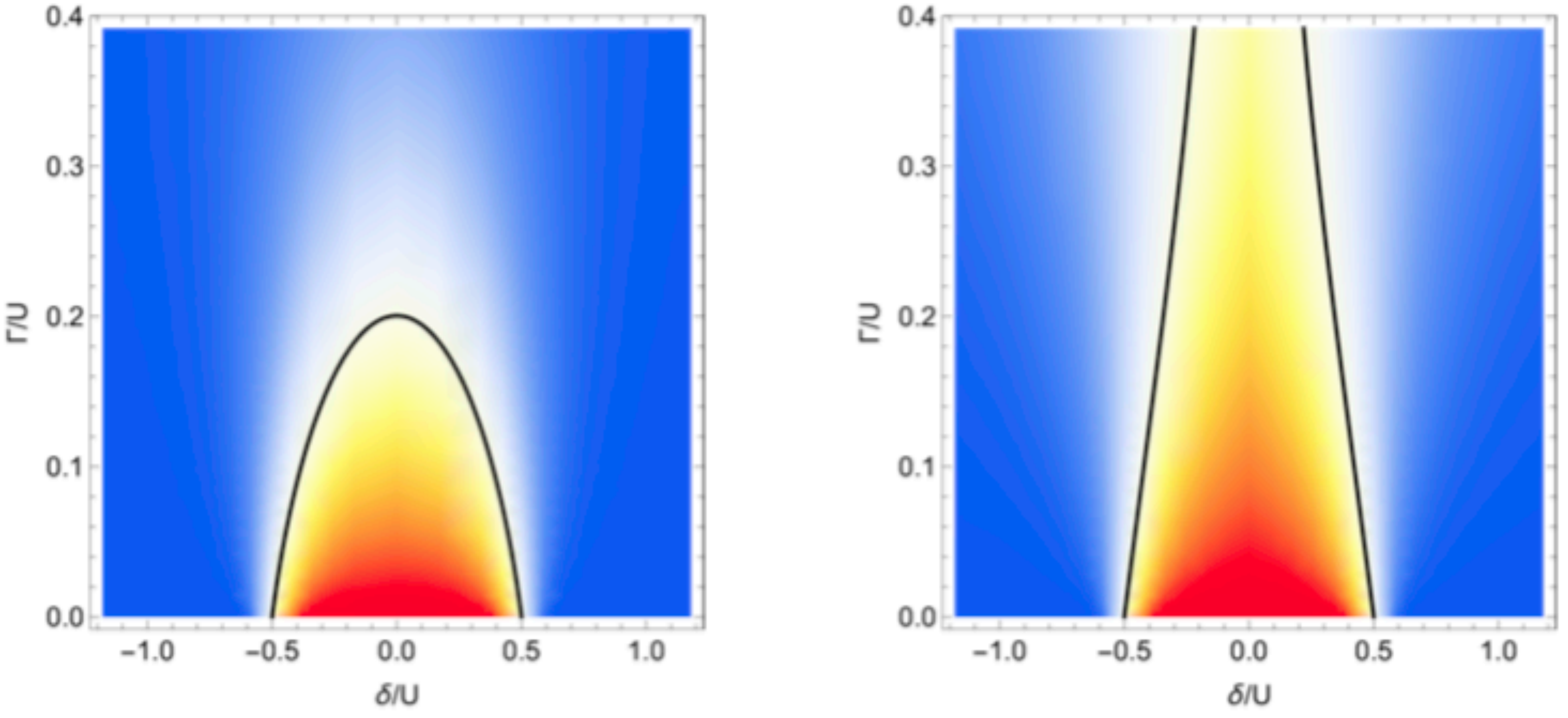


(a) Phase diagram at $\phi = 0$ (b) Phase diagram at $\phi = \pi$



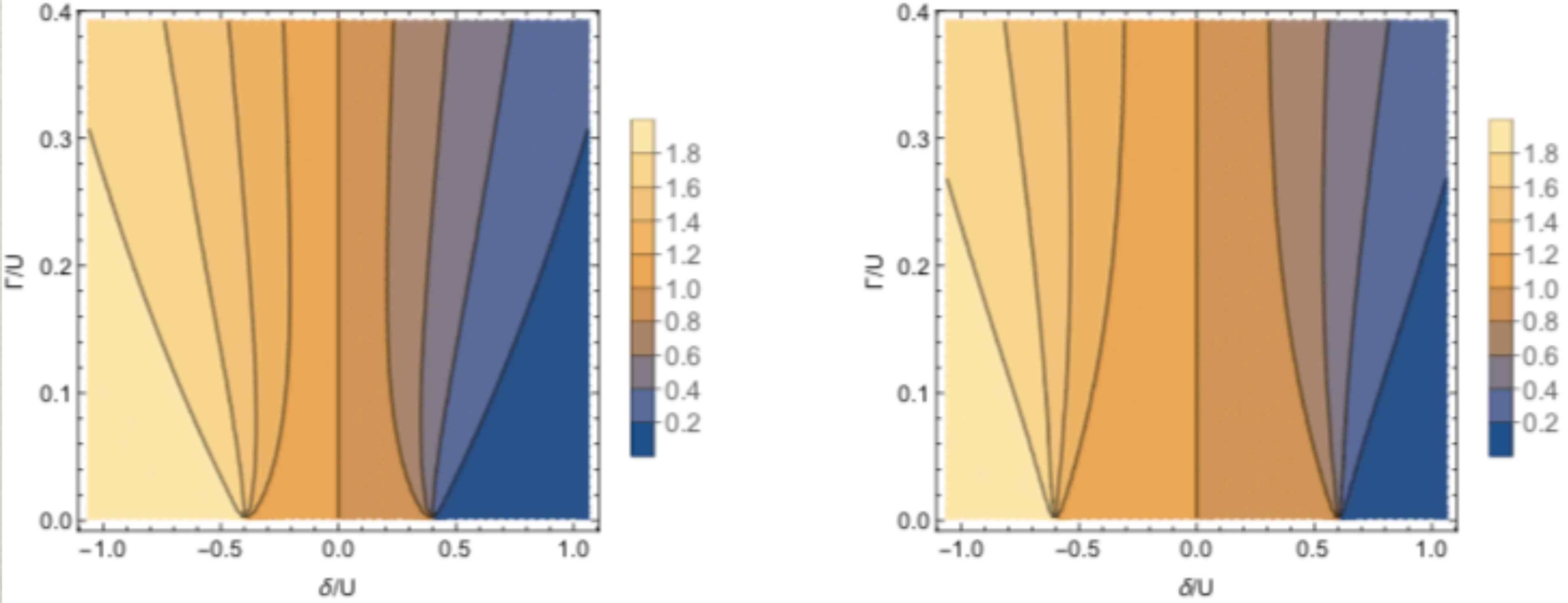
(g) n_{imp} for $S = 0$ (h) n_{imp} for $S = 1/2$

Figure 10: Results for $U/\Delta = 2.5$.



(a) Phase diagram at $\phi = 0$

(b) Phase diagram at $\phi = \pi$



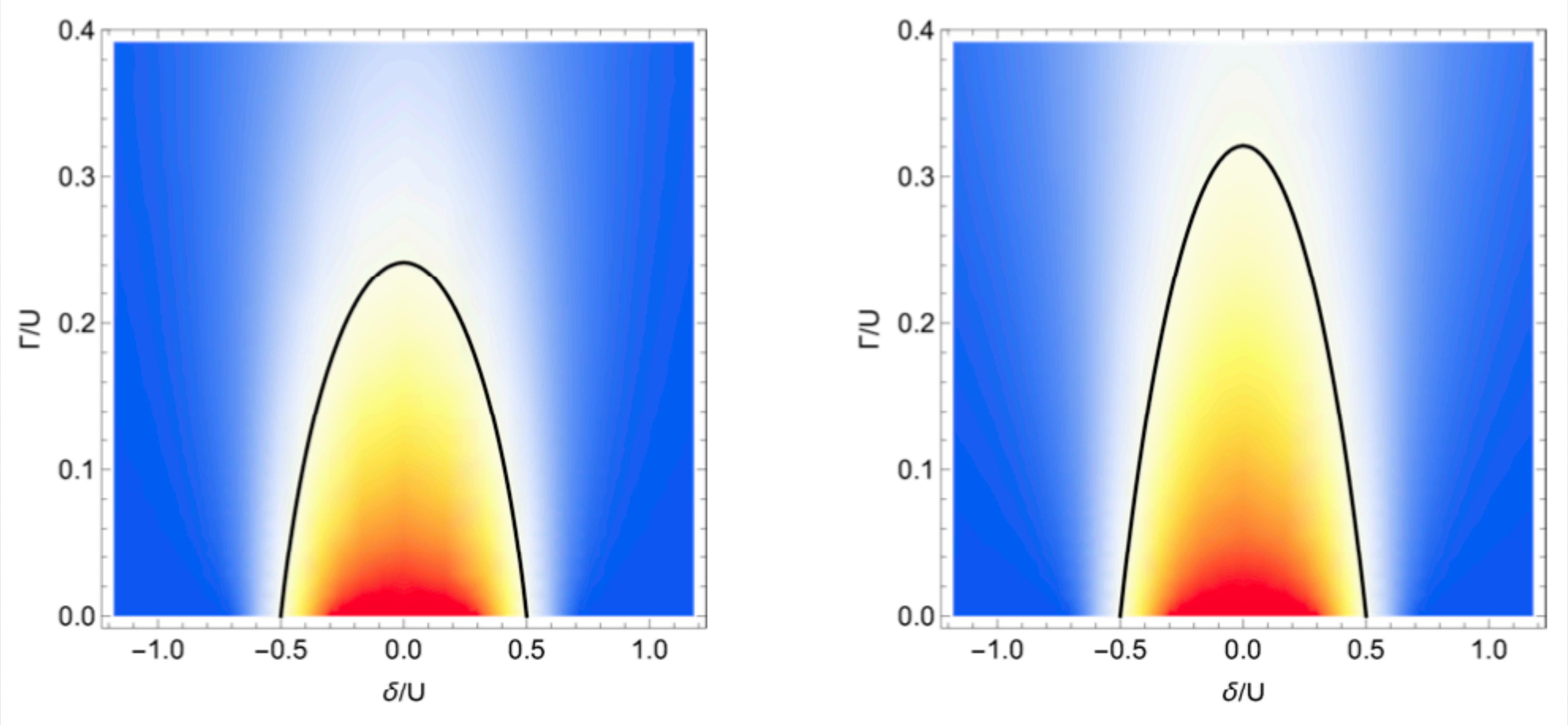
(g) n_{imp} for $S = 0$

(h) n_{imp} for $S = 1/2$

Figure 11: Results for $U/\Delta = 10$.

EFFECTS OF CHANNEL ASYMMETRY

$$\Delta(z) = \sum_{\alpha=1,2} \frac{|V_\alpha|^2}{z^2 - [(\epsilon-\mu)^2 + \Delta^2]} \begin{pmatrix} z + (\epsilon - \mu) & -\Delta e^{i\phi_\alpha} \\ -\Delta e^{-i\phi_\alpha} & z - (\epsilon - \mu) \end{pmatrix}$$

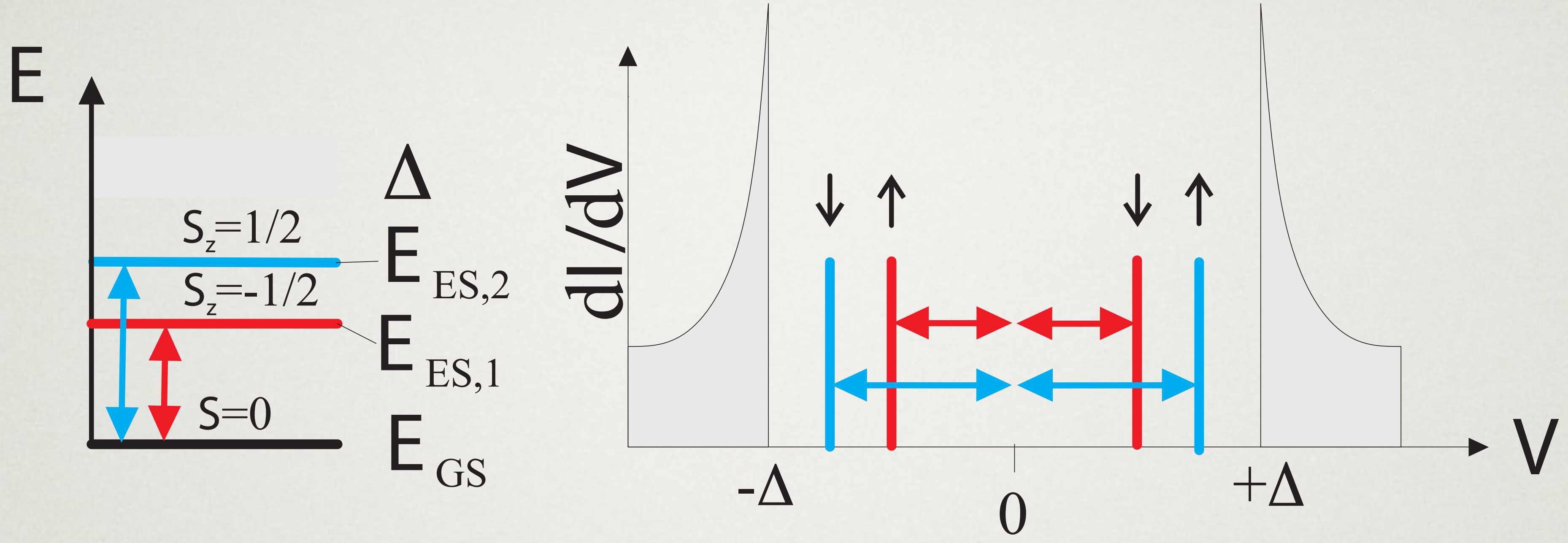


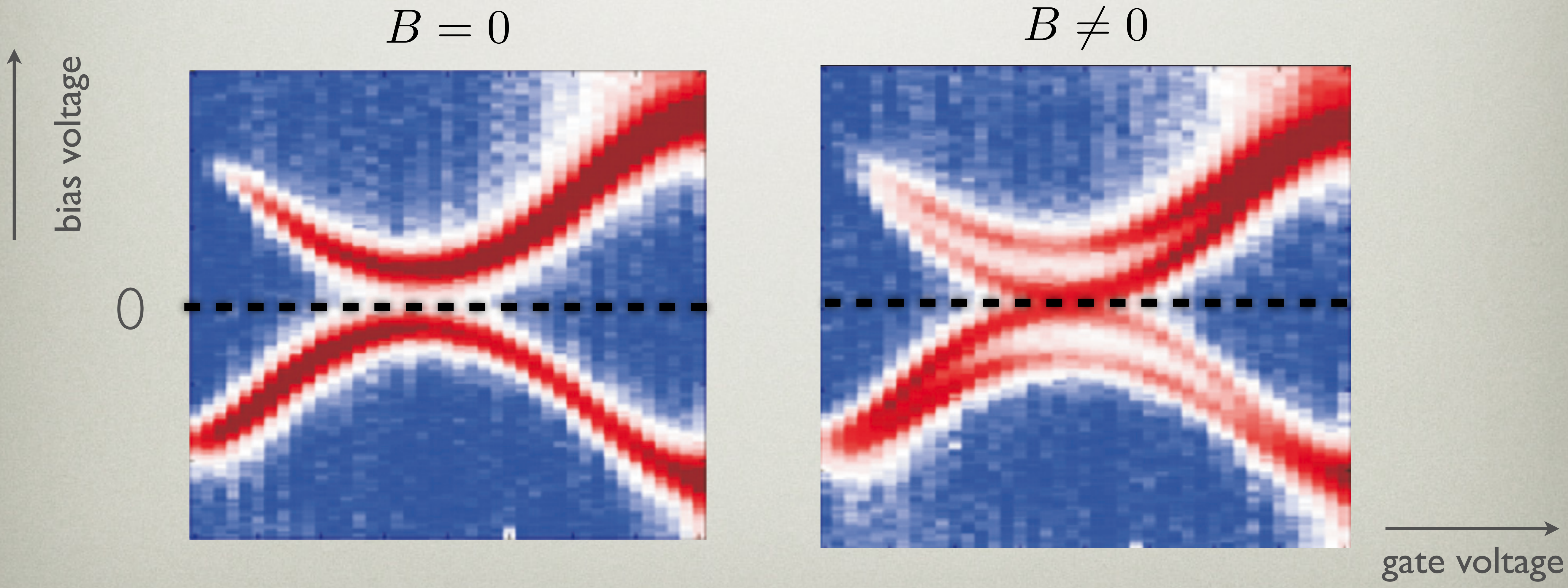
(a) Phase diagram at $\phi = 0$

(b) Phase diagram at $\phi = \pi$

Figure 13: Results for $U/\Delta = 5$, $\Gamma_1/\Gamma_2 = 5$.

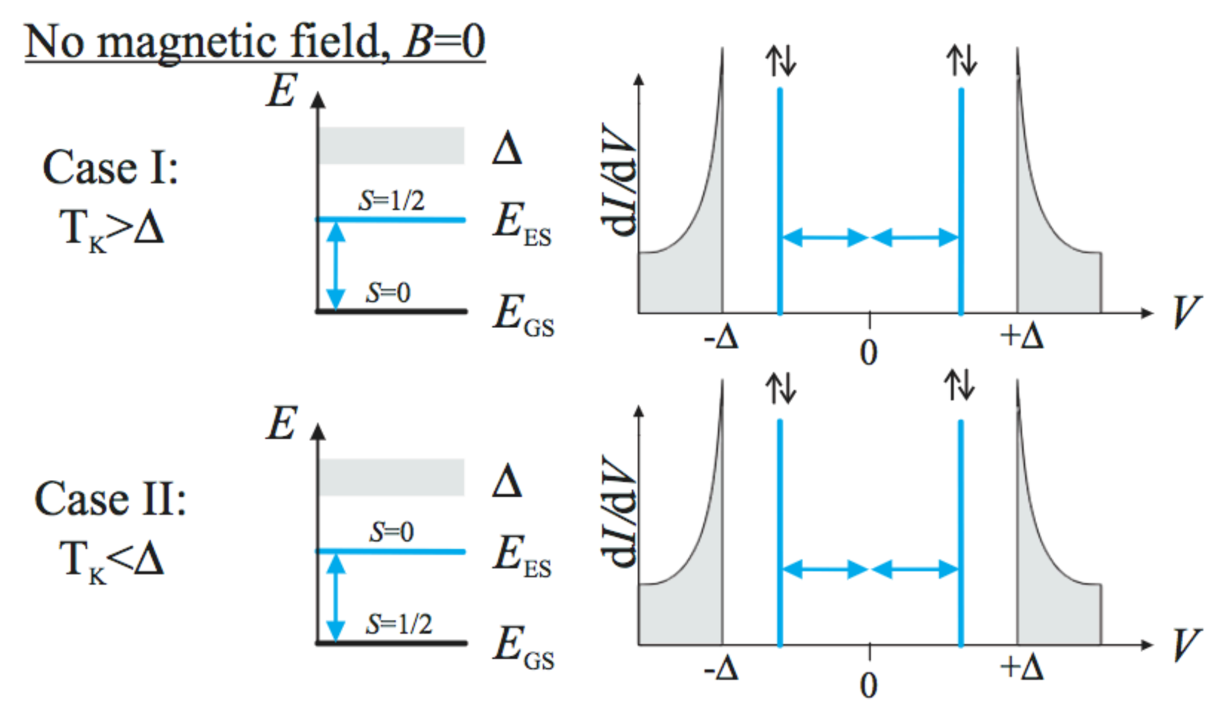
ZEEMAN SPLITTING OF YSR STATES

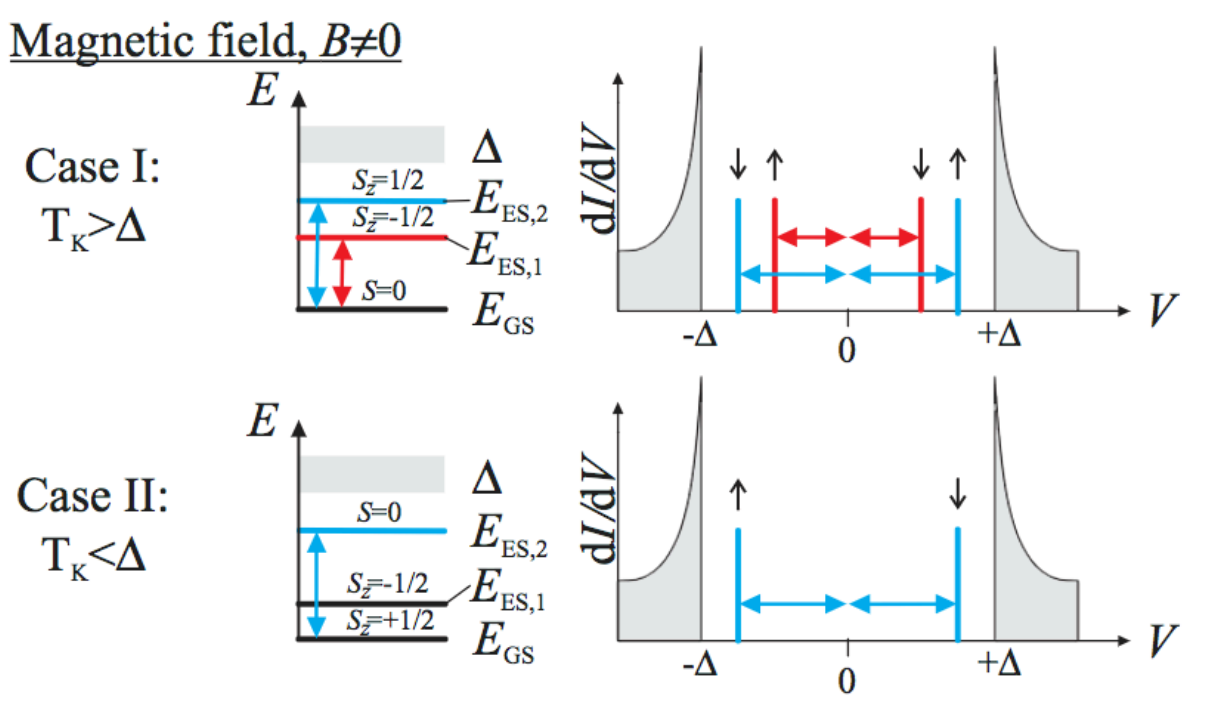


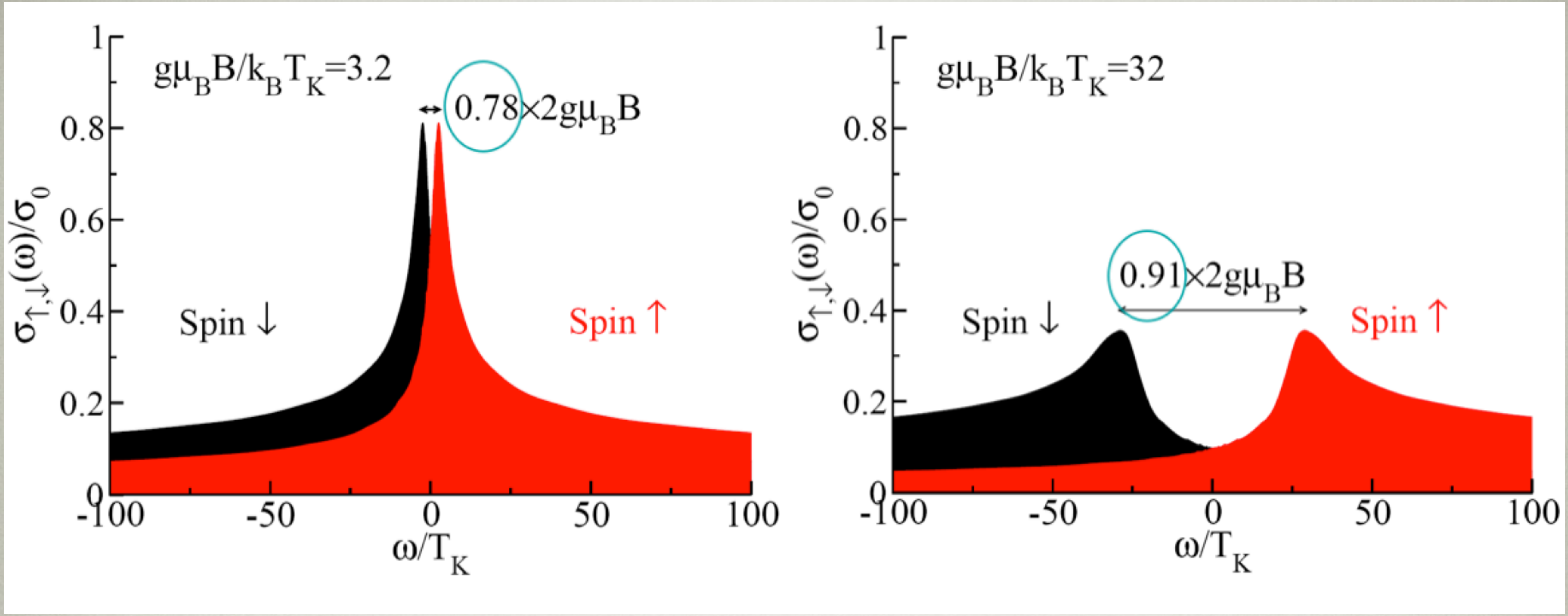


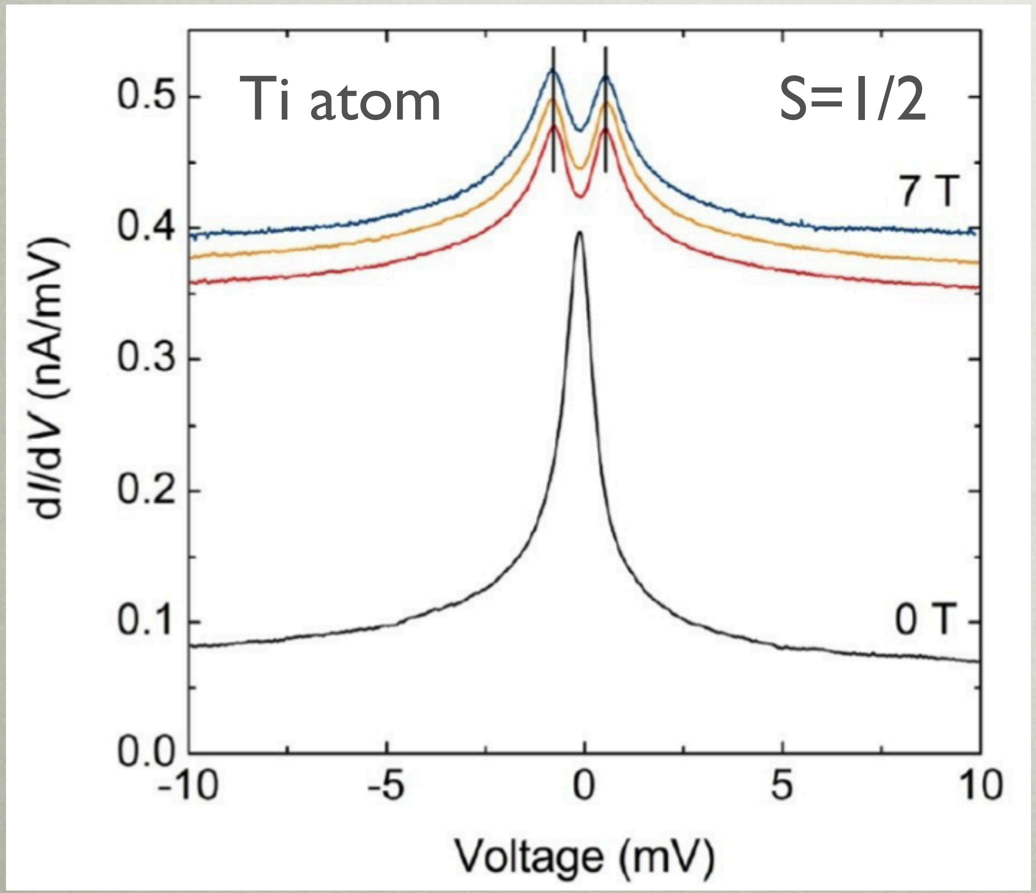
Lee, Jiang, Houzet, Aguado, Lieber, De Franceschi, Nature Nanotech. 9, 79 (2014)

Relation between many-body states and single-particle spectral function



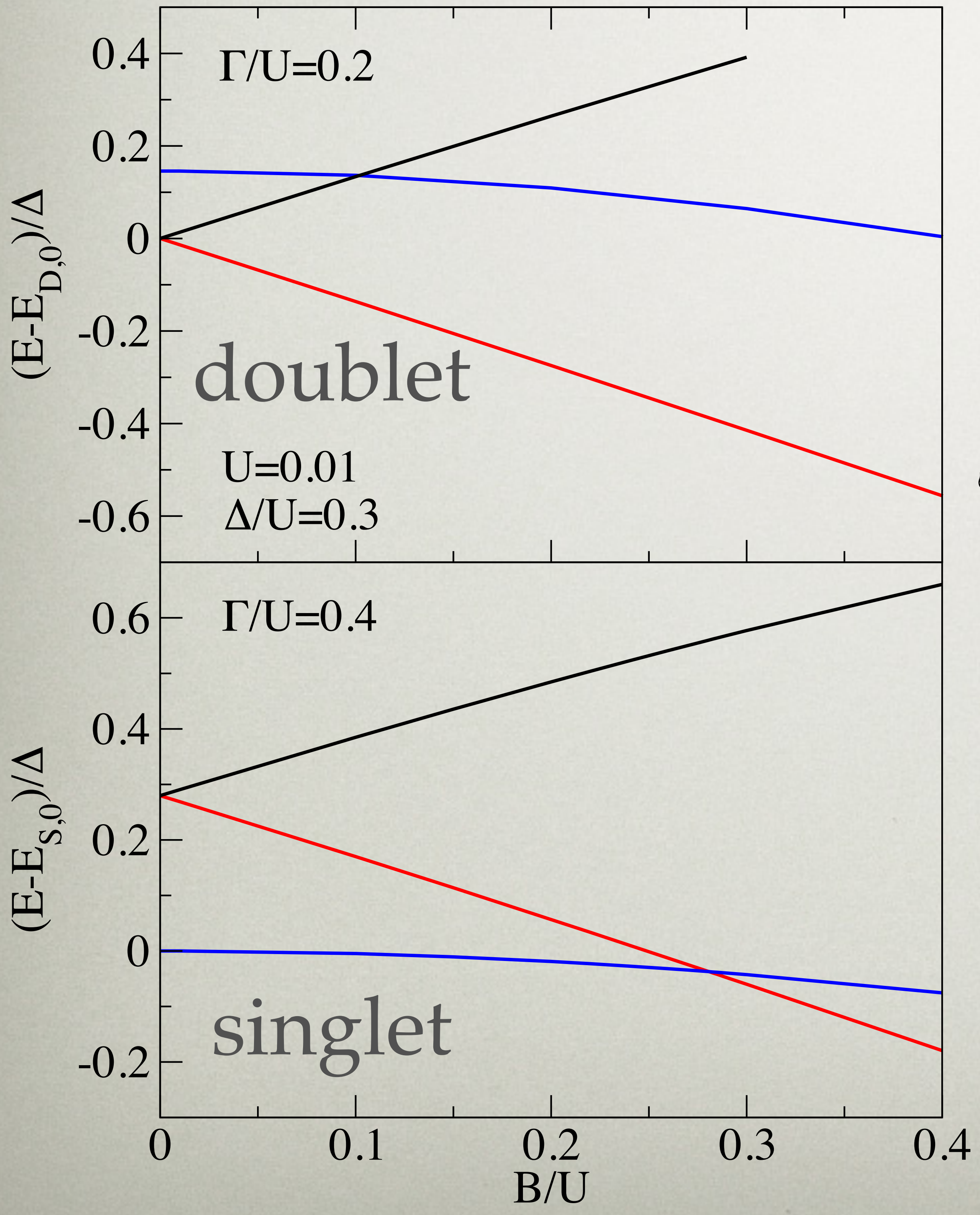




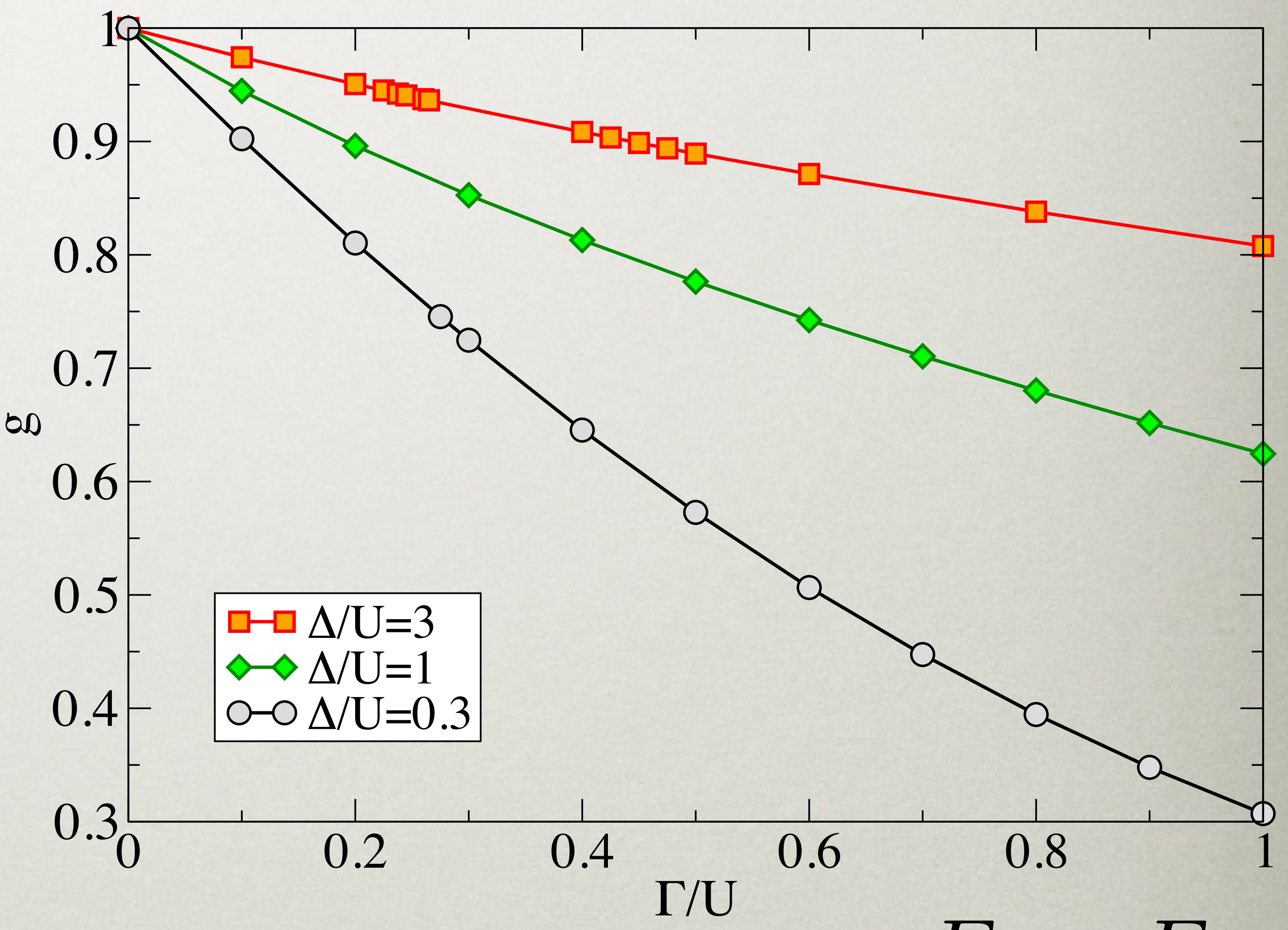


S. Otte et al., Nature Physics 4, 847 (2008)

MAGNETIC FIELD EFFECTS ON SHIBA STATES



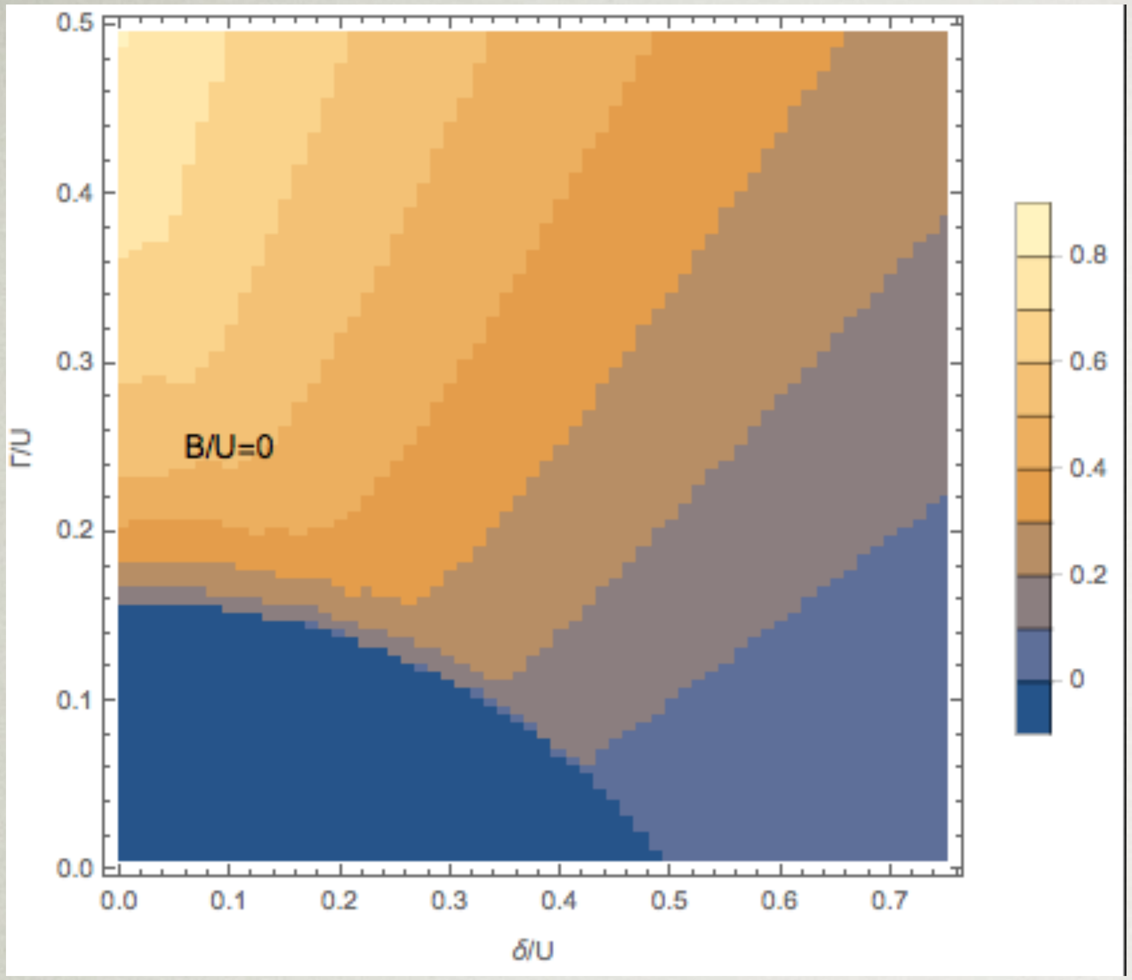
$$H_{\mathrm{mag}} = g_0 \mu_B B S_{\mathrm{imp},z}$$

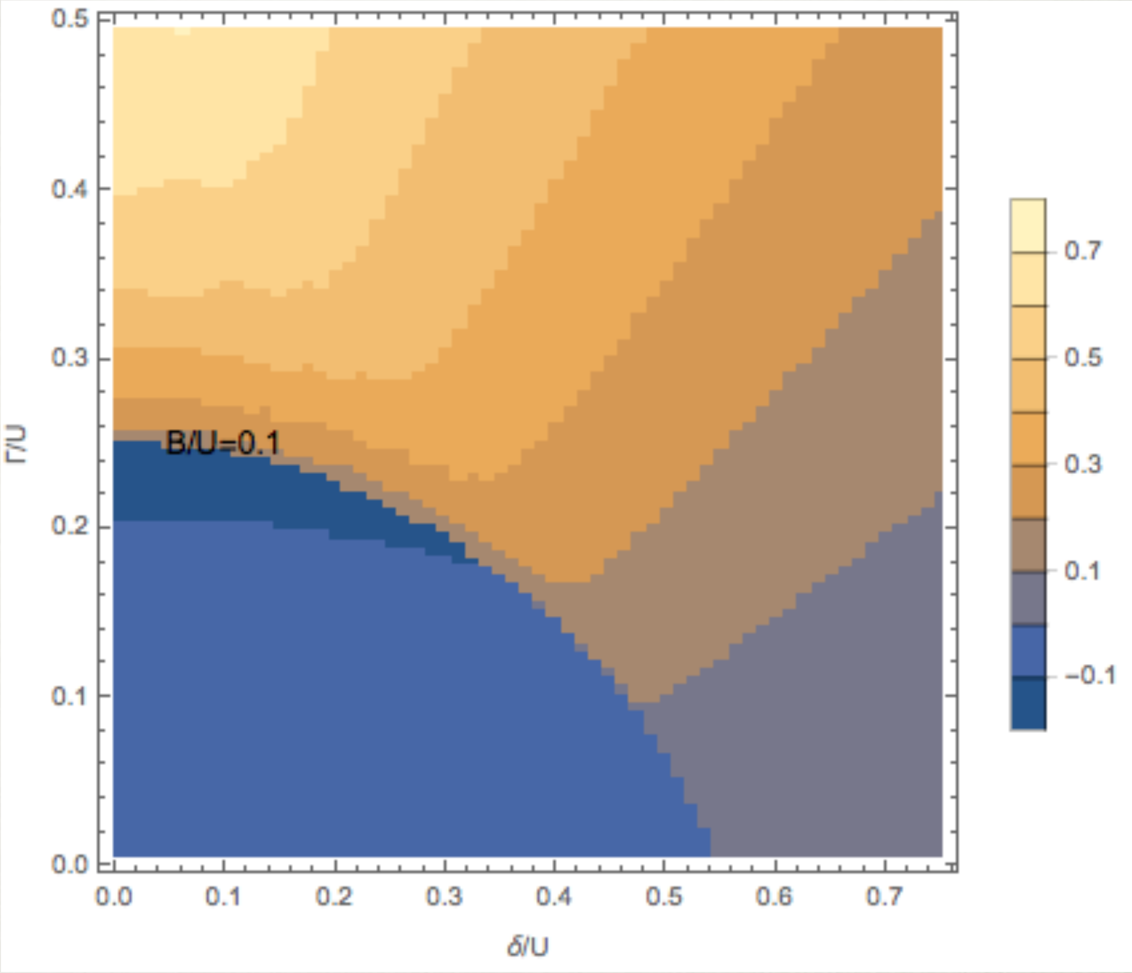


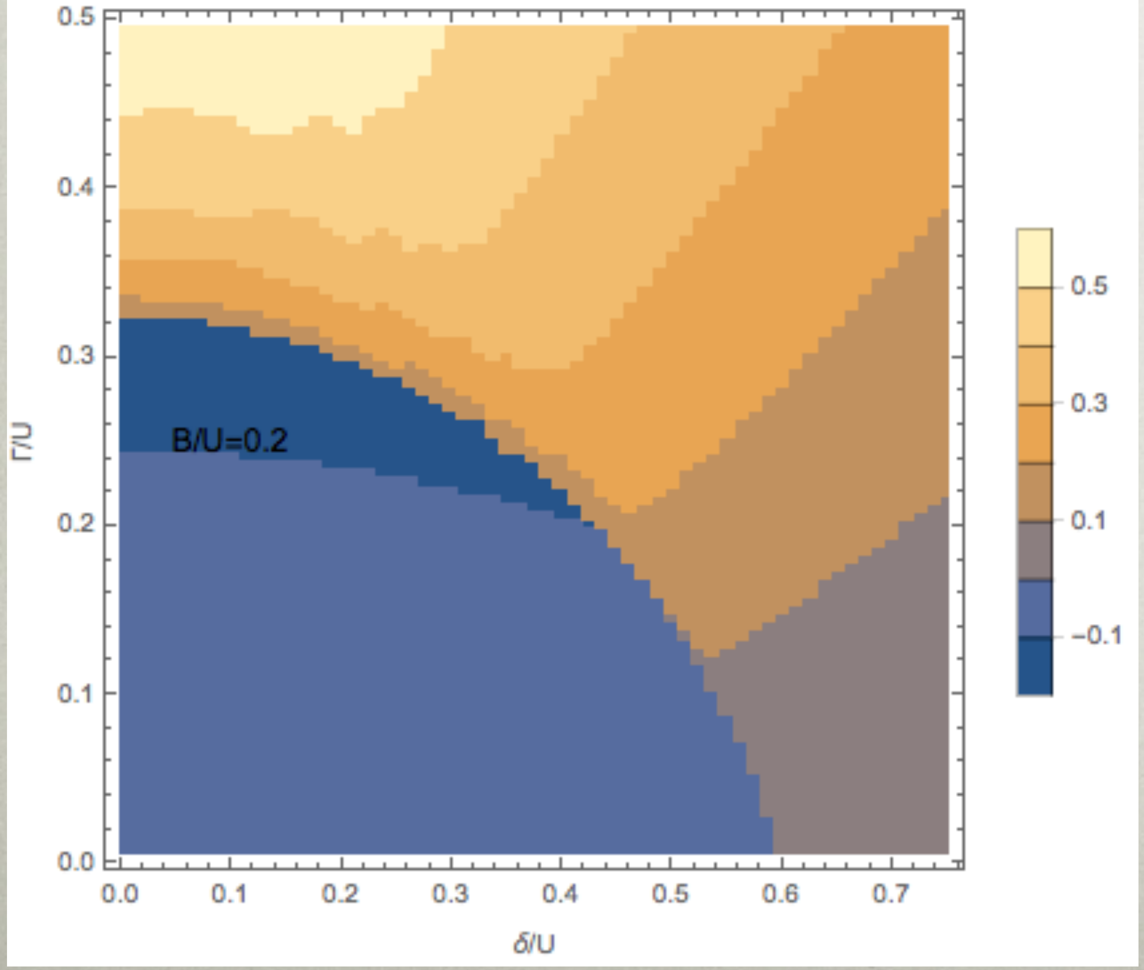
relative g factor

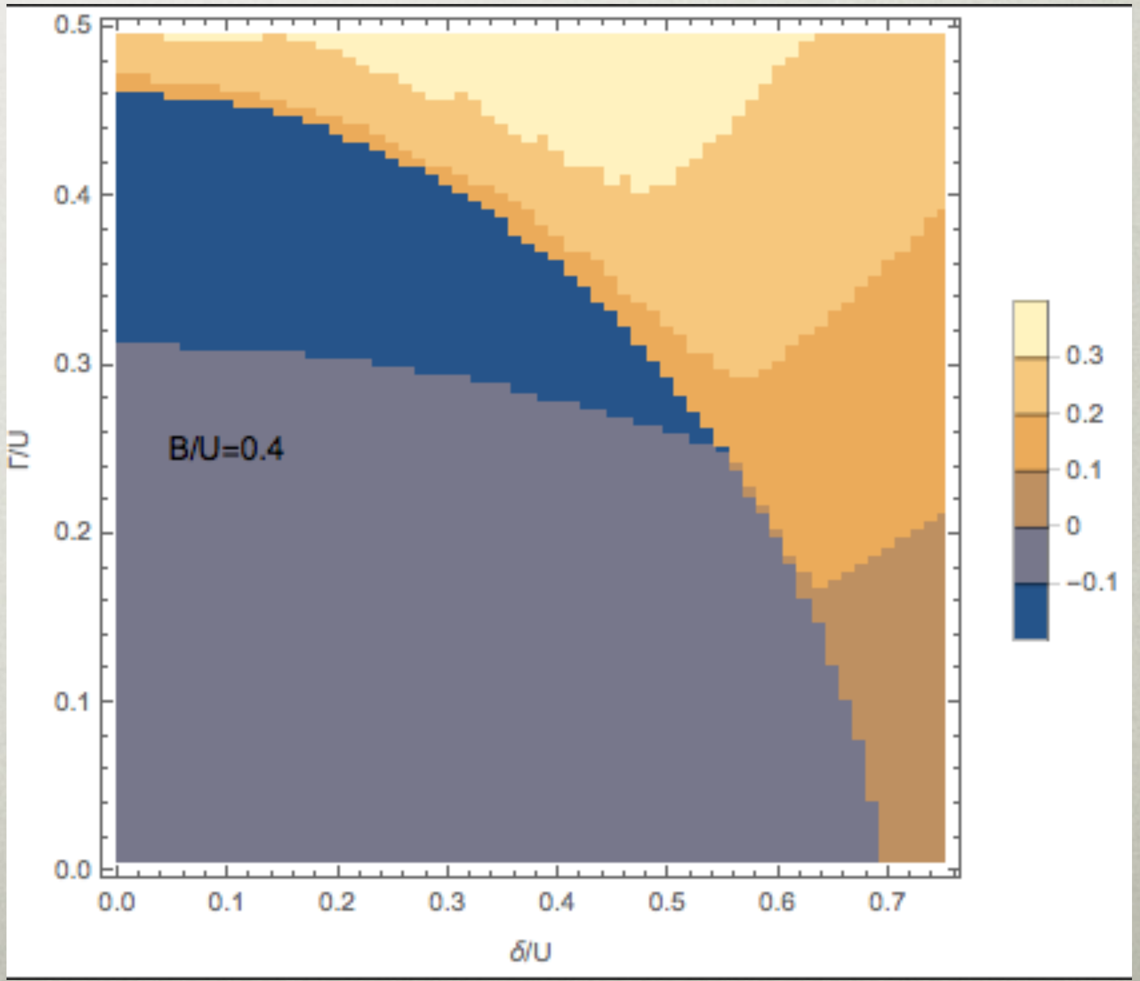
$$g = \frac{E_\uparrow - E_\downarrow}{g_0 \mu_B B}$$

strongly renormalized
by Kondo exchange coupling!

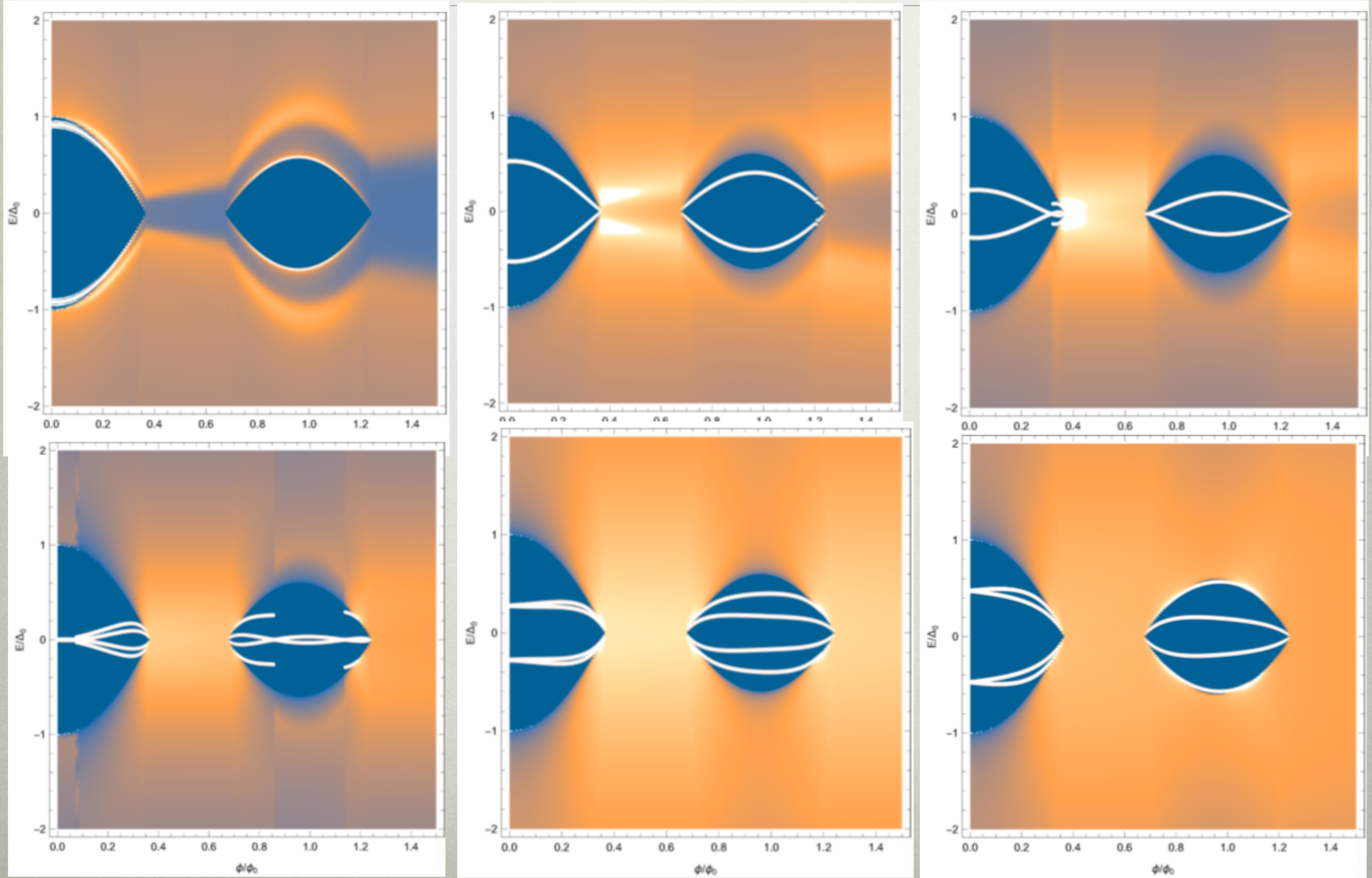

B/U=0
Γ/U
δ/U
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.6
0.4
0.2
0


B/U=0.1
Γ/U
δ/U
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.7
0.5
0.3
0.1
−0.1


B/U=0.2
Γ/U
δ/U
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.5
0.3
0.1
−0.1


B/U=0.4
Γ/U
δ/U
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.3
0.2
0.1
0
−0.1

FULL-SHELL NANOWIRES

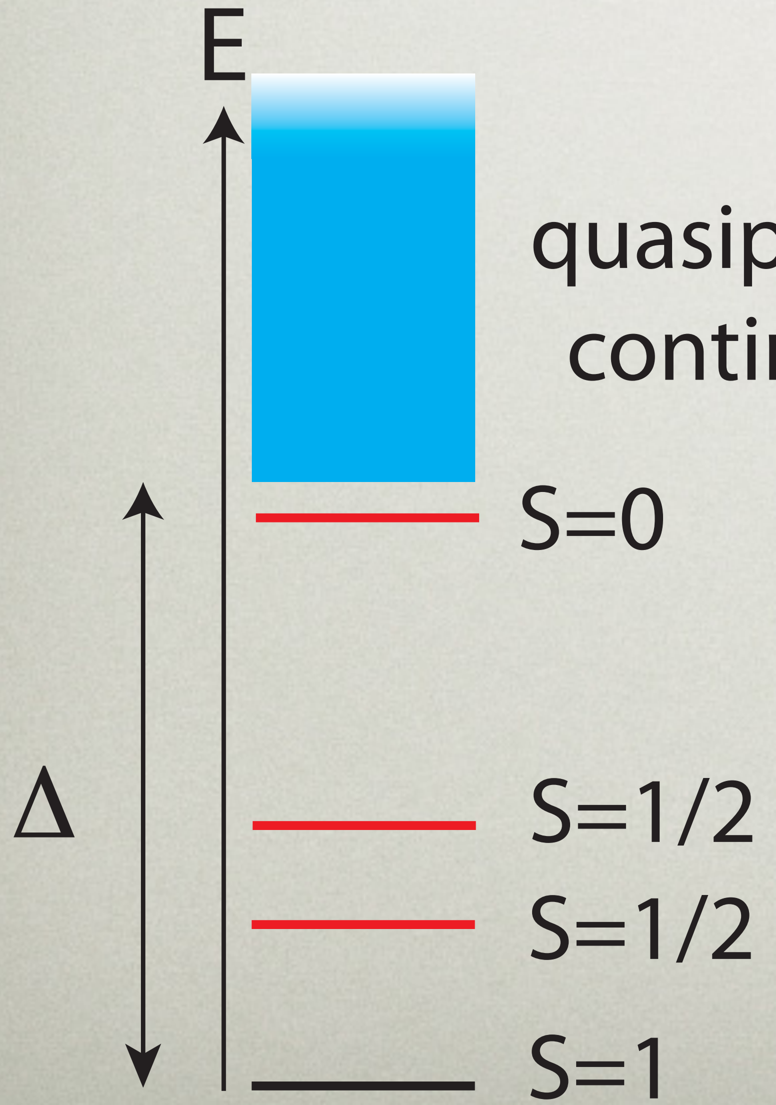


SHIBA STATES IN HIGH-SPIN IMPURITIES

$$H_{\mathrm{imp}} = \sum_{i=1}^{N_{\mathrm{ch}}} J_i \, \mathbf{S}_{\mathrm{imp}} \cdot \mathbf{s}_i$$

coupling to
multiple “channels”
with different
orbital symmetries

Example: S_{imp}=1



Transitions with $\Delta S_z = \pm 1/2$ are observable in tunneling spectroscopy

MAGNETIC ANISOTROPY FOR S≥1

(ALSO KNOWN AS “ZERO-FIELD SPLITTING”)

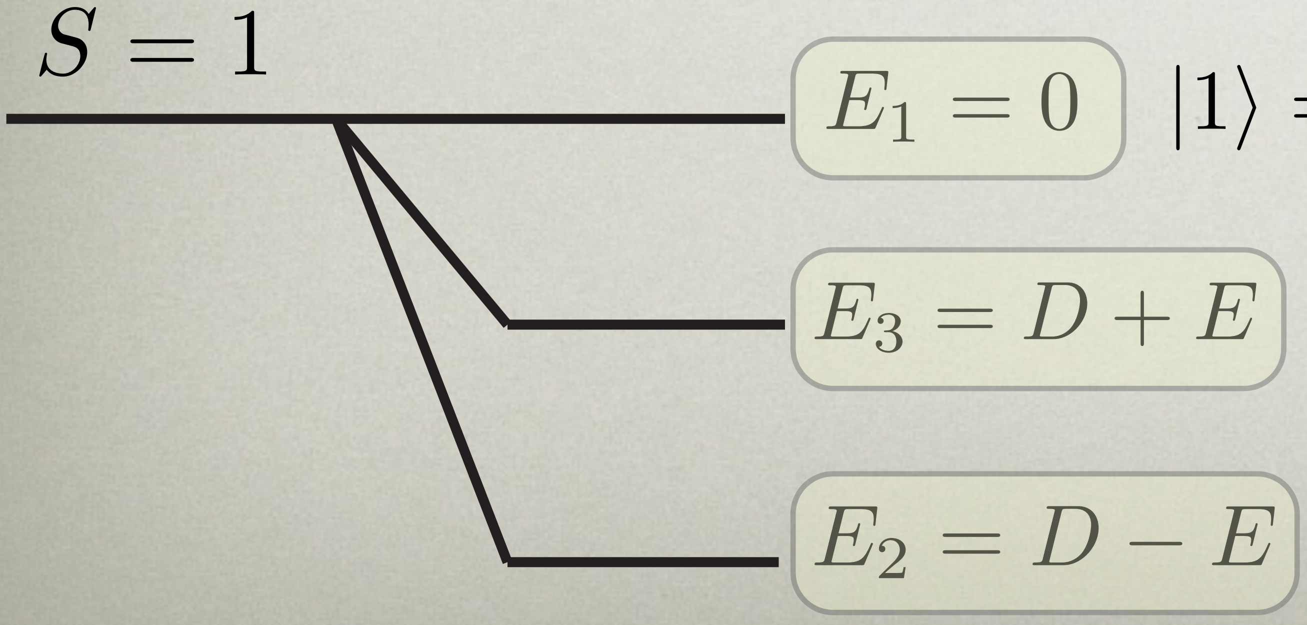
$$\begin{aligned} H_{\text{aniso}} &= DS_z^2 + E(S_x^2 - S_y^2) \\ &= DS_z^2 + E(S_+^2 + S_-^2) \end{aligned}$$

longitudinal anisotropy

transverse anisotropy

Example (S=1):

$$H_{\text{aniso}} = \begin{pmatrix} D & 0 & E \\ 0 & 0 & 0 \\ E & 0 & D \end{pmatrix}$$

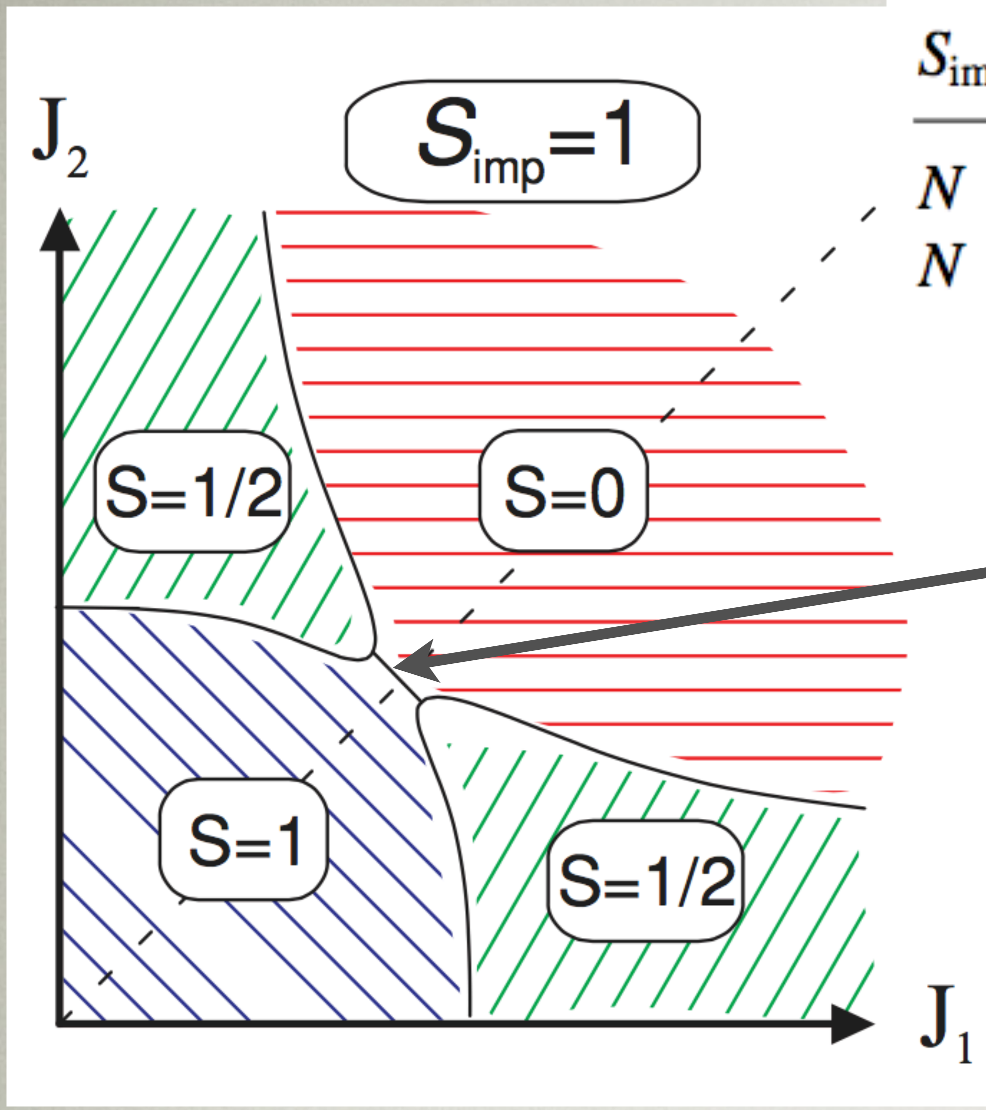


$S = 1$

$E_1 = 0$ $\quad |1\rangle = |S_z = 0\rangle$

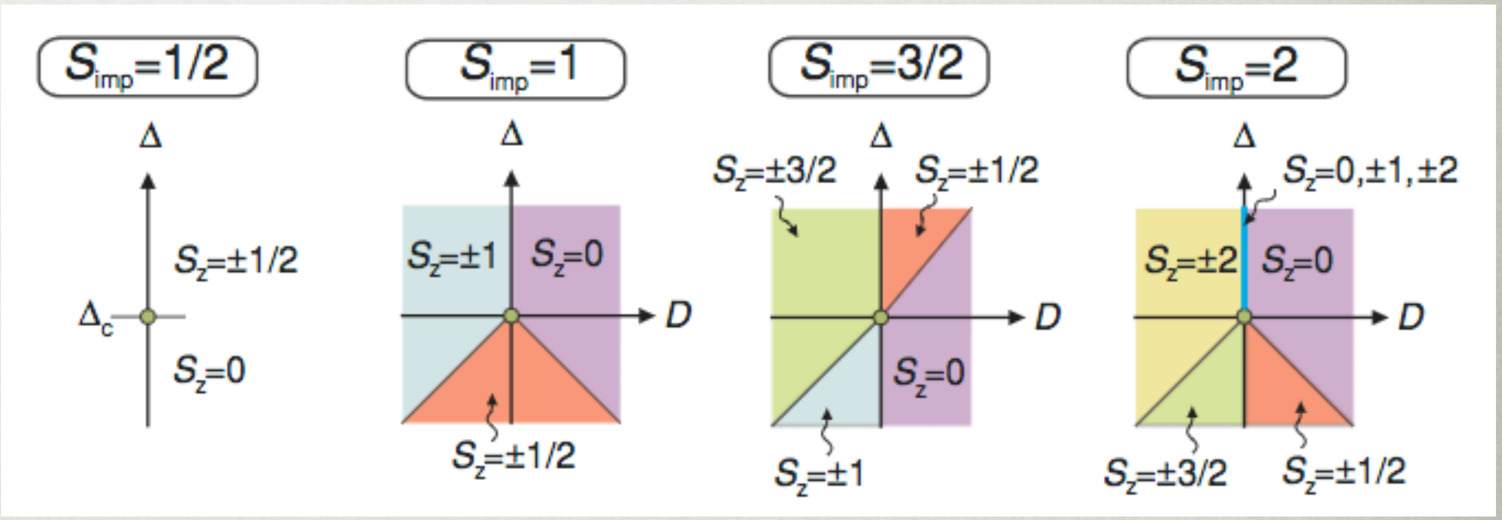
$E_3 = D + E$ $\quad |3\rangle = \frac{1}{\sqrt{2}}\left(|S_z = -1\rangle + |S_z = 1\rangle\right)$

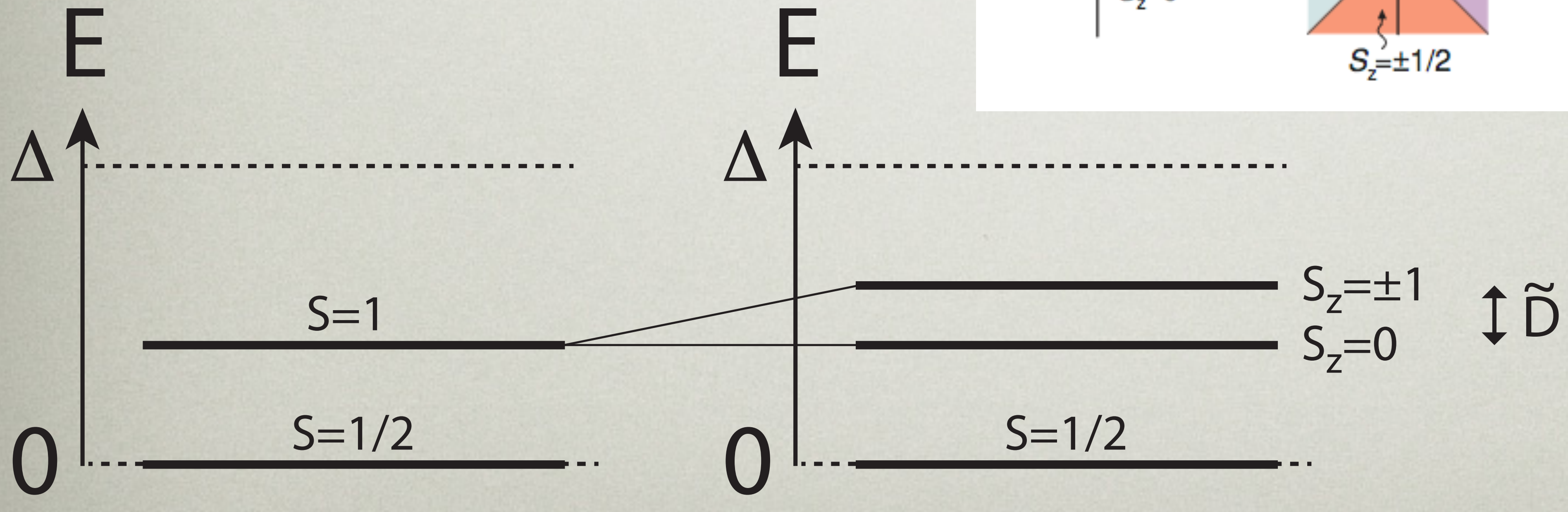
$E_2 = D - E$ $\quad |2\rangle = \frac{1}{\sqrt{2}}\left(|S_z = -1\rangle - |S_z = 1\rangle\right)$



S_{imp}	1/2	1	3/2	2	5/2
$N = 1$	3.7	5.9	10.3	19.8	43
$N = 2$	0.70	5.7	11.3	23	51

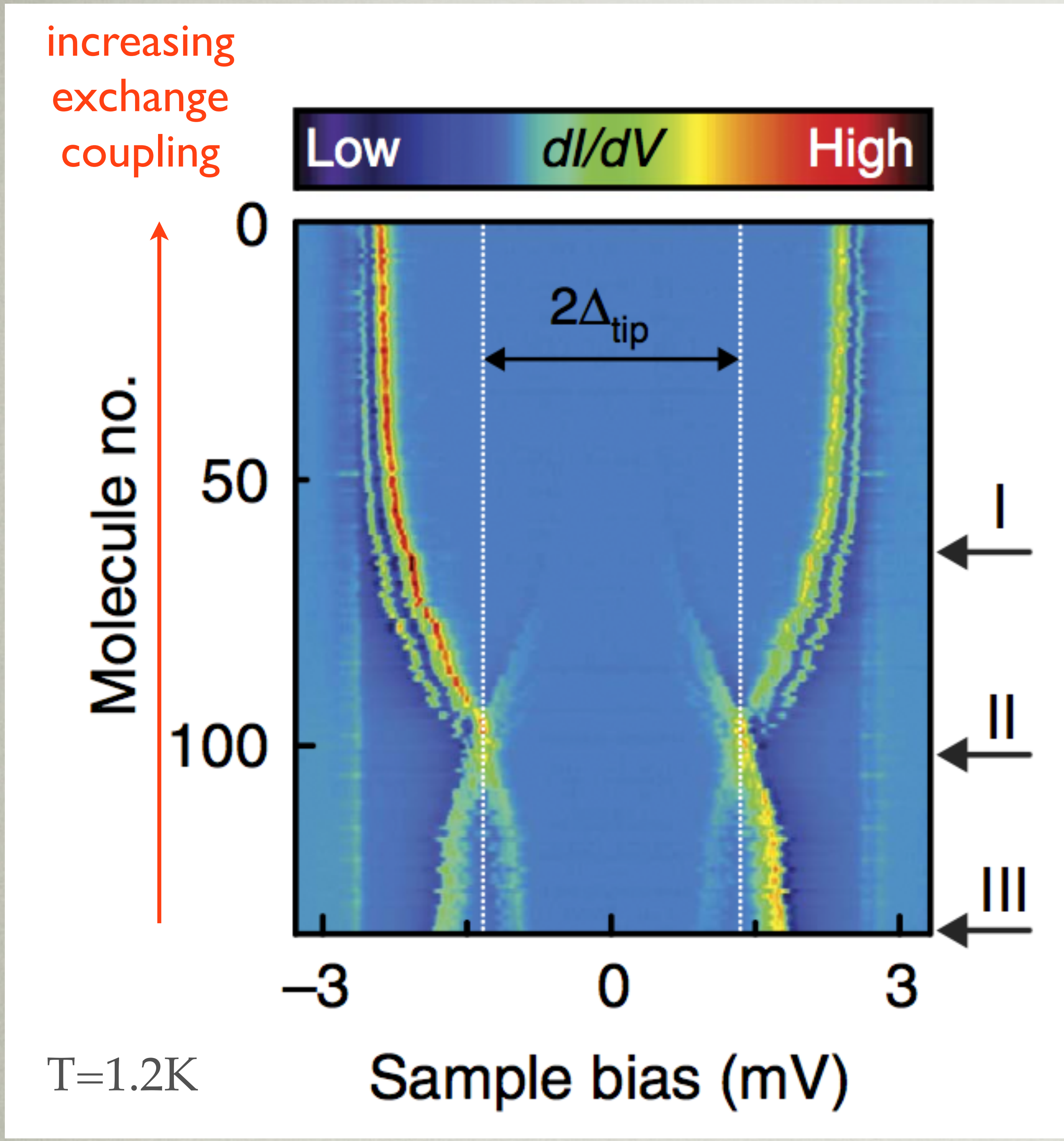
$$\frac{\Delta_c}{T_K} = 5.7$$

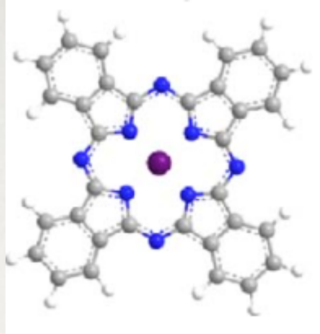




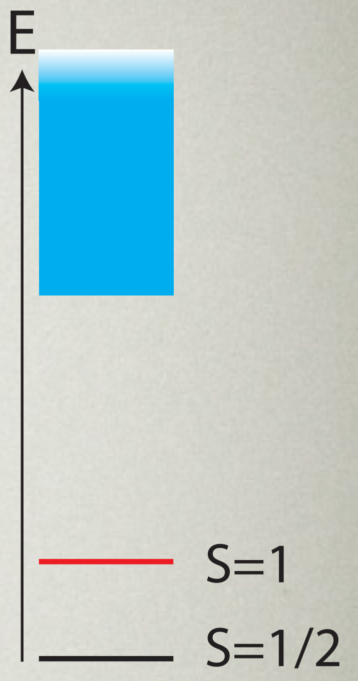
renormalized
from bare D

Žitko, Bodensiek, Pruschke (2011)



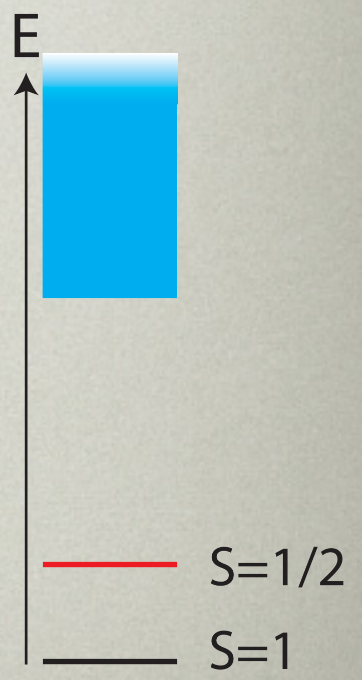


Kondo screened

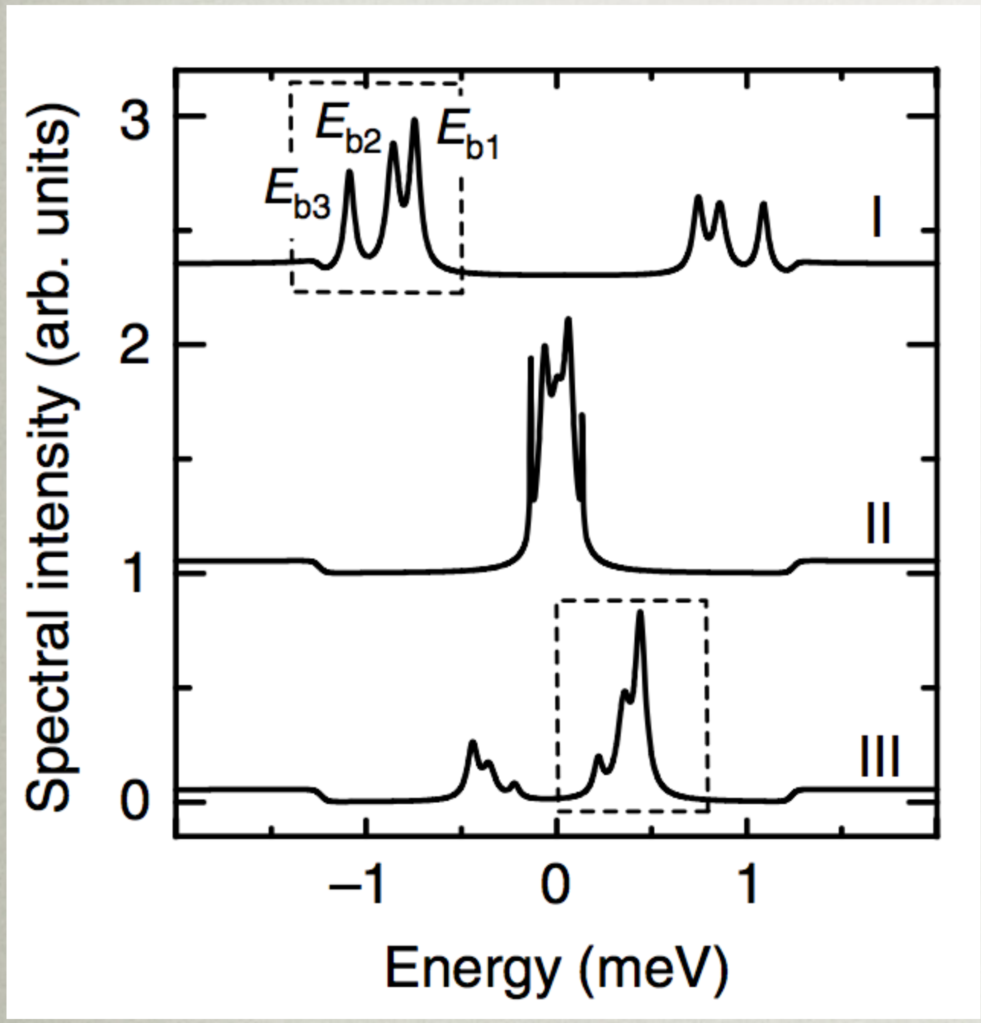


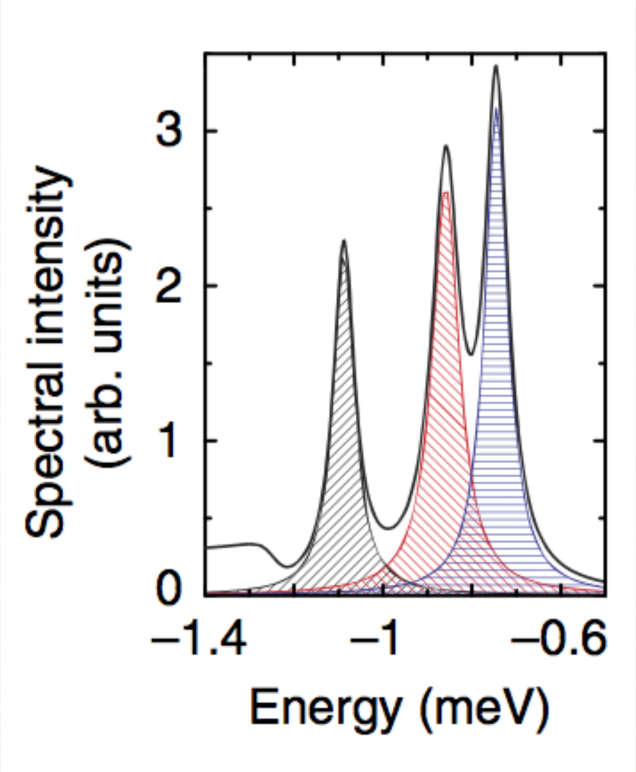
quantum
phase transition

free spin



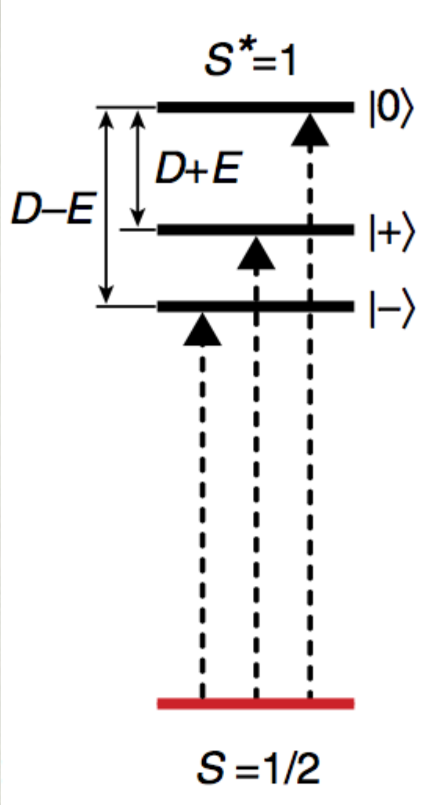
N. Hatter, B.W. Heinrich, M. Ruby, J. I. Pascual, K. J. Franke, Nat. Comm. 6:8988 (2015)

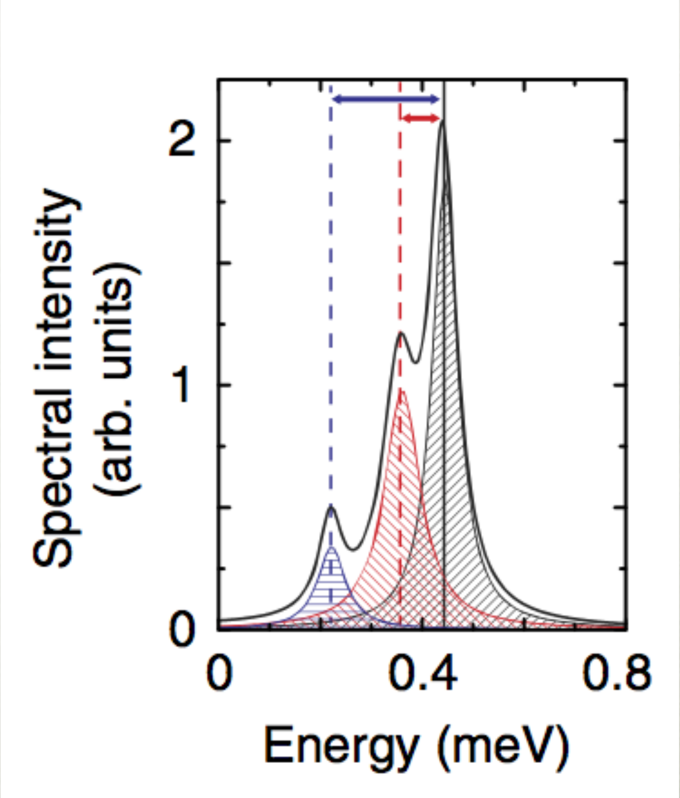




Kondo screened

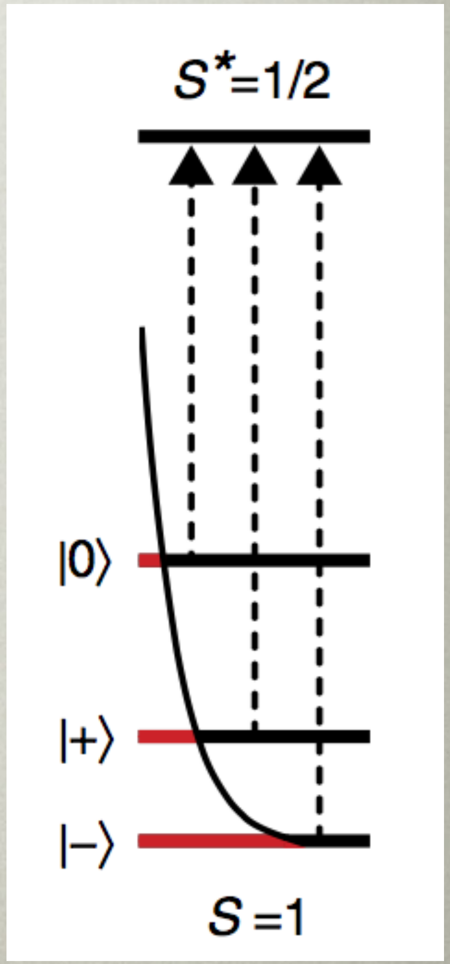
equal weights





free spin

Boltzmann distributed weights



N. Hatter, B.W. Heinrich, M. Ruby, J. I. Pascual, K. J. Franke, Nat. Comm. 6:8988 (2015)