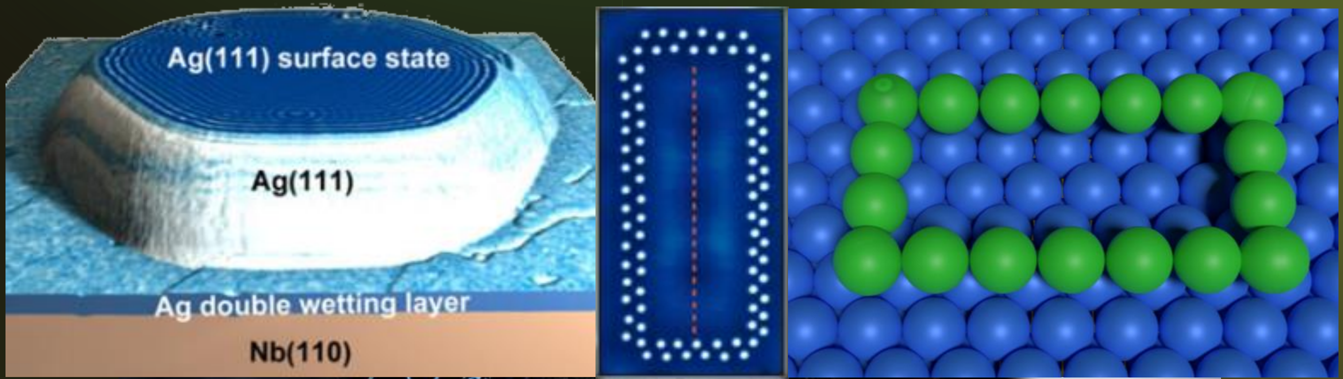
Artificial atomic structures on superconductors for engineering quantum states: Theoretical insights

THORE POSSKE

THE HAMBURG CENTRE FOR ULTRAFAST IMAGING

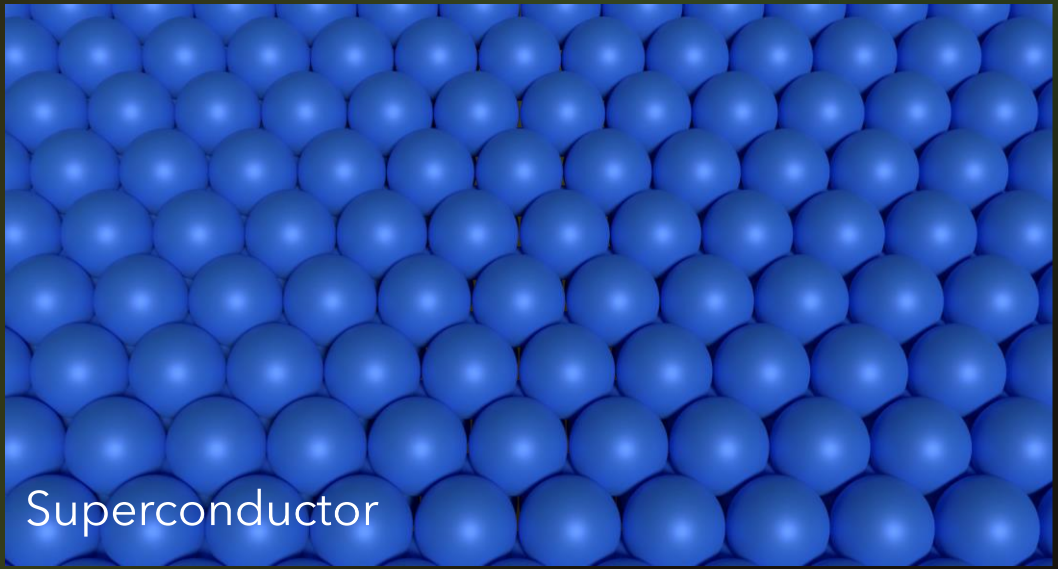
I INSTITUTE FOR THEORETICAL PHYSICS, UNIVERSITÄT HAMBURG

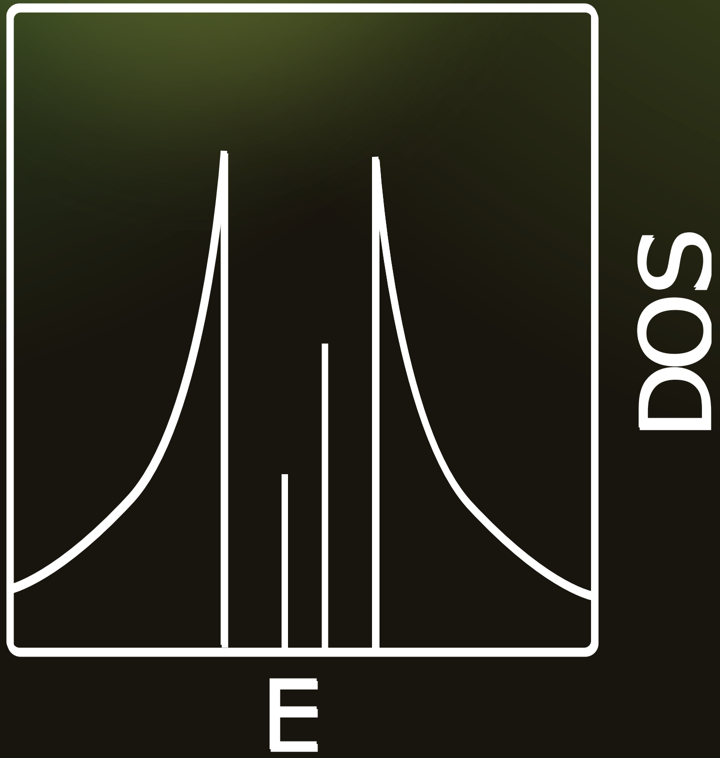


Superconductors as platform for engineering quantum states

Superconducting gap shields from electronic noise

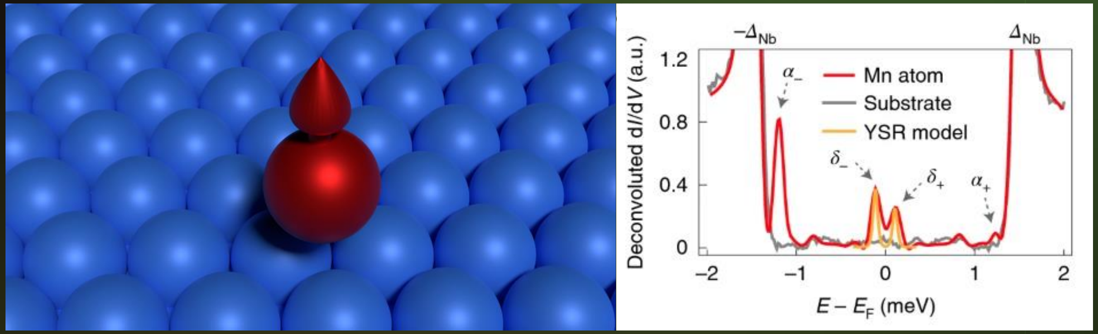
Atomically precise control by scanning tunneling microscopy





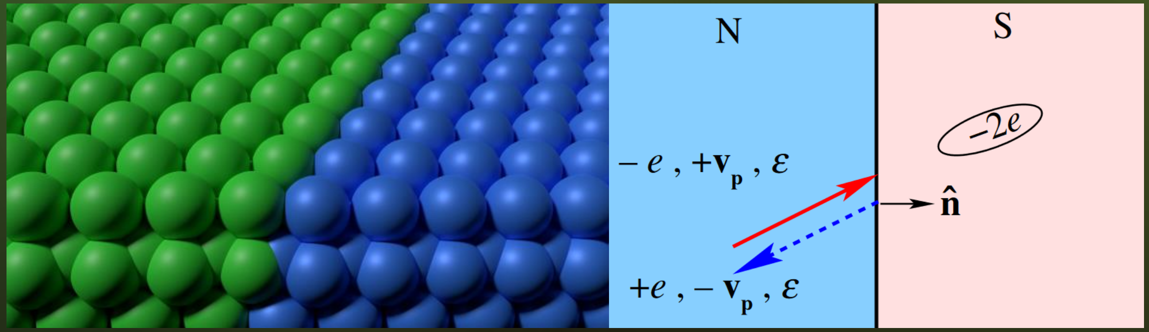
In gap states in superconductors

Yu-Shiba Rusinov states



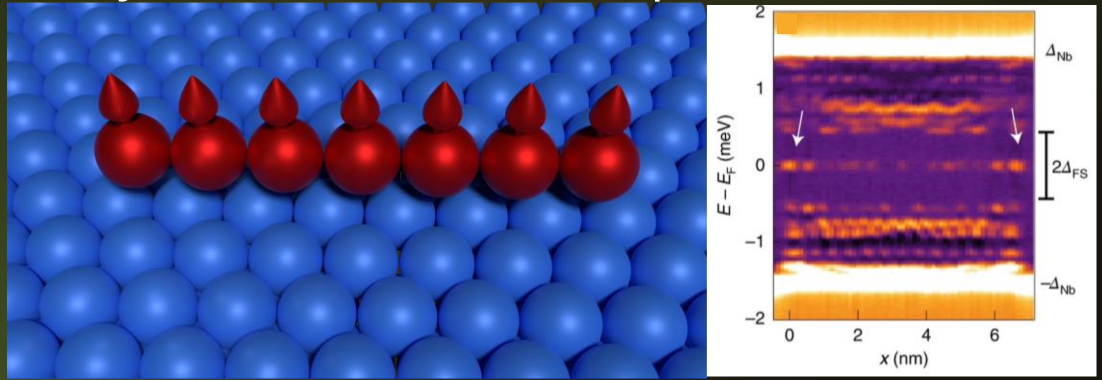
Schneider et al., *Nat. Nano* **17**, 384 (2022)

Andreev bound states



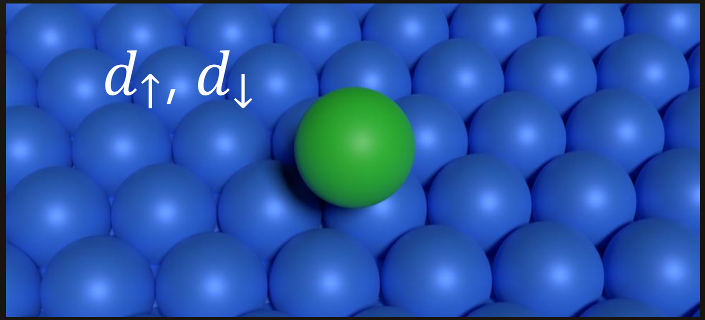
Sauls, Phil. Trans.R. Soc. **A376**, 20180140 (2018)

Majoranas and their precursors



Schneider et al., *Nat. Nano* **17**, 384 (2022)

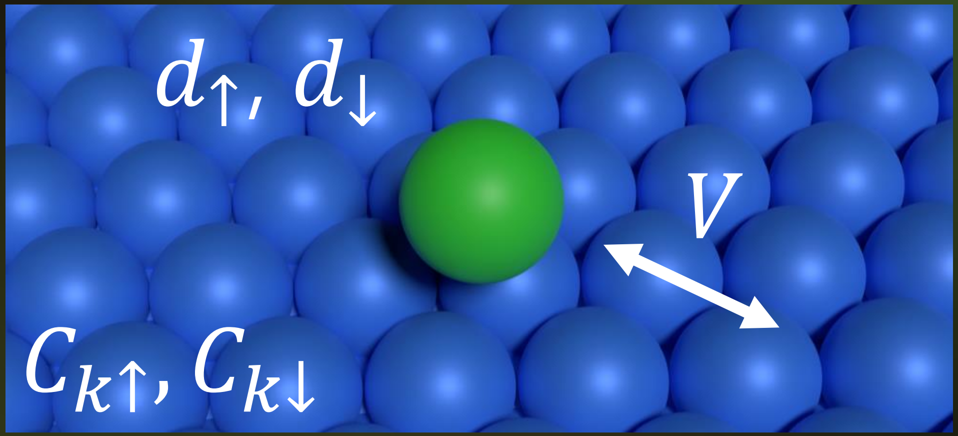
Machida-Shibata states



Schneider et al. arXiv:2212.00657 (2022)

Spin-degenerate level on a superconductor

Kazushige Machida, Fumiaki Shibata (1972)



$$\mathcal{H} = \sum_{k\sigma} \epsilon_k C^\dagger_{k\sigma} C_{k\sigma} - \Delta \sum_{k} (C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} + C_{-k\downarrow} C_{k\uparrow}) + \sum_{k\sigma} V_{kd} (C^\dagger_{k\sigma} d_\sigma + d_\sigma^\dagger C_{k\sigma}) + E \sum_{\sigma} n_{d\sigma}$$

Progress of Theoretical Physics, Vol. 47, No. 6, June 1972

Bound States Due to Resonance Scattering in Superconductor

Kazushige MACHIDA and Fumiaki SHIBATA

Department of Physics, Tokyo University of Education, Tokyo

(Received December 27, 1971)

It is shown exactly that the bound state in the energy gap of superconductors is produced by the resonance scattering due to a single non-magnetic impurity.

In an appropriate renormalization procedure, we can show the growth of an impurity band in the case of impurities of finite concentration and a possibility for gapless superconductivity is indicated.

Exact solution

$$\omega^2 \left(1 + \frac{2\Gamma}{\sqrt{\Delta^2 - \omega^2}}\right) = E^2 + \Gamma^2$$

$$\Gamma = V^2 \pi \times SC\ Density\ of\ states$$

Where is the in-gap state?

Hybridization Γ much larger than superconducting gap Δ. $\Gamma \approx 100 - 1000\,\Delta$

$$\omega^2\left(1+\frac{2\Gamma}{\sqrt{\Delta^2-\omega^2}}\right)=E^2+\Gamma^2$$

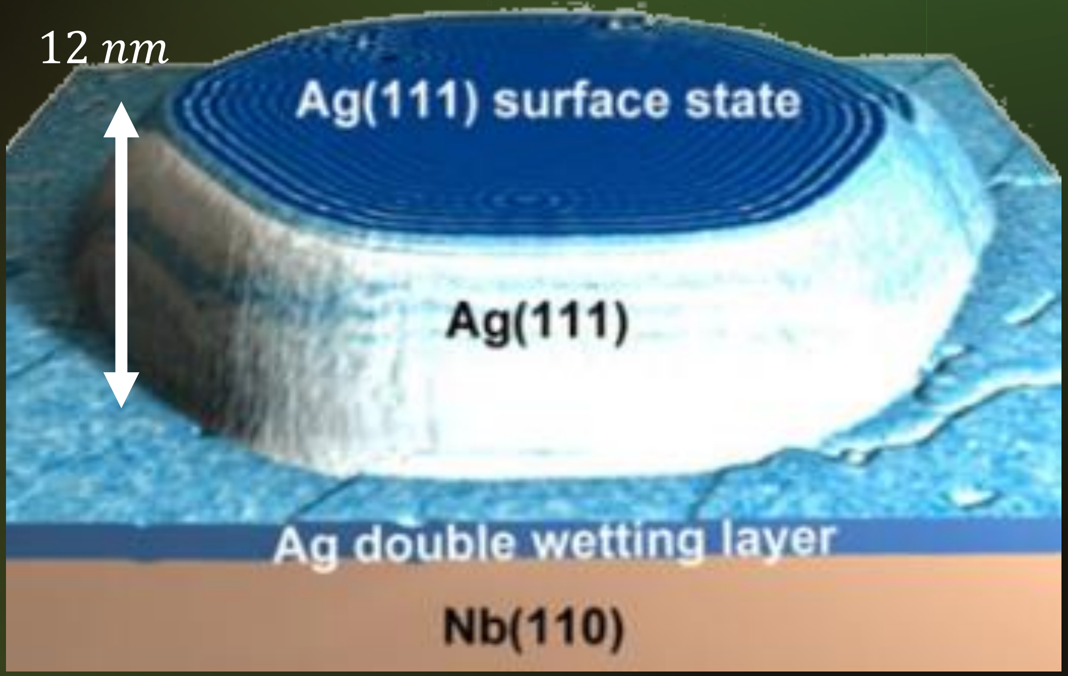
$$\omega \approx \Delta$$

“ In most physical situations […] the bound state lies essentially at the gap edge. […] Shiba […] concluded […] that they] can be neglected in discussion of physical properties.

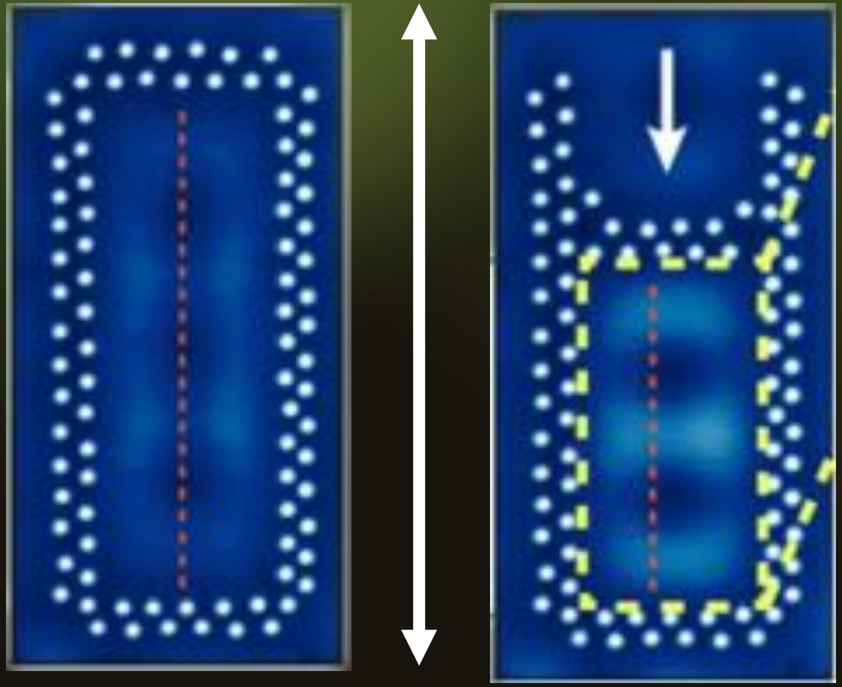
A. V. Balatsky, I. Vekhter, and Jian-Xin Zhu
Rev. Mod. Phys. **78**, 373 (2006)

Experimental setup for Machida-Shibata states

$12\ nm$



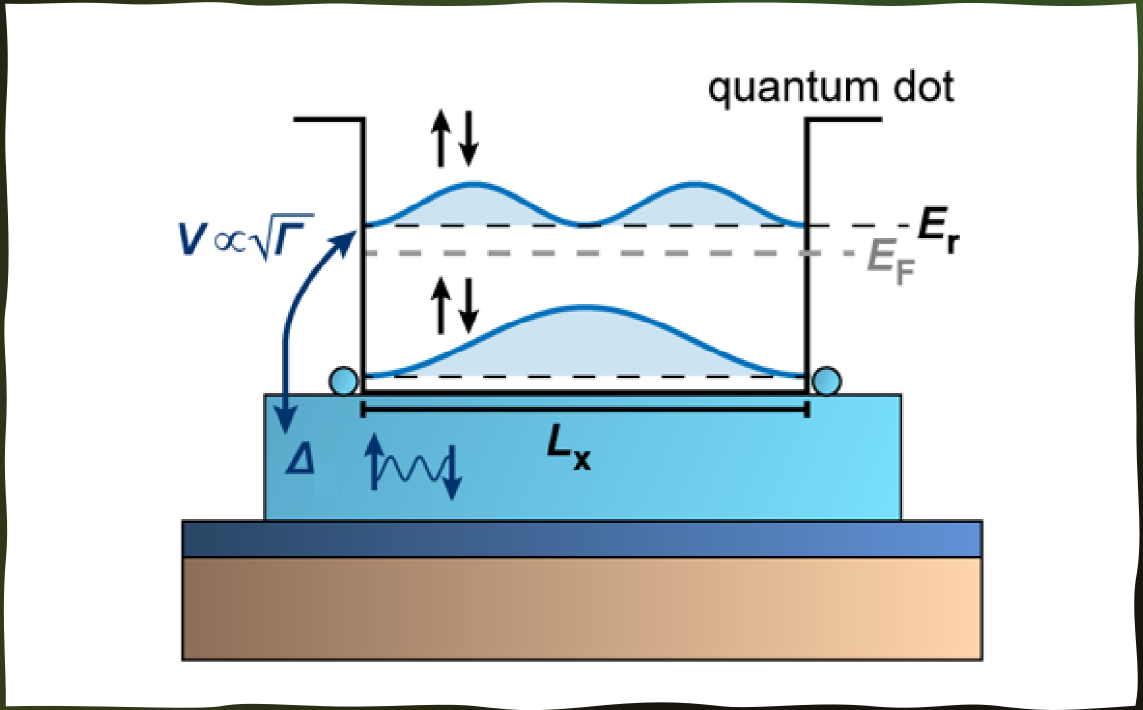
$24\ nm$



$\Delta_{Nb} = 1.50\ meV$
$\Delta = 1.35\ meV$

Schneider et al. arXiv:2212.00657 (2022)

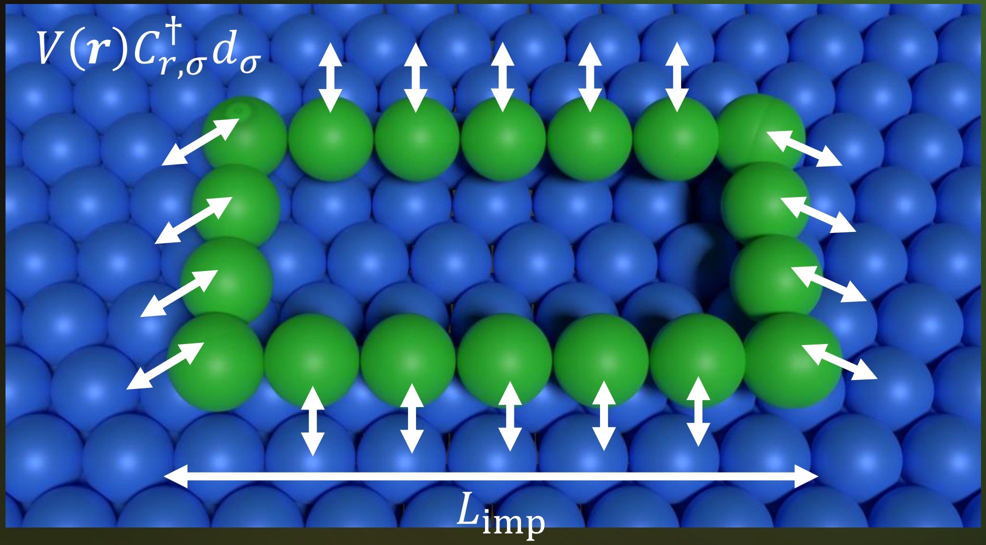
Experimental setup for Machida-Shibata states



1) Particle-in-a-box state couples to superconductor only close to boundary
2) Capacitive screening by superconductor
3) Energy tunable by quantum dot length

Schneider et al. arXiv:2212.00657 (2022)

Model of extended impurity



$$\mathcal{H}_{coupling} = \sum_{\mathbf{k},\sigma} V(\mathbf{k})C^{\dagger}_{\mathbf{k},\sigma}d_{\sigma} + h.c.$$

Solve Green's functions equation of motions

$$G_{d_\sigma,d_\sigma^\dagger}(\omega) = \frac{\omega + E_{\mathrm{r}} + \sum_{\mathbf{k}} |V(\mathbf{k})|^2 \frac{(\omega-\epsilon_{\mathbf{k}})}{(\omega^2-\epsilon_{\mathbf{k}}{}^2-\Delta_{\mathrm{s}}{}^2)}}{\left(\omega + E_{\mathrm{r}} - \sum_{\mathbf{k}} \frac{|V(\mathbf{k})|^2(\omega-\epsilon_{\mathbf{k}})}{(\omega^2-\epsilon_{\mathbf{k}}{}^2-\Delta_{\mathrm{s}}{}^2)}\right)\left(\omega - E_{\mathrm{r}} - \sum_{\mathbf{k}} \frac{|V(\mathbf{k})|^2(\omega+\epsilon_{\mathbf{k}})}{(\omega^2-\epsilon_{\mathbf{k}}{}^2-\Delta_{\mathrm{s}}{}^2)}\right) - \left(\sum_{\mathbf{k}} \frac{\Delta_s V(\mathbf{k})^2}{(\omega^2-\epsilon_{\mathbf{k}}{}^2-\Delta_{\mathrm{s}}{}^2)}\right)\left(\sum_{\mathbf{k}} \frac{\Delta_s V(\mathbf{k})^{*2}}{(\omega^2-\epsilon_{\mathbf{k}}{}^2-\Delta_{\mathrm{s}}{}^2)}\right)}$$

Localized or delocalized impurity?

$V(\mathbf{k}) = \boldsymbol{const}.$ within $k \approx \pm 1/L_{imp}$

Induced superconducting coherence length

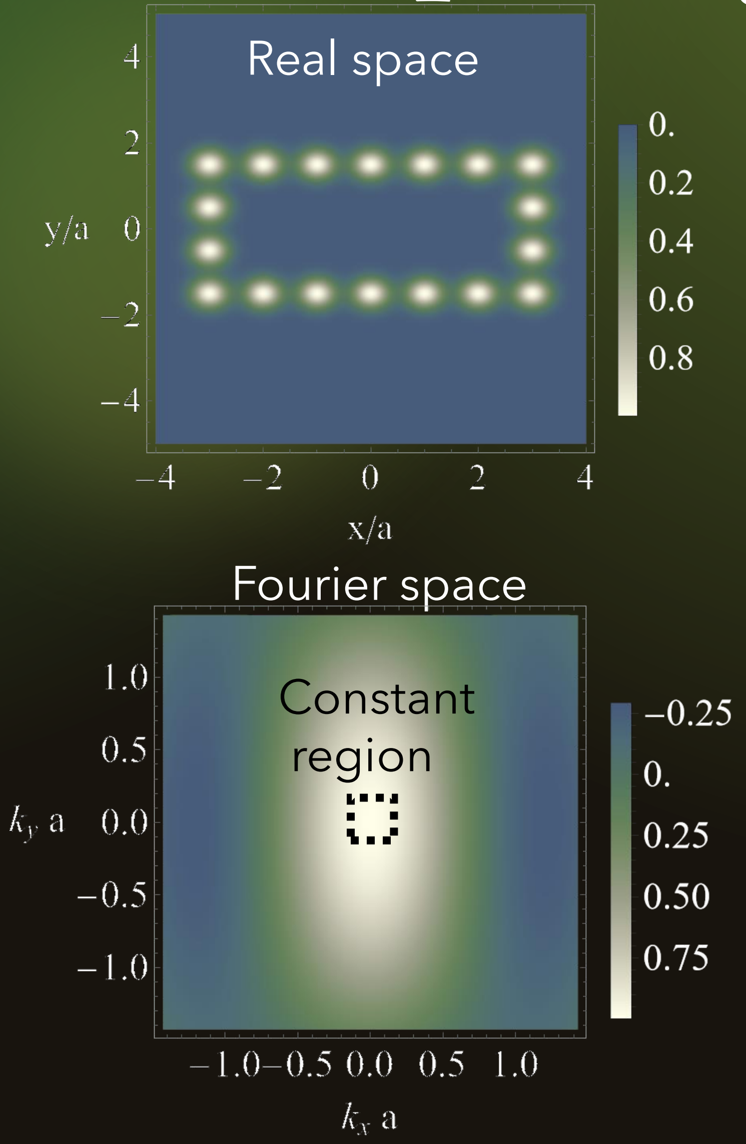
$$\xi_{Ag} = \frac{v_F}{\Delta} = 253 \ - 789\, nm$$

Impurity localized if

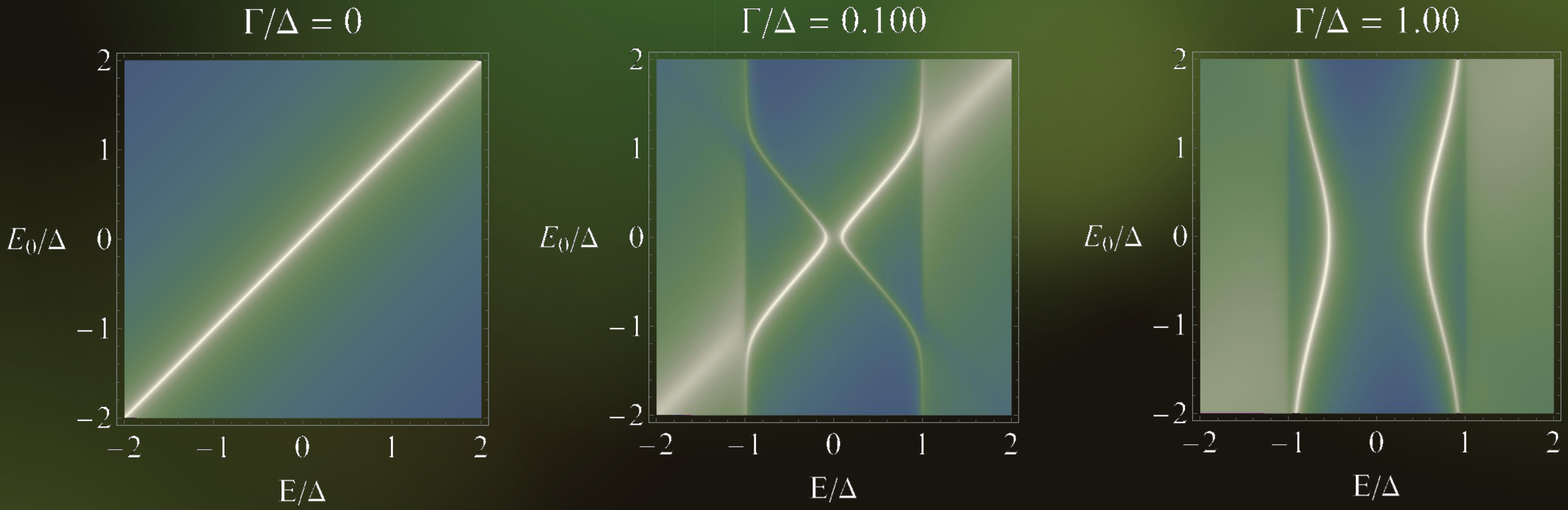
$$L_{imp} = 24\, nm \ll \xi_{Ag}$$

$$\mathrm{DOS}(E) = -\frac{1}{\pi}\mathrm{Im}\left[\frac{\omega + E_\mathrm{r} + \frac{\Gamma\omega}{\sqrt{{\Delta_\mathrm{s}}^2 - \omega^2}}}{\omega^2\left(1 + \frac{2\Gamma}{\sqrt{{\Delta_\mathrm{s}}^2 - \omega^2}}\right) - {E_\mathrm{r}}^2 - \Gamma^2}\right]$$

Villas, A. *et al. Phys. Rev. B* **101**, 235445 (2020).



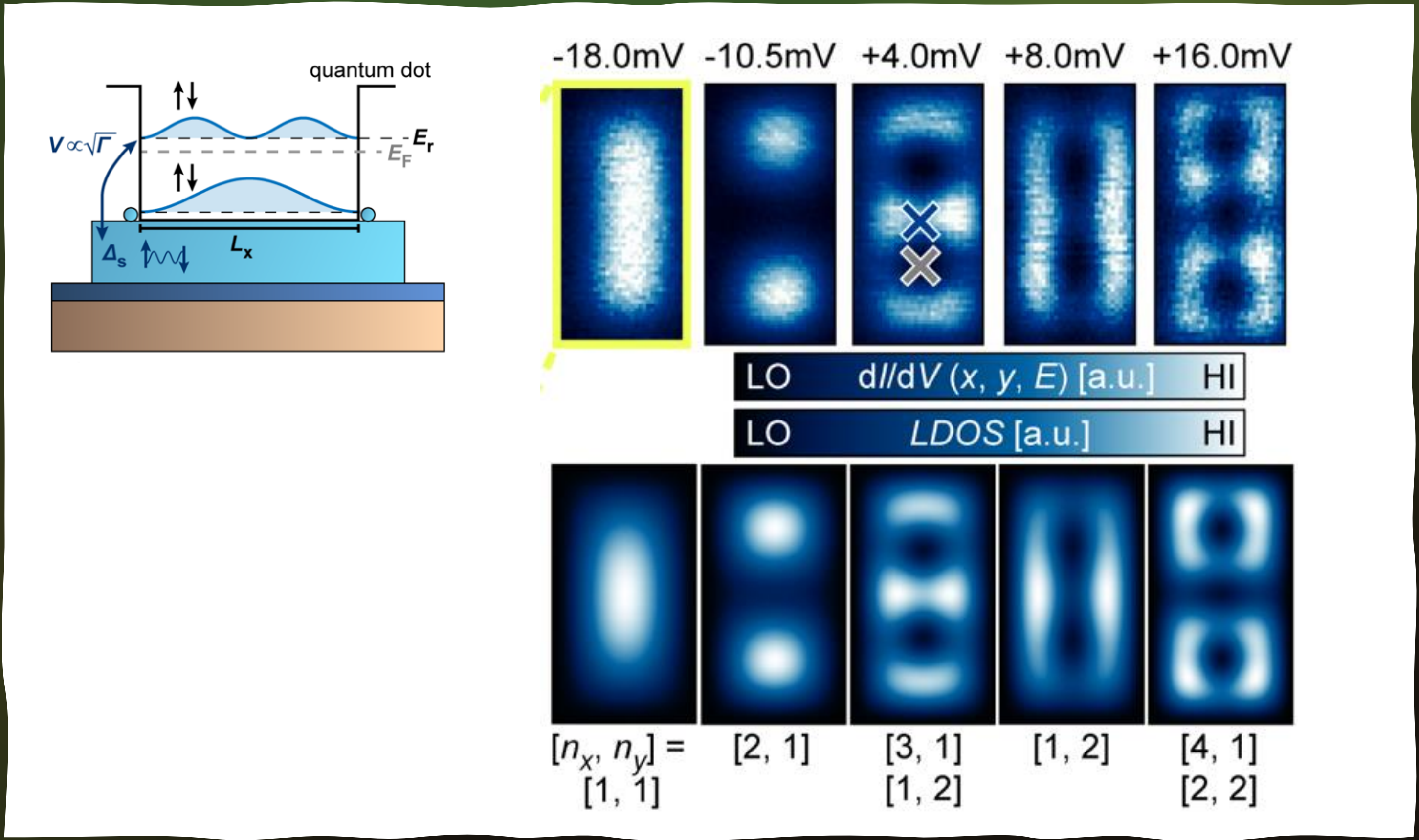
DOS of a localized impurity



$$\mathscr{H} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} C^{\dagger}_{\boldsymbol{k}\sigma} C_{\boldsymbol{k}\sigma} - \Delta \sum_{\boldsymbol{k}} (C^{\dagger}_{\boldsymbol{k}\uparrow} C^{\dagger}_{-\boldsymbol{k}\downarrow} + C_{-\boldsymbol{k}\downarrow} C_{\boldsymbol{k}\uparrow}) + \sum_{\boldsymbol{k}\sigma} V_{\boldsymbol{k}d} (C^{\dagger}_{\boldsymbol{k}\sigma} d_{\sigma} + d_{\sigma}^{\dagger} C_{\boldsymbol{k}\sigma}) + E \sum_{\sigma} n_{d\sigma}$$

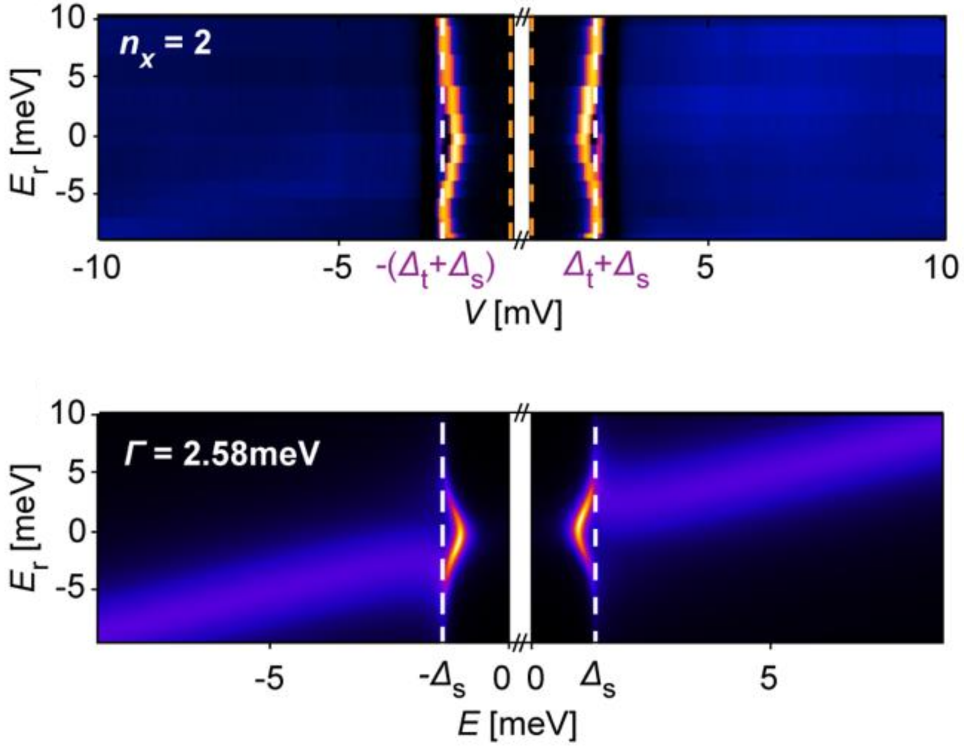
$$\Gamma = V^2 \pi \times SC\ Density\ of\ states$$

Measurements

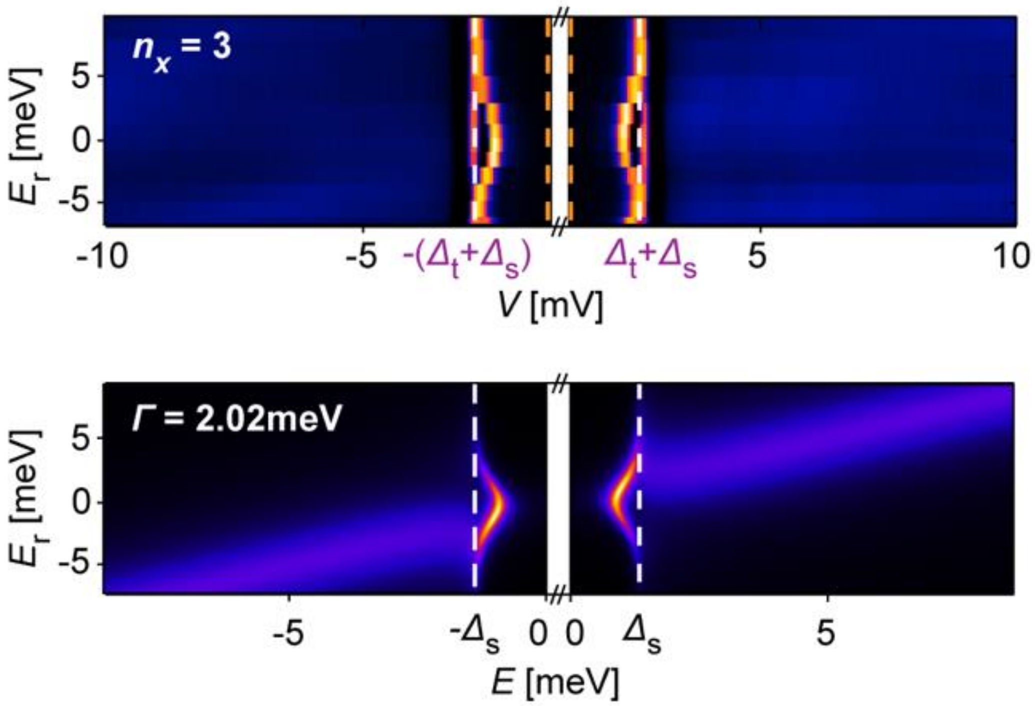


Measurements

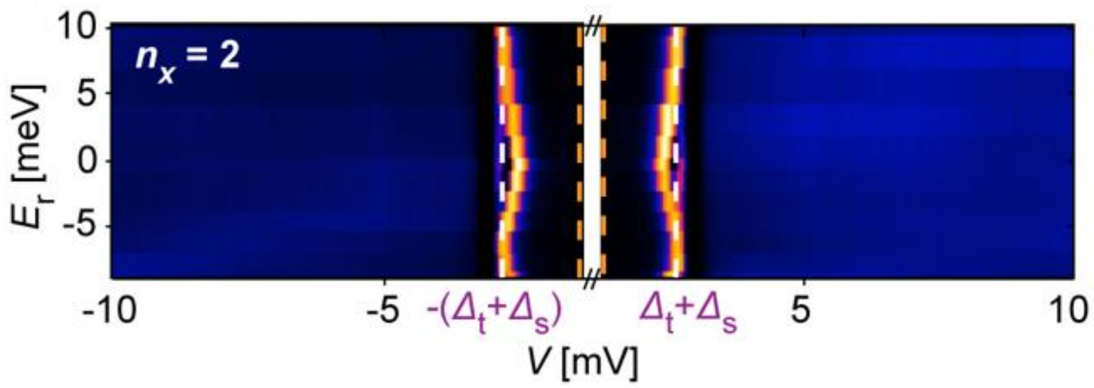
$n_x = 2$

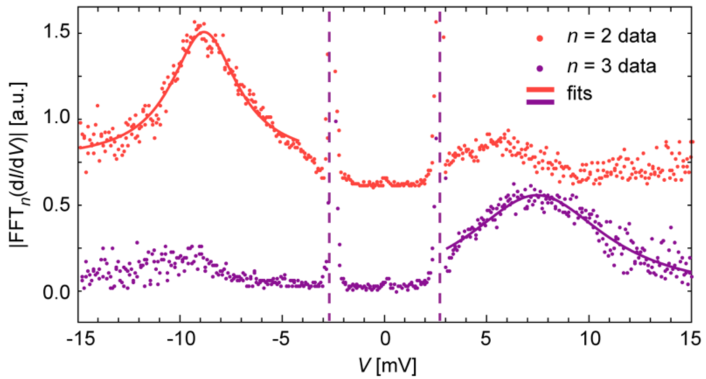


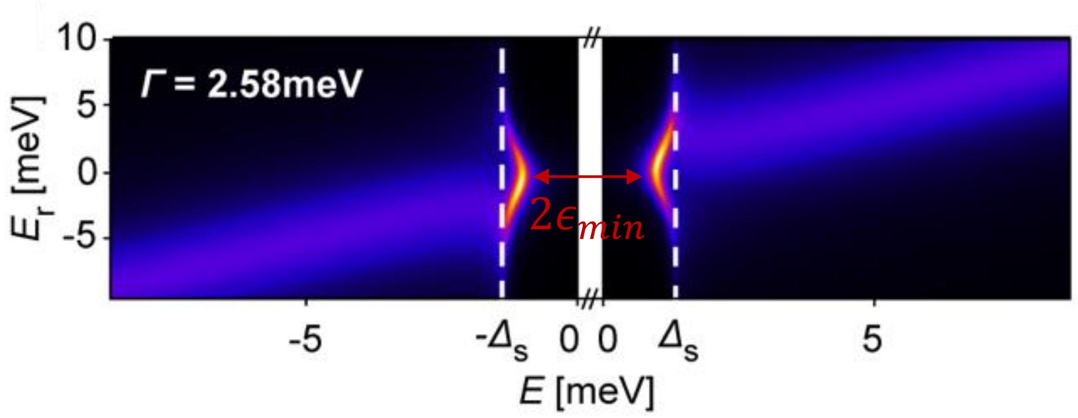
$n_x = 3$

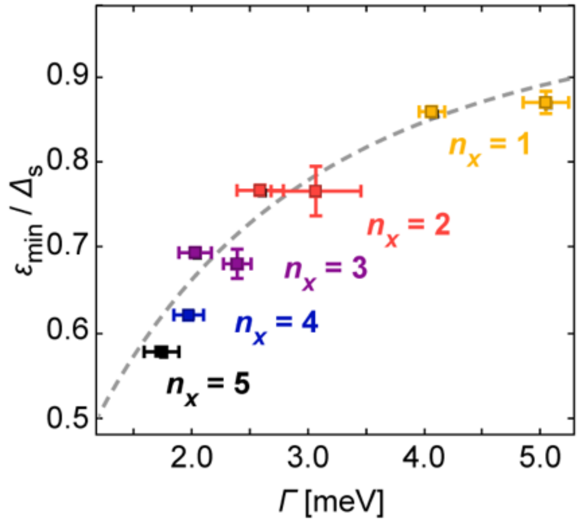


Measurements

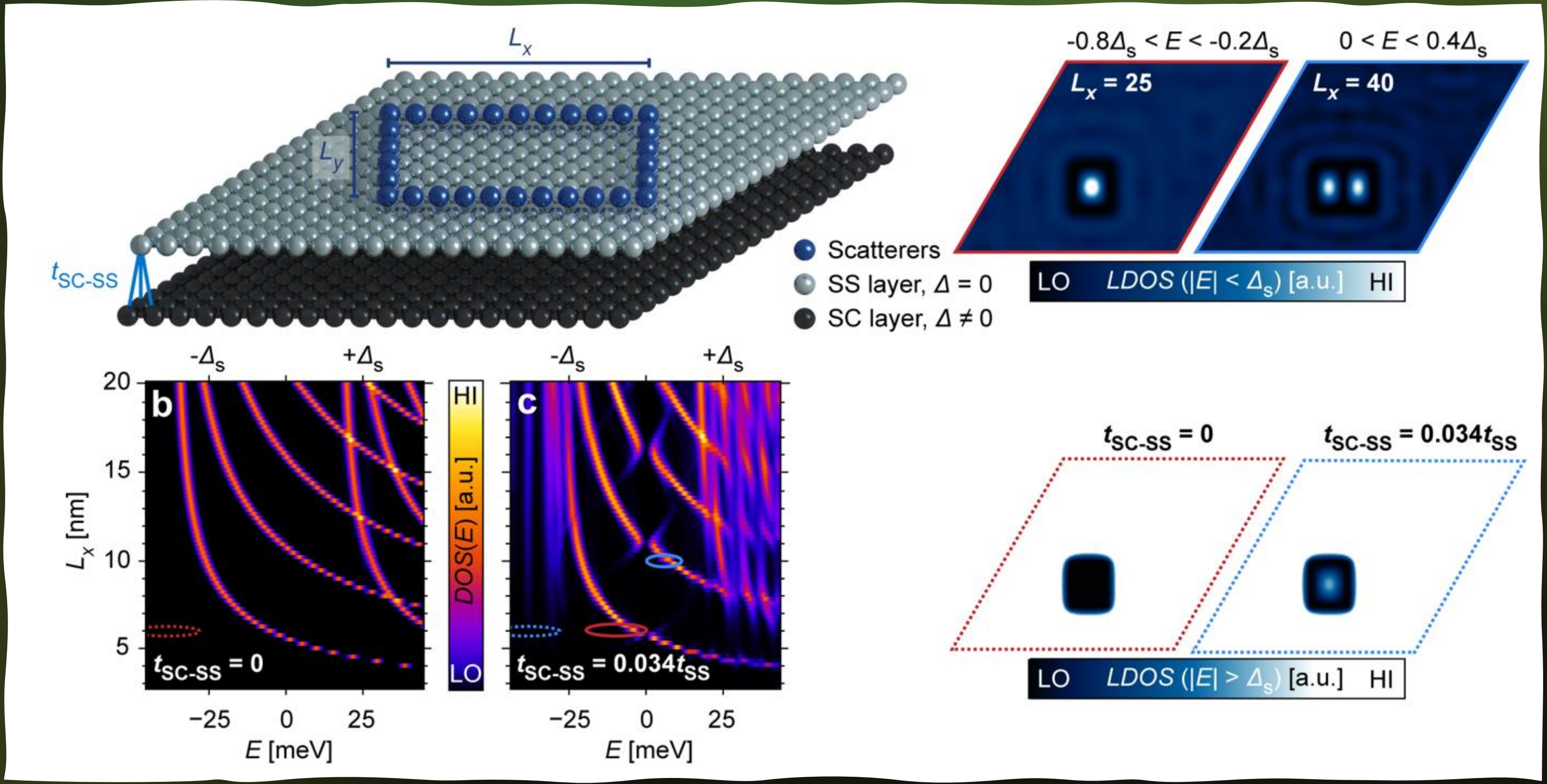






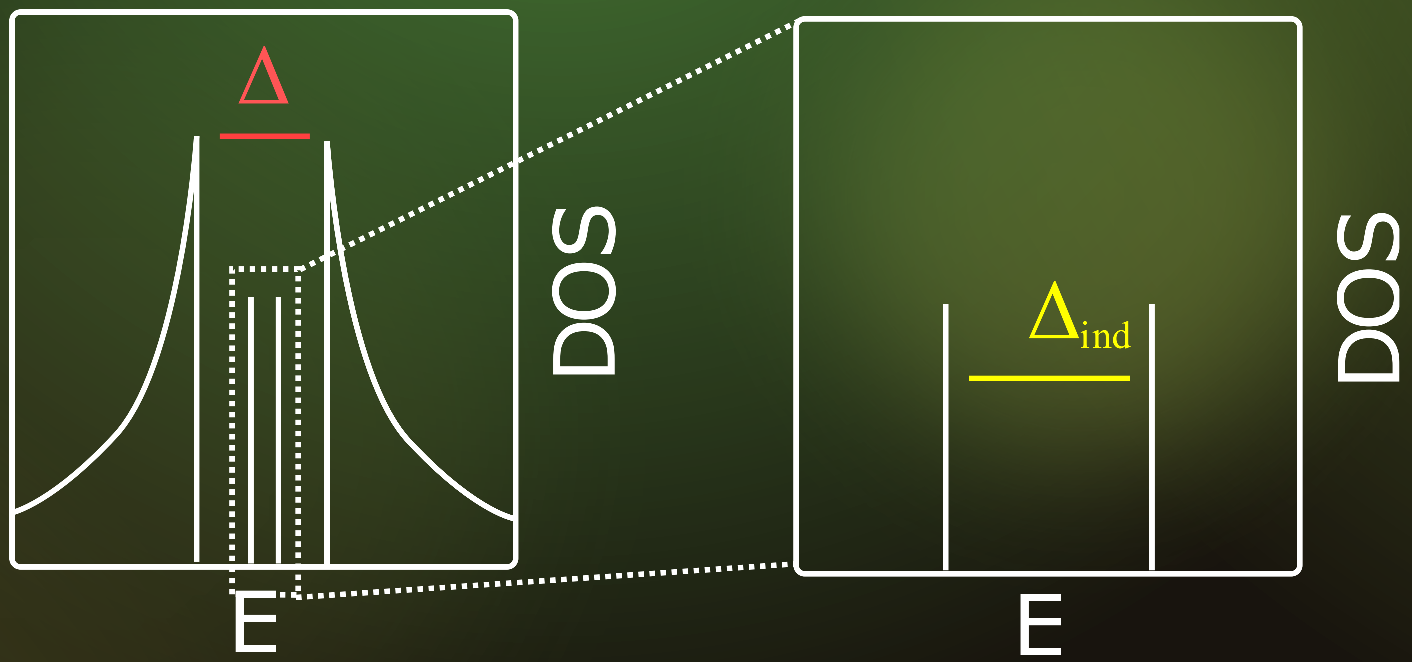


Tight binding model for MS states



Schneider et al. arXiv:2212.00657 (2022)

Single level superconductivity



Low energy theory
(Schrieffer-Wolff)

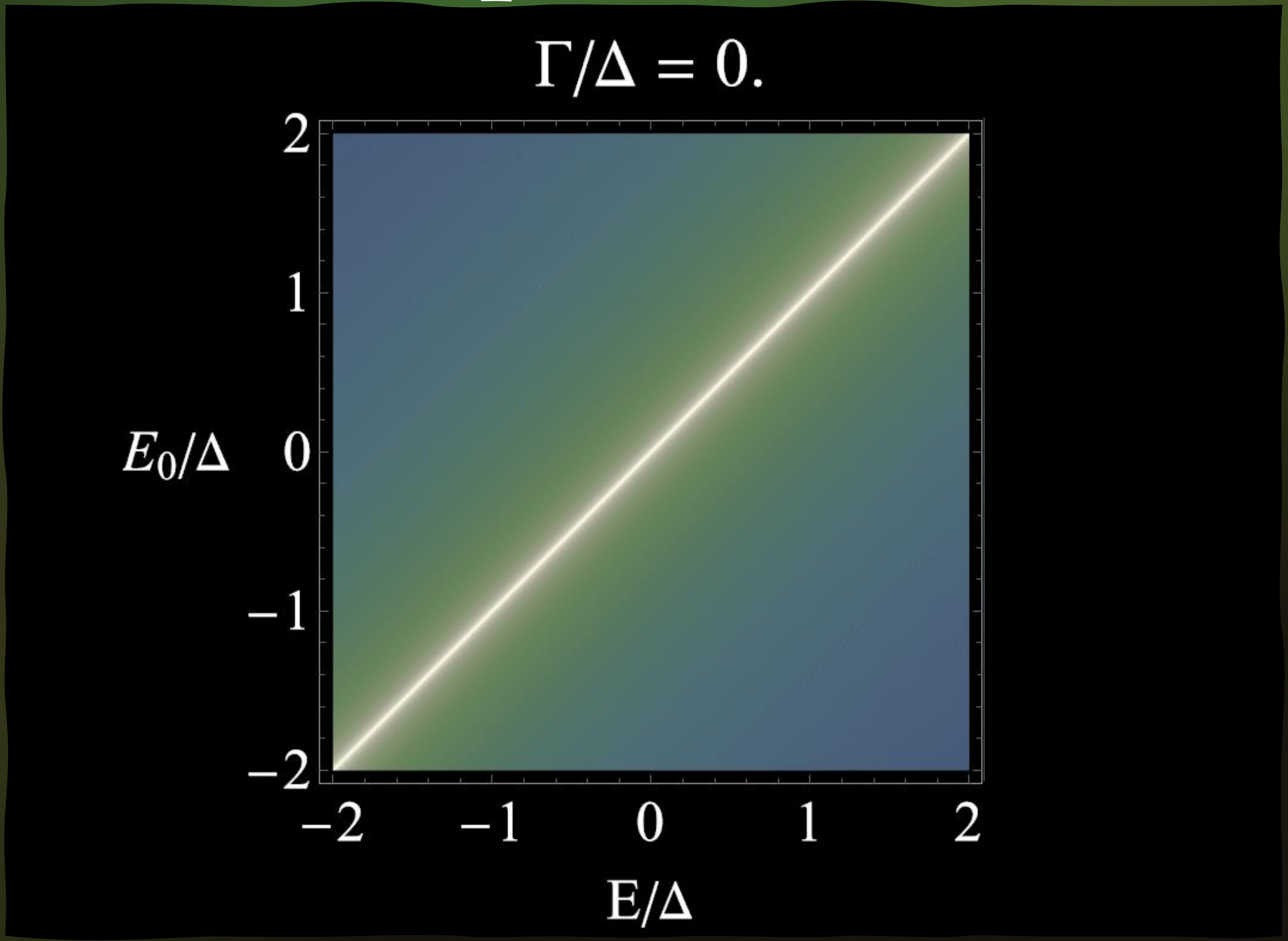
$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} V\left(c^\dagger_{k,\sigma} d_\sigma + d^\dagger_\sigma c_{k,\sigma}\right) + \sum_\sigma E_0 d^\dagger_\sigma d_\sigma - \Delta_{\mathrm{s}} \sum_k \left(c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} + c_{-k,\downarrow} c_{k,\uparrow}\right)$$

$$\mathcal{H}'_{\mathrm{D}} = \sum_\sigma (E_{\mathrm{r}} + E_{\mathrm{shift}}) d^\dagger_\sigma d_\sigma - (\Delta_{\mathrm{ind}} d_\uparrow d_\downarrow + \mathrm{h.c.})$$

$$\Delta_{\mathrm{ind}} \lesssim \Gamma \frac{\Delta_{\mathrm{s}}}{\sqrt{\Delta_{\mathrm{s}}^2 - E_0^2}}$$

$$E_{\mathrm{shift}} = E_{\mathrm{r}} \frac{\Delta_{\mathrm{ind}}}{\Delta_{\mathrm{s}}}$$

Single level superconductivity



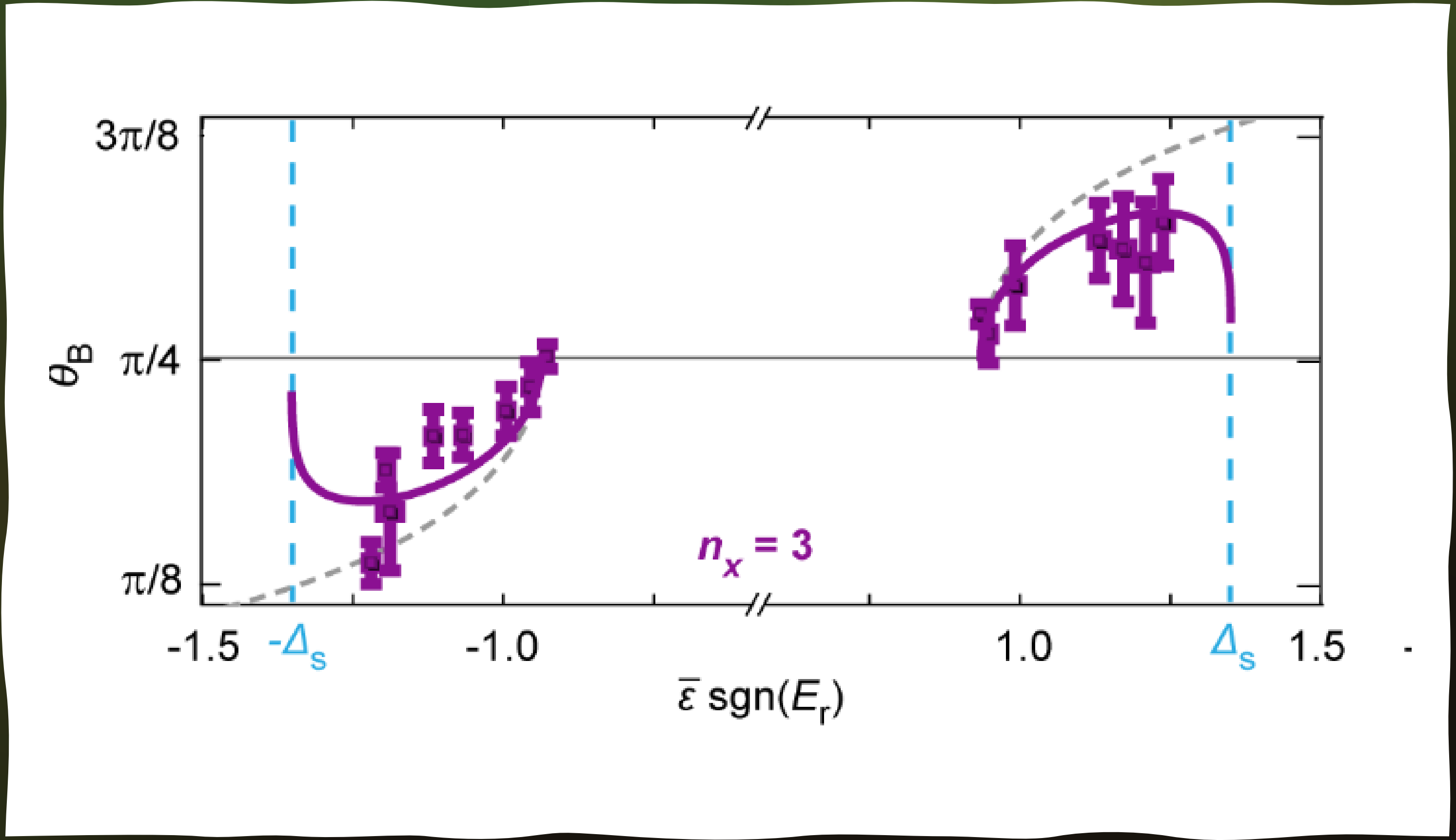
Single level superconductivity details

MSS energies: $\varepsilon = \pm\sqrt{{E_\mathrm{r}}^2(1-\Delta_\mathrm{ind}/\Delta_\mathrm{s})^2+{\Delta_\mathrm{ind}}^2}$

Particle-hole weight: $|v|^2 = \frac{1}{2} - \frac{E_\mathrm{r}\left(1-\frac{\Delta_\mathrm{ind}}{\Delta_\mathrm{s}}\right)}{2\varepsilon}$ $|u|^2 = 1 - |v|^2$

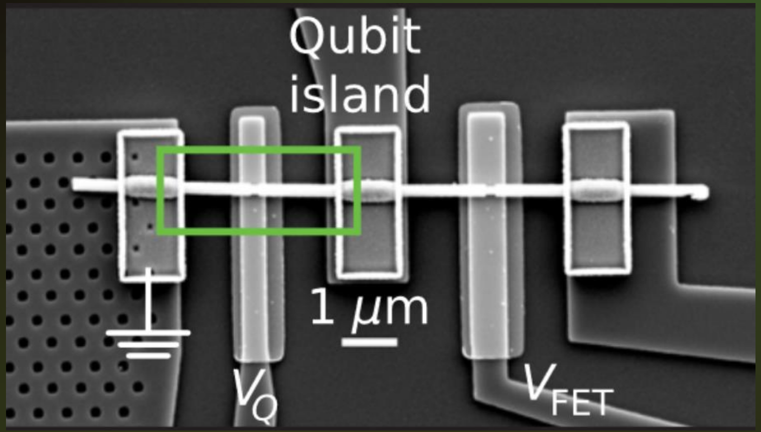
Bogoliubov mixing angle: $\theta_\mathrm{B}(\varepsilon) = \mathrm{ArcTan}\left(\sqrt{|u|^2/|v|^2}\right)$

Low energy theory validity regime

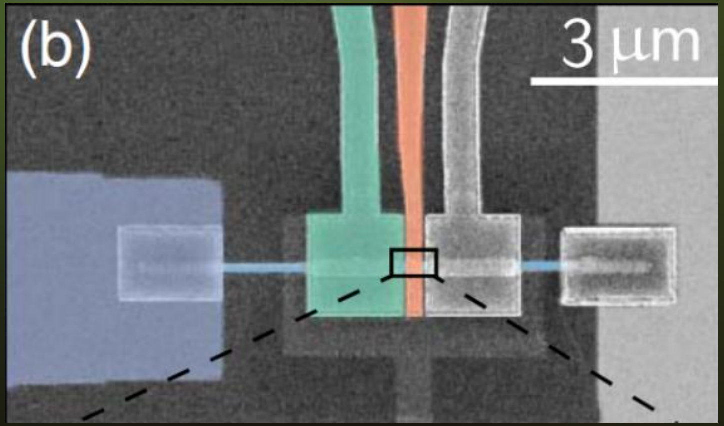


Schneider et al. arXiv:2212.00657 (2022)

Using Machida-Shibata states in transmon/gatemon qubits?



Kringhøj et al. PRL **124**, 246803 (2020)

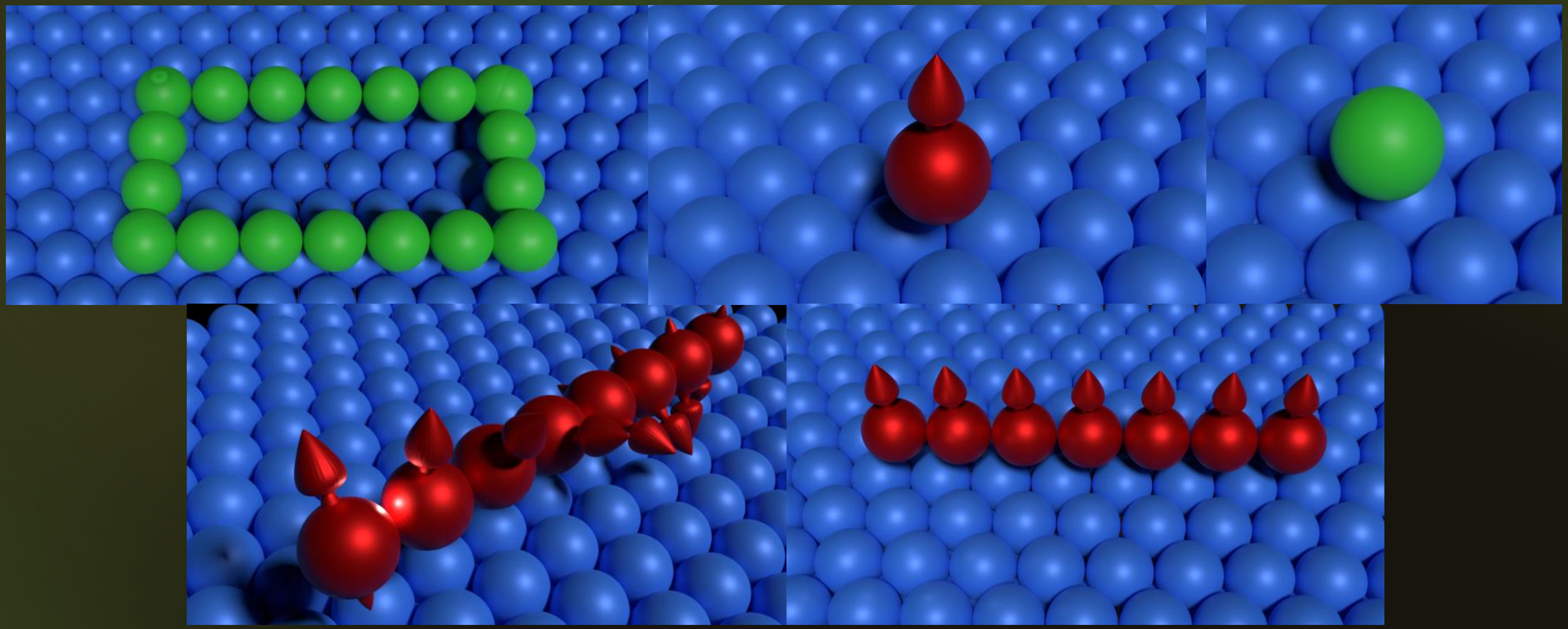


Bargerbos et al. Phys. Rev. Lett. 124, 24680 (2020)

Suggested suppressed voltage noise and strong anharmonicity

Outlook: Lego kit of in-gap states?

Combination of Machida-Shibata, Yu-Shiba-Rusinov, and Majorana zero modes for versatile 2D quantum matter



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- Lucas Schneider (UHH)
- Khai That Ton
- **Ioannis Ioannidis (UHH)**
- **Jannis Neuhaus-Steinmetz (UHH)**

Thank you!

Kazushige Machida

"I thought for long time that transition metal non-magnetic impurities produce the in-gap state, but the location of it is so near the superconducting gap edge, thus it is impossible to prove
its existence. But by your ingenious method you have finally checked it to be true experimentally.
[…]
I hope that this time reversal preserving Machida-Shibata state turns out to be of some use for the future as application or fundamental physics."

Summary

- The Machida-Shibata state adds to the existing subgap quantum states in a superconductor
- Spin-degeneracy and low-linewidth inside the gap are generic features useful for applications in quantum techonolgies
- Atomic design of 2D quantum matter on superconductors comes closer