Title: Automated Characterization of Engineered Quantum Materials

Speakers: Eliska Greplova

Collection: Machine Learning for Quantum Many-Body Systems

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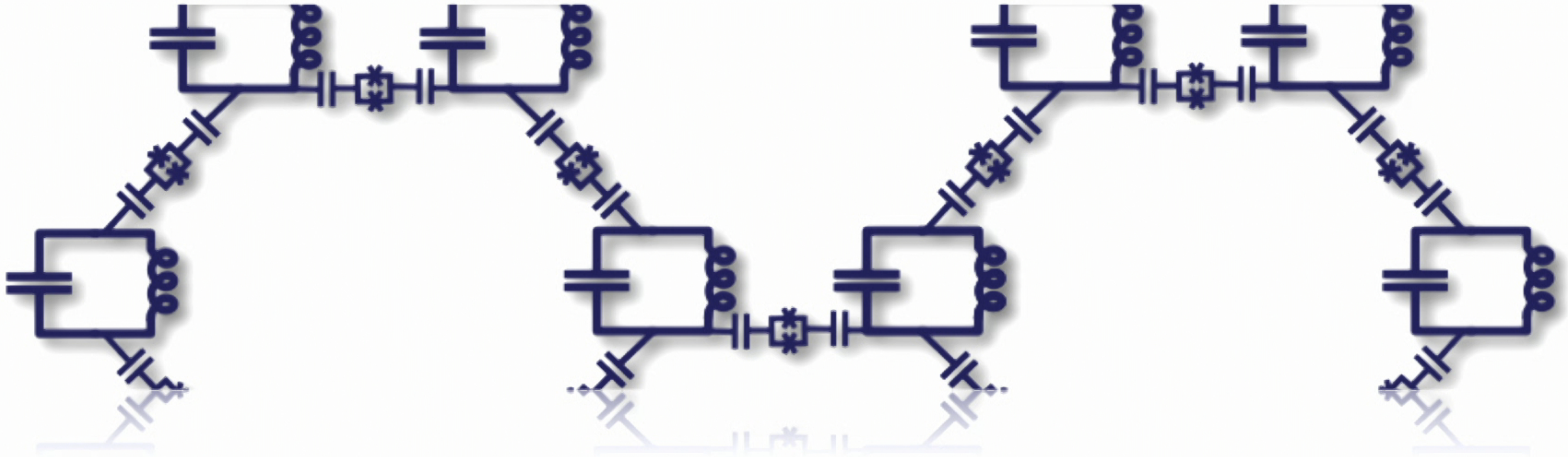

Automated Characterization of Engineered Quantum Materials

Eliska Greplova, **Rouven Koch, Jozef Bucko**, David van Driel, Alberto Bordin, Frank Schäfer, Jose Lado,
Annika Kurzmann, Rebekka Garreis, Chuyao Tong, Frantisek Herman,Thomas Ihn.

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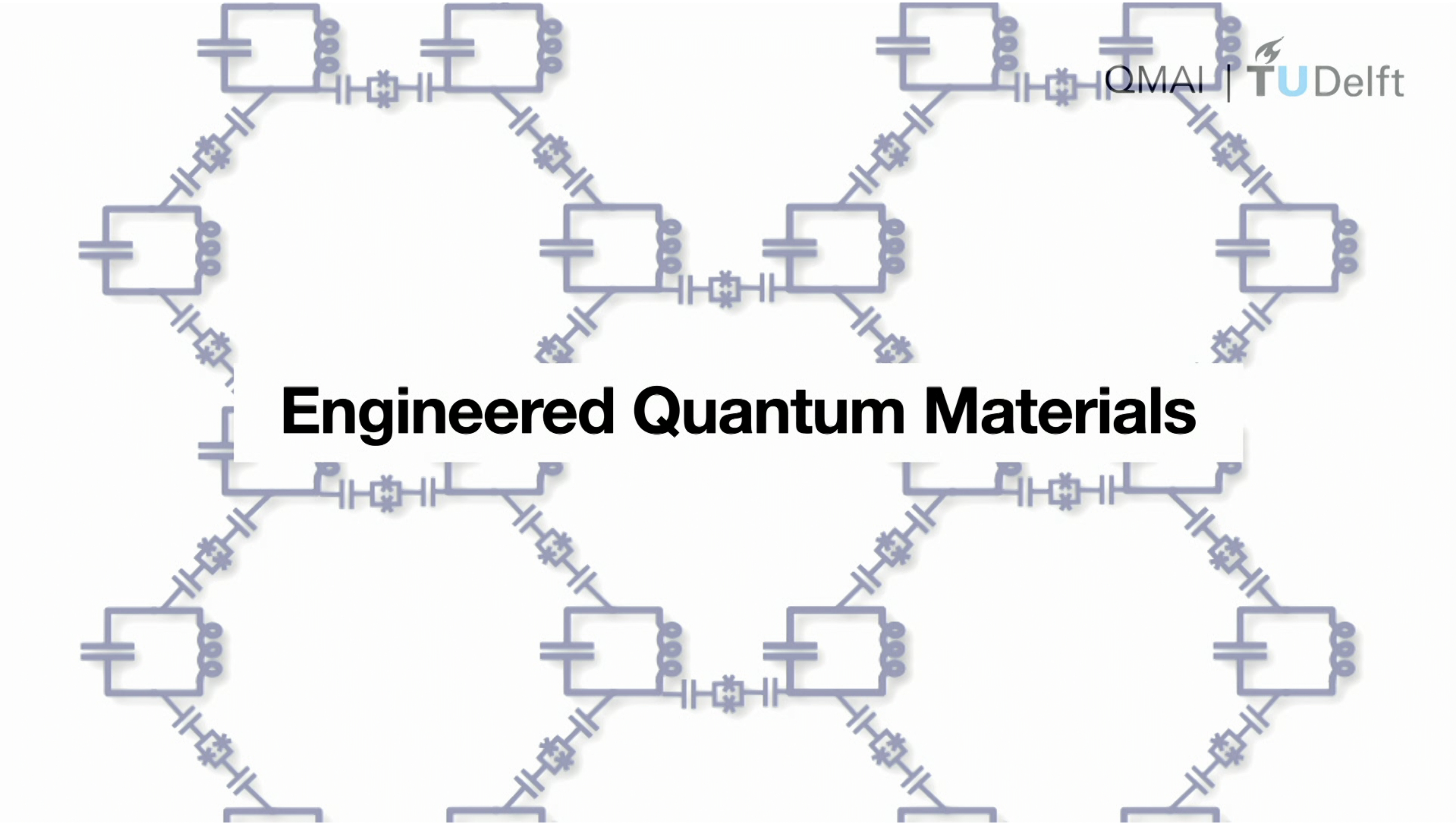
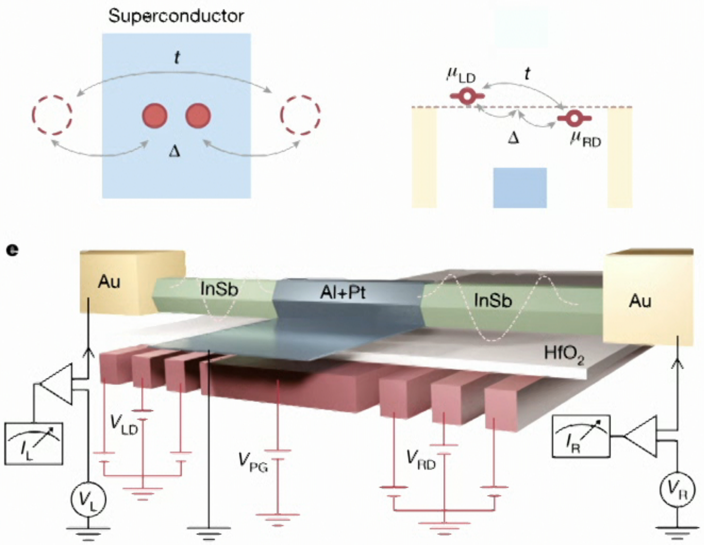


Engineered Quantum Materials

Kitaev Chain



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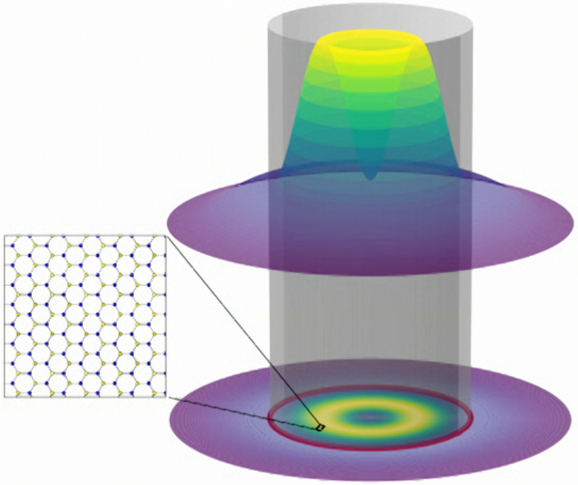
Dvir, T., Wang, G., van Loo, N. *et al.* Realization of a minimal Kitaev chain in coupled quantum dots. *Nature* **614**, 445–450 (2023). https://doi.org/10.1038/s41586-022-05585-1

Bilayer graphene



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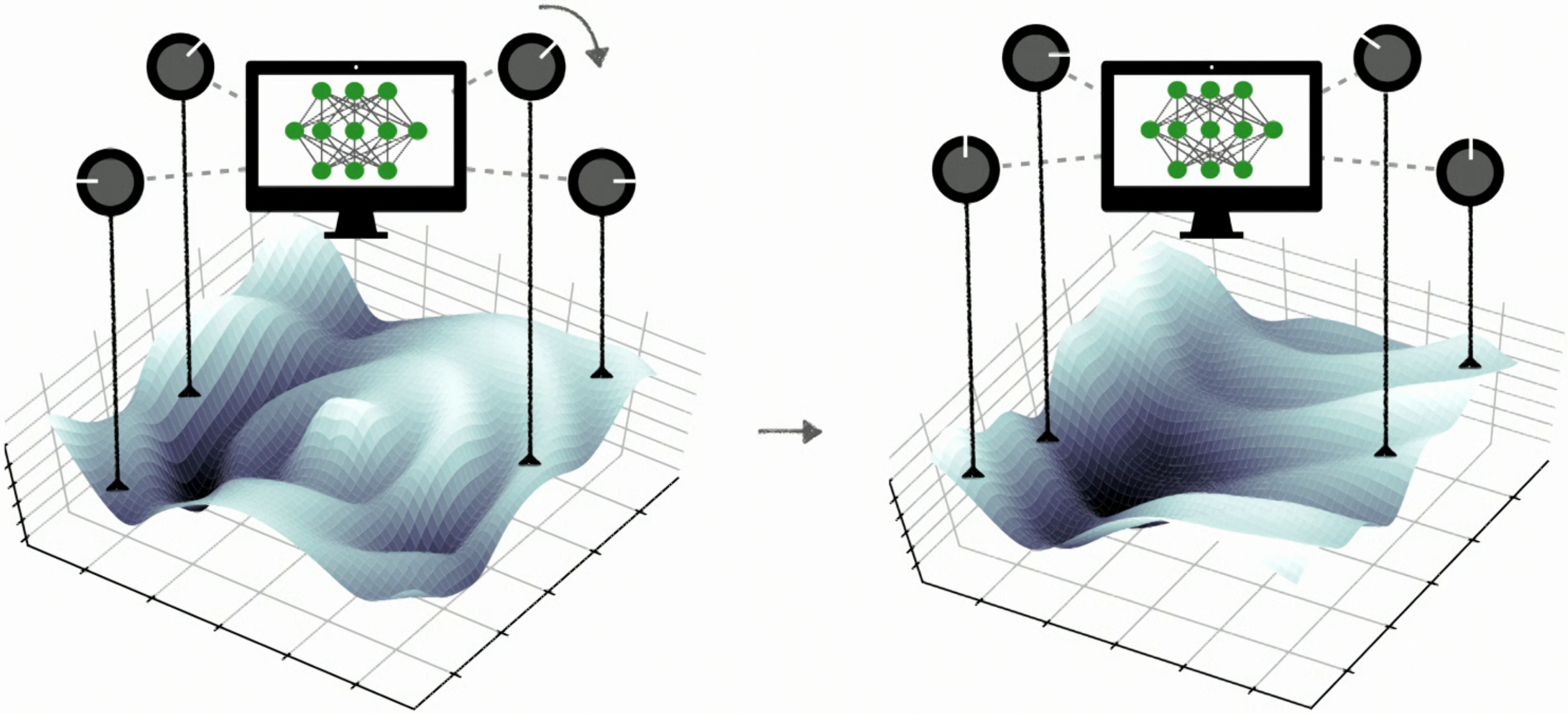
Tuning Engineered Quantum Materials



EG. "Solving optimization tasks in condensed matter." *Nature Machine Intelligence* 2.10 (2020): 557-558.

Tuning Engineered Quantum Materials

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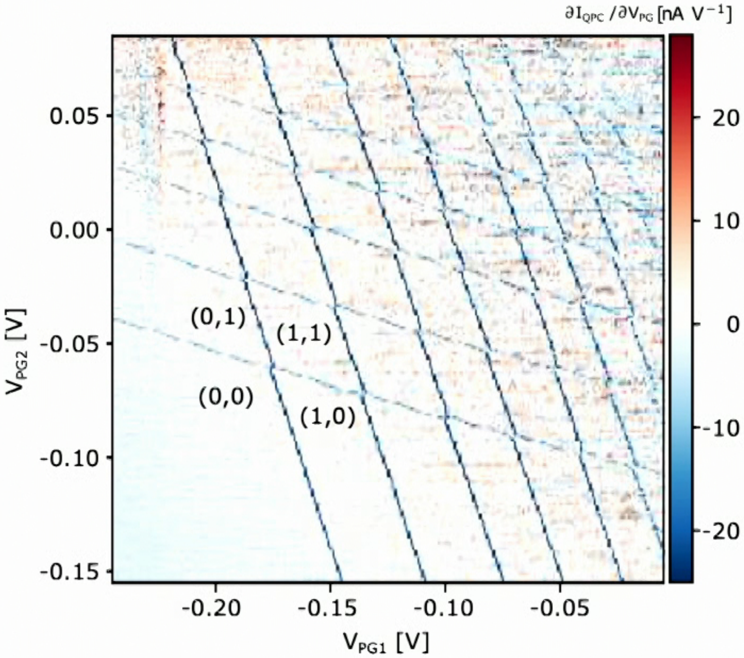
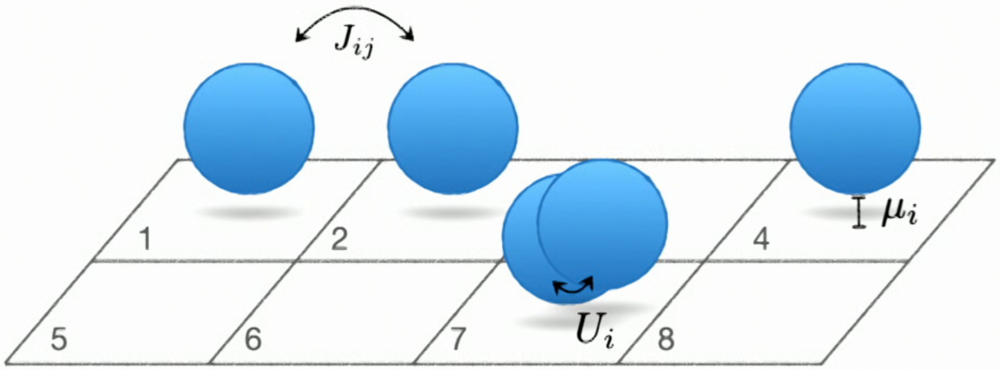


Fast feature analysis in the measured quantum data

Durrer, R., Kratochwil, B., Koski, J. V., Landig, A. J., Reichl, C., Wegscheider, W., ... & **EG**. (2020). Automated tuning of double quantum dots into specific charge states using neural networks. *Physical Review Applied*, *13*(5), 054019.



Learning parameters governing underlying physics

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Hamiltonian Learning as a ML Problem

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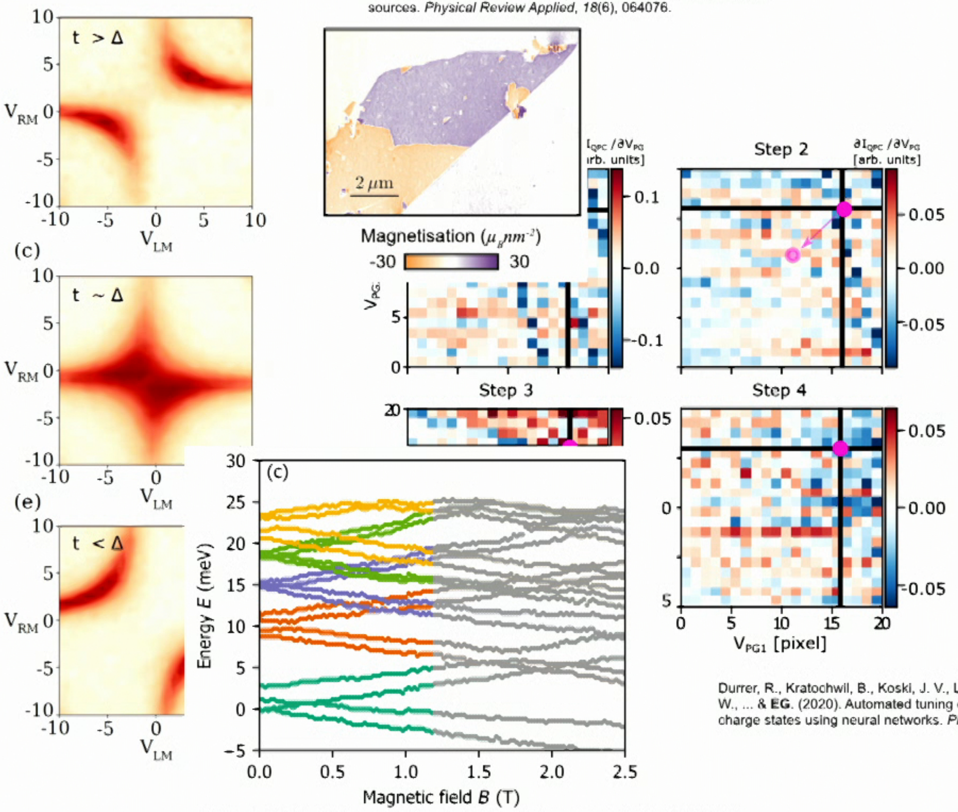

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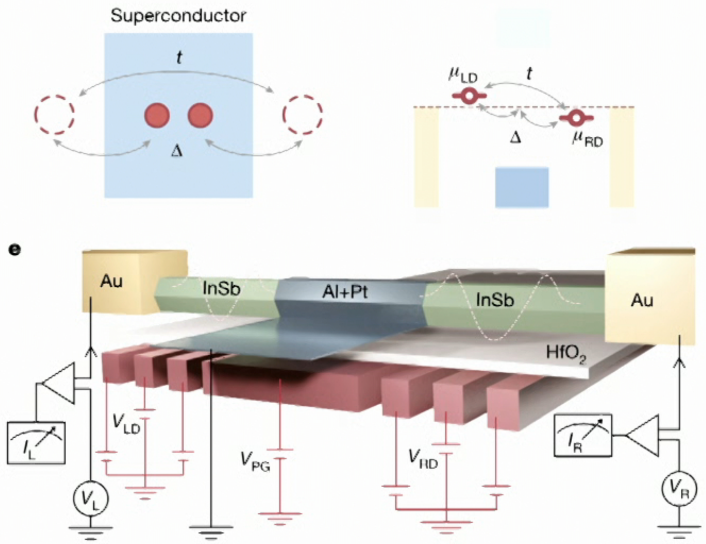
→ ⚙ → **H**

Kitaev Chain



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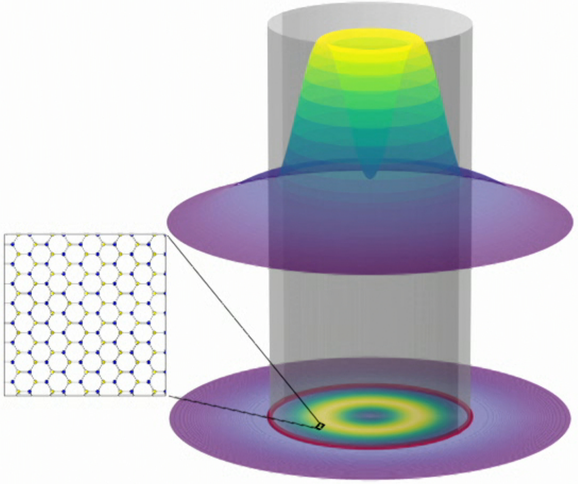
Bilayer graphene



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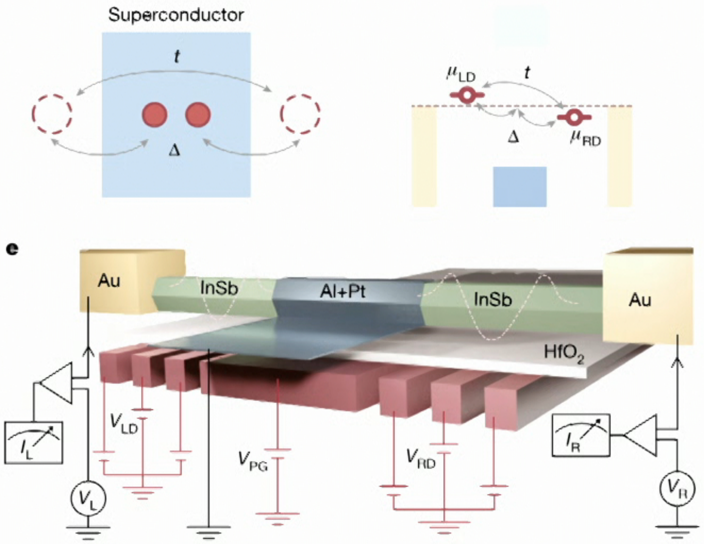
Kitaev Chain

Conditional Generative Model



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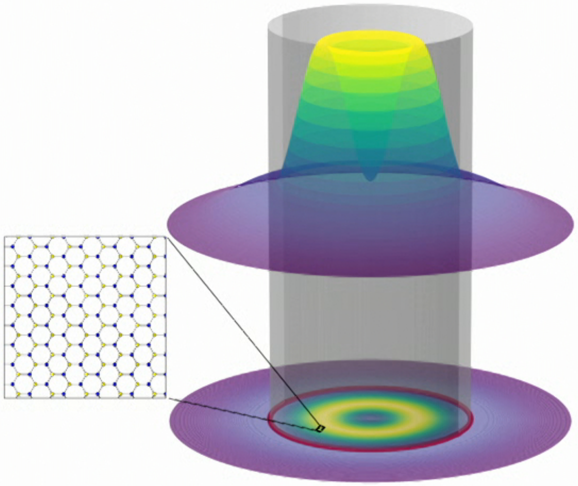
Bilayer graphene

Custom Global Optimizer



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Part I: Adversarial Hamiltonian Learning in a minimal Kitaev chain


Rouven Koch


David van Driel


Alberto Bordin

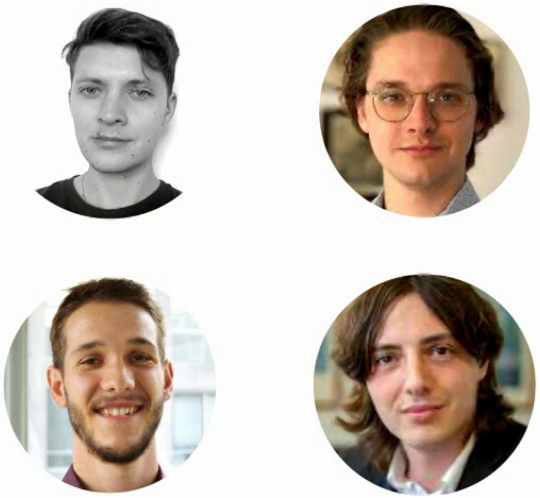

Jose Lado

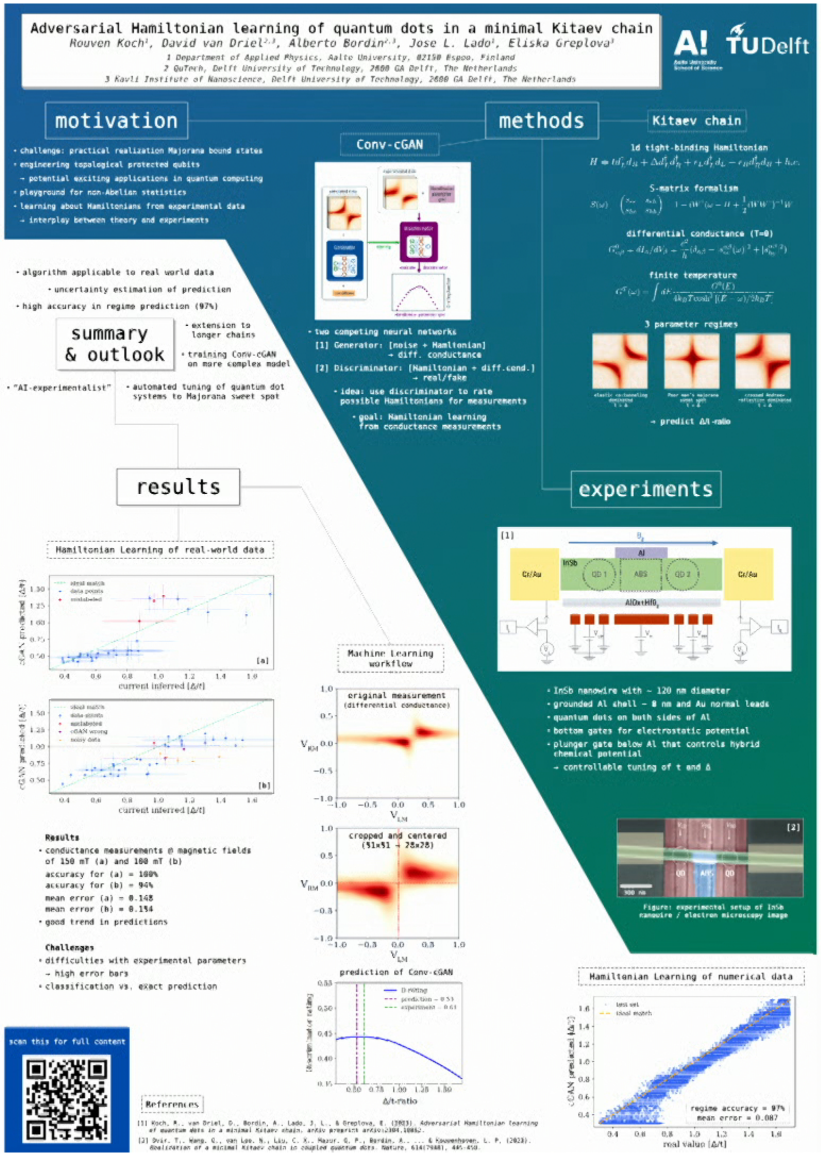
QMAI

Aalto University

QuTech

Part I: Adversarial Hamiltonian Learning in a minimal Kitaev chain





Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain

Rouven Koch[1], David van Driel[2,3], Alberto Bordin[2,3], Jose L. Lado[1], Eliska Greplova[3]
1 Department of Applied Physics, Aalto University, 02150 Espoo, Finland
2 QuTech, Delft University of Technology, 2600 GA Delft, The Netherlands
3 Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands

motivation

- challenge: practical realization Majorana bound states
- engineering topological protected qubits
  - → potential exciting applications in quantum computing
- playground for non-Abelian statistics
- learning about Hamiltonians from experimental data
  - → interplay between theory and experiments

methods

Conv-cGAN

- two competing neural networks

[1] Generator: [noise + Hamiltonian] → diff. conductance

[2] Discriminator: [Hamiltonian + diff.cond.] → real/fake

- idea: use discriminator to rate possible Hamiltonians for measurements
- goal: Hamiltonian learning from conductance measurements

Kitaev chain

1d tight-binding Hamiltonian

$$H = t d_L^\dagger d_R + \Delta d_L^\dagger d_R^\dagger + \epsilon_L d_L^\dagger d_L - \epsilon_R d_R^\dagger d_R + h.c.$$

S-matrix formalism

$$S(\omega) = \begin{pmatrix} s_{ee} & s_{eh} \\ s_{he} & s_{hh} \end{pmatrix} = 1 - iW^\dagger\left(\omega - H + \frac{i}{2}WW^\dagger\right)^{-1}W$$

differential conductance (T=0)

$$G^0_{\alpha\beta} = dI_\alpha/dV_\beta = \frac{e^2}{h}\left(\delta_{\alpha\beta} - |s^{\alpha\beta}_{ee}(\omega)|^2 + |s^{\alpha\beta}_{he}|^2\right)$$

finite temperature

$$G^T(\omega) = \int dE \frac{G^0(E)}{4k_BT\cosh^2[(E-\omega)/2k_BT]}$$

3 parameter regimes

elastic co-tunneling dominated t > Δ

Poor man's majorana sweet spot t = Δ

crossed Andreev reflection dominated t < Δ

→ predict Δ/t-ratio

experiments

- InSb nanowire with ~ 120 nm diameter
- grounded Al shell ~ 8 nm and Au normal leads
- quantum dots on both sides of Al
- bottom gates for electrostatic potential
- plunger gate below Al that controls hybrid chemical potential
  - → controllable tuning of t and Δ

Figure: experimental setup of InSb nanowire / electron microscopy image

results

Hamiltonian Learning of real-world data

Results

- conductance measurements @ magnetic fields of 150 mT (a) and 100 mT (b)

  accuracy for (a) = 100%
  accuracy for (b) = 94%
  mean error (a) = 0.148
  mean error (b) = 0.154

- good trend in predictions

Challenges

- difficulties with experimental parameters
  - → high error bars
- classification vs. exact prediction

Machine Learning workflow

original measurement (differential conductance)

cropped and centered (51x51 → 28x28)

prediction of Conv-cGAN

Hamiltonian Learning of numerical data

regime accuracy = 97%
mean error = 0.087

summary & outlook

- algorithm applicable to real world data
- uncertainty estimation of prediction
- high accuracy in regime prediction (97%)
- extension to longer chains
- training Conv-cGAN on more complex model
- "AI-experimentalist"
- automated tuning of quantum dot systems to Majorana sweet spot

scan this for full content

References

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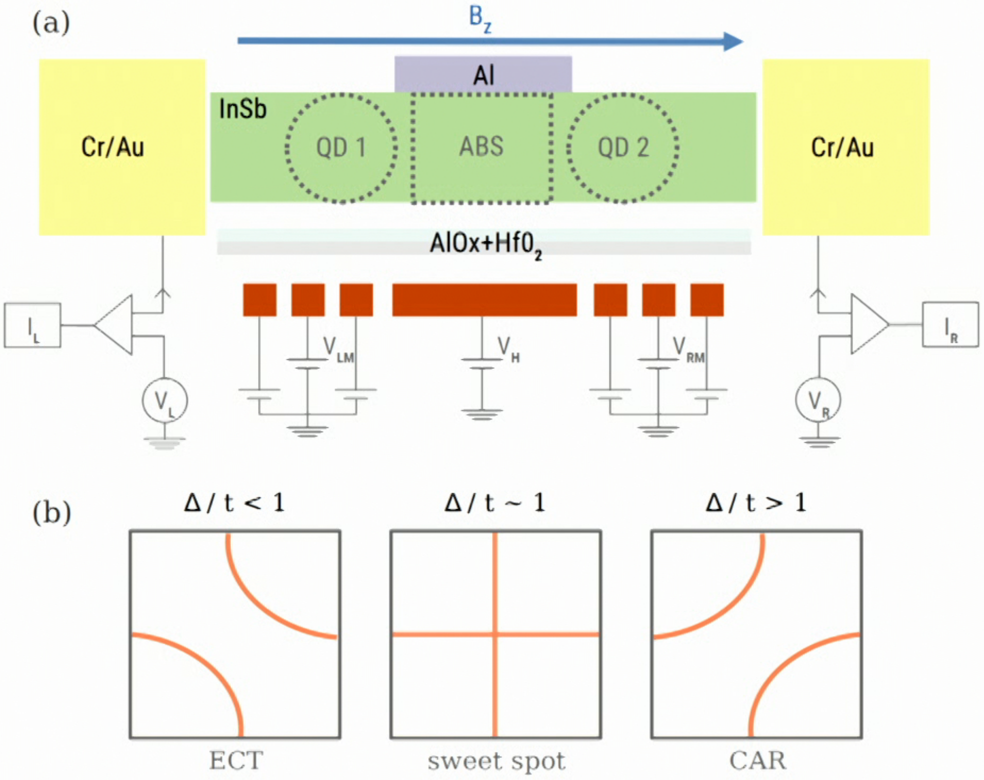
[2] Dvir, T., Wang, G., van Loo, N., Liu, C. X., Mazur, G. P., Bordin, A., ... & Kouwenhoven, L. P. (2023). Realization of a minimal Kitaev chain in coupled quantum dots. Nature, 614(7948), 445-450.

Tuning Engineered Kitaev Mini-Chain

$$H = t d_L^\dagger d_R + \Delta d_L^\dagger d_R^\dagger + \epsilon_L d_L^\dagger d_L + \epsilon_R d_R^\dagger d_R + h.c.$$

Elastic Co-tunnelling (ECT)

Cross-Andreev Reflection (CAR)



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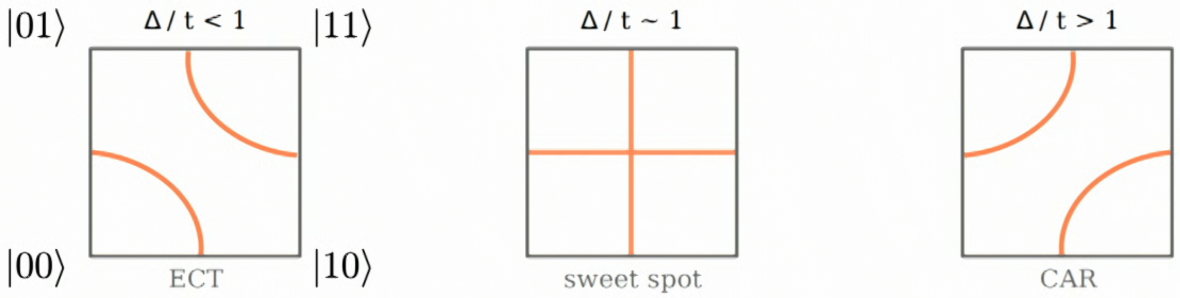
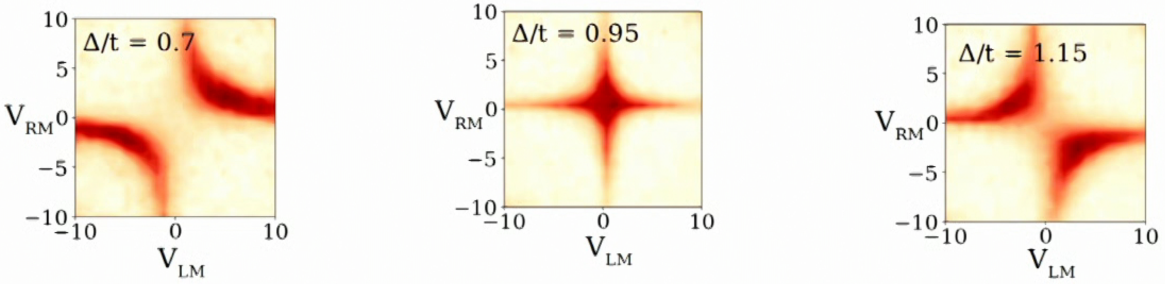
Part 1: Tuning Engineered Kitaev Mini-Chain





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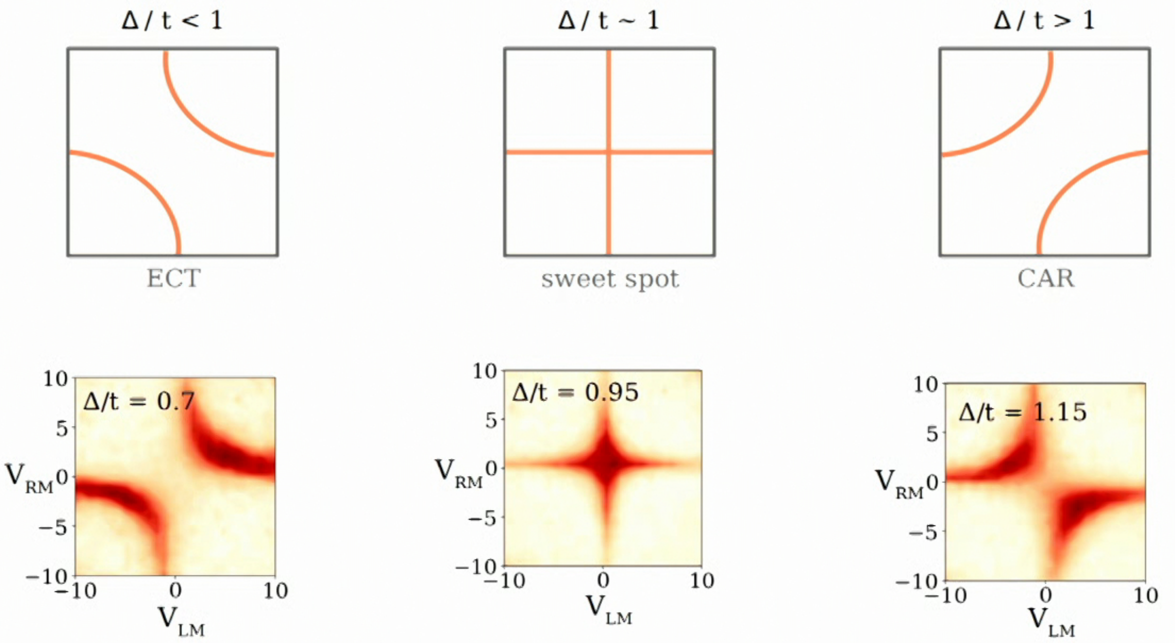

Either directly measured or simulated with S-matrix formalism

Koch, R., van Driel, D., Bordin, A., Lado, J. L., & **EG**. (2023). Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain. *arXiv preprint arXiv:2304.10852*.

Hamiltonian Learning Task

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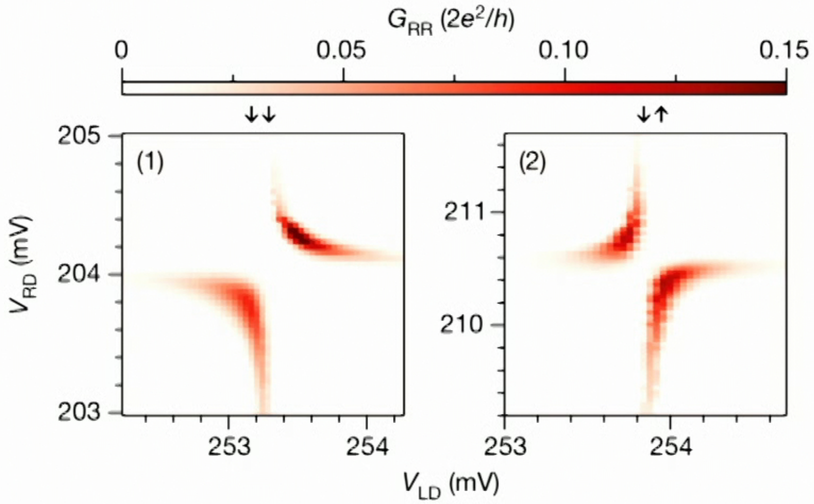

$$\rightarrow \quad H(\Delta/t)$$

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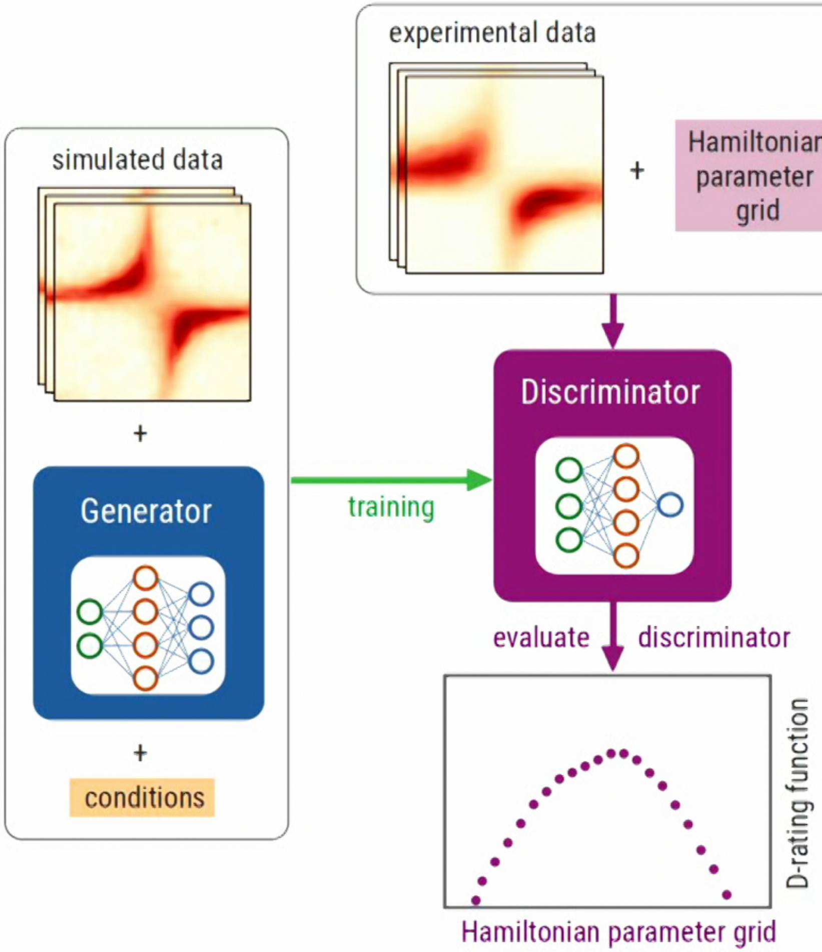

Conditional Convolutional GAN Workflow

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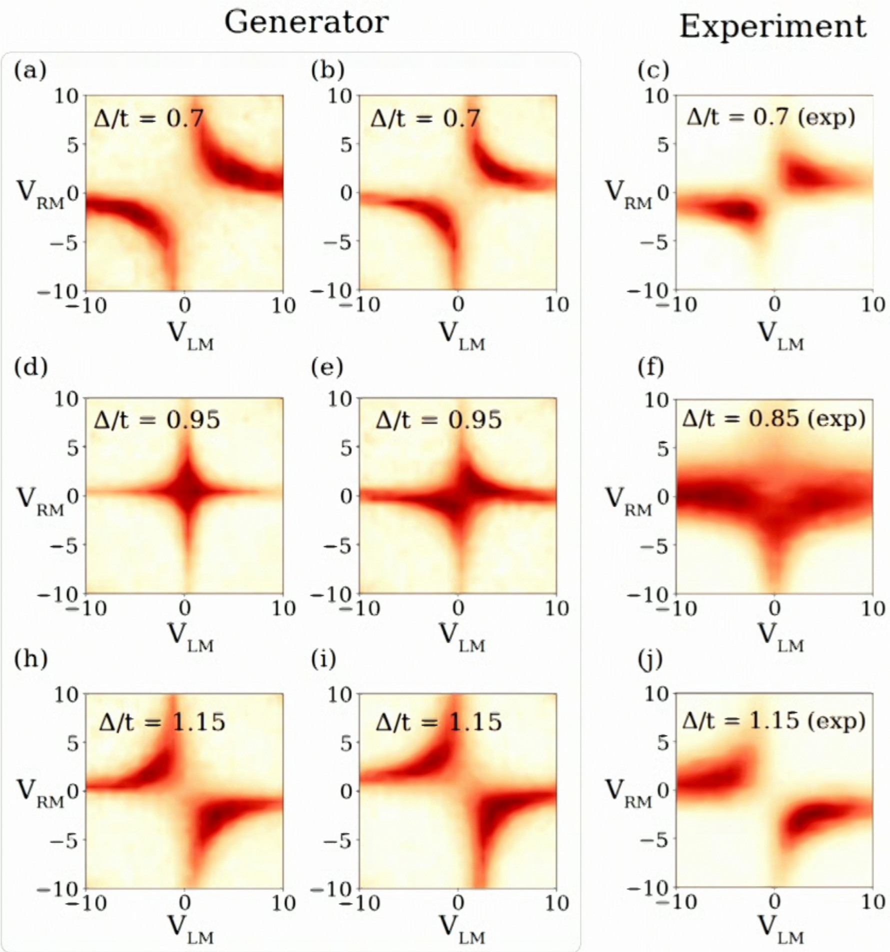

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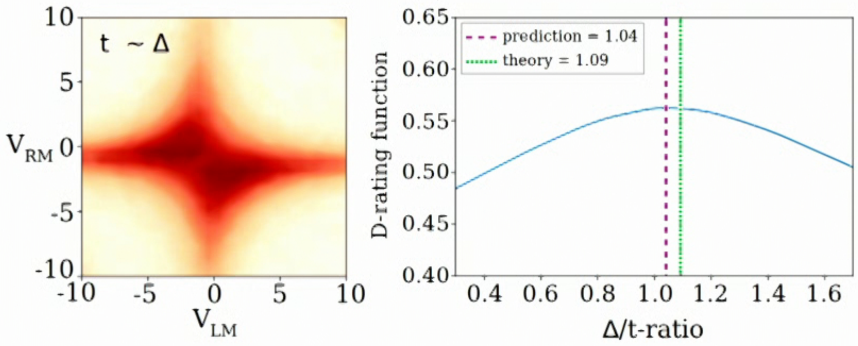
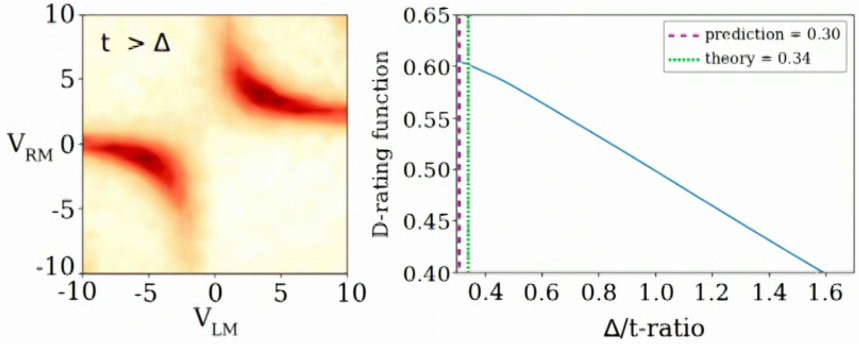
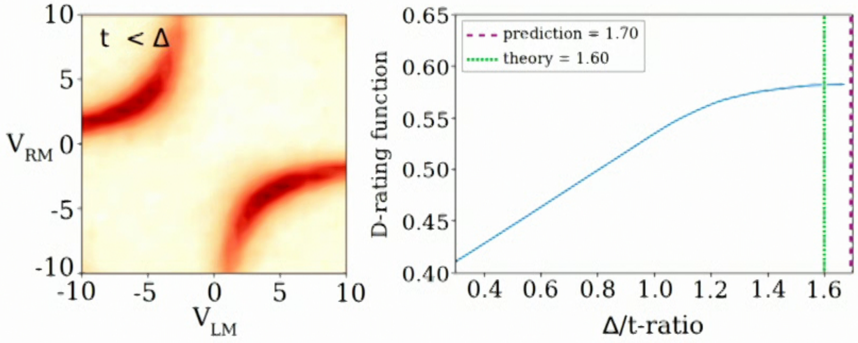
Generator outputs vs experimental measurements

Discriminator prediction distributions for simulated data







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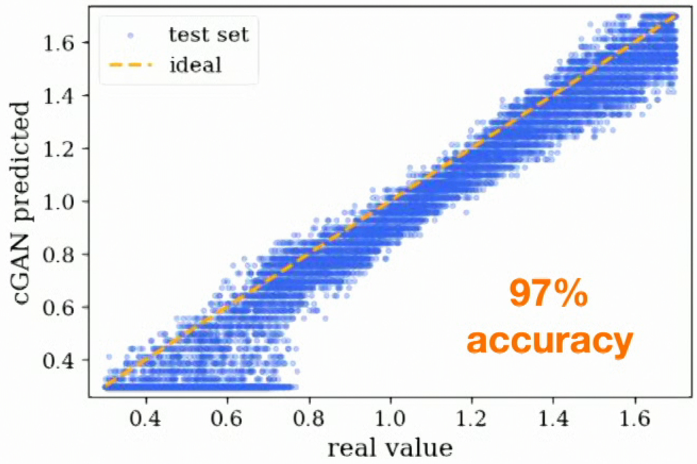

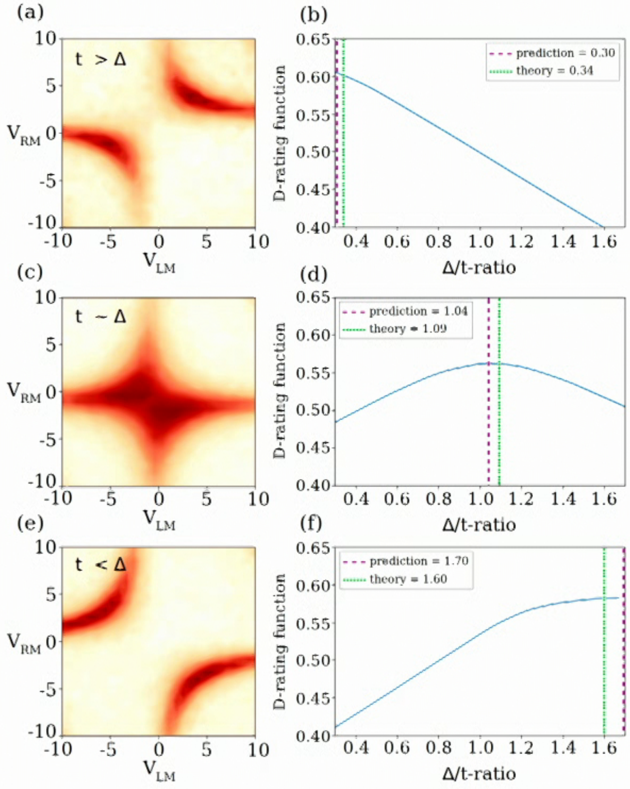

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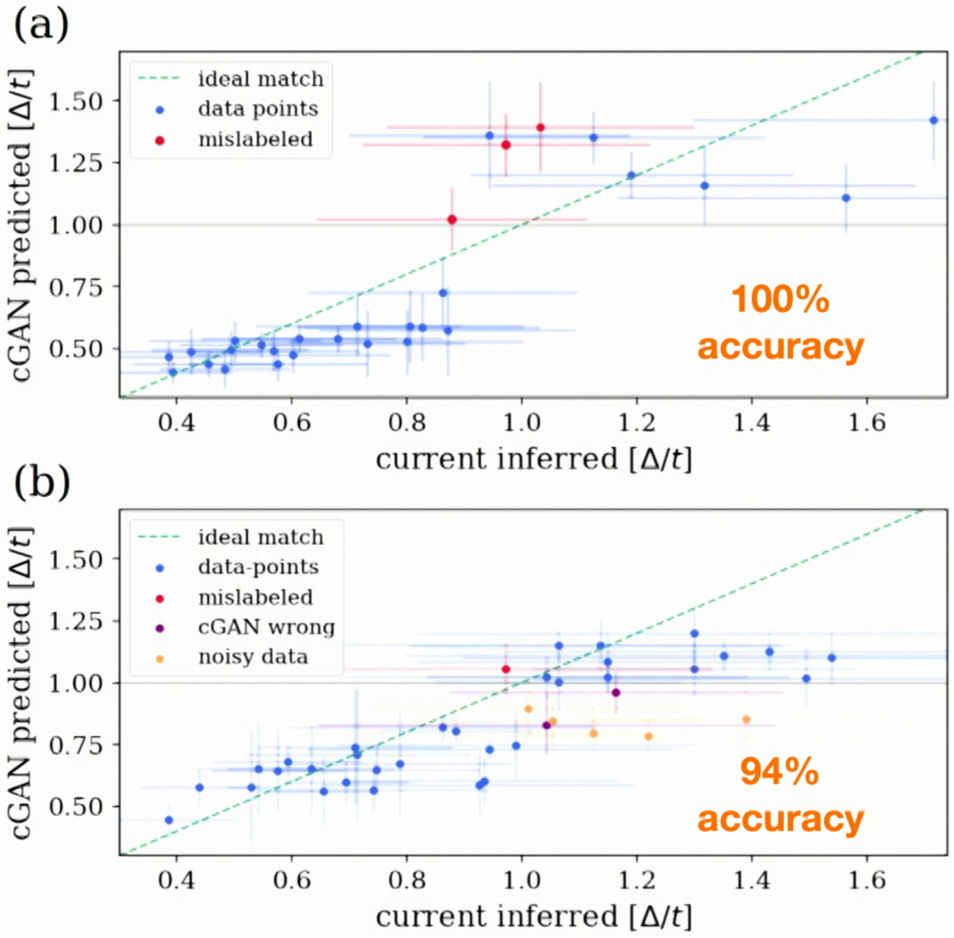
Discriminator prediction distributions for excremental data



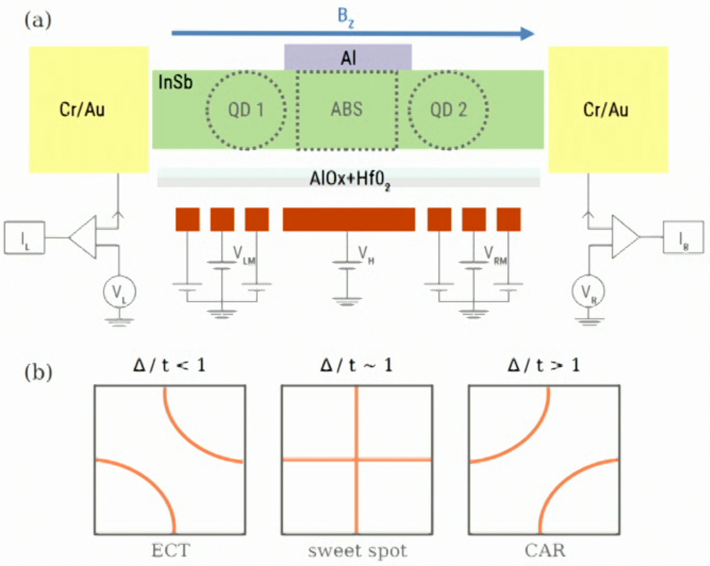
100% accuracy

94% accuracy

GAN correctly identified measurements with wrong experimental label!

Koch, R., van Driel, D., Bordin, A., Lado, J. L., & **EG**. (2023). Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain. *arXiv preprint arXiv:2304.10852*.

Part I Conclusion: Adversarial Hamiltonian Learning in a minimal Kitaev chain



We characterized topological Kitaev chain states autonomously with higher precision than human experts.

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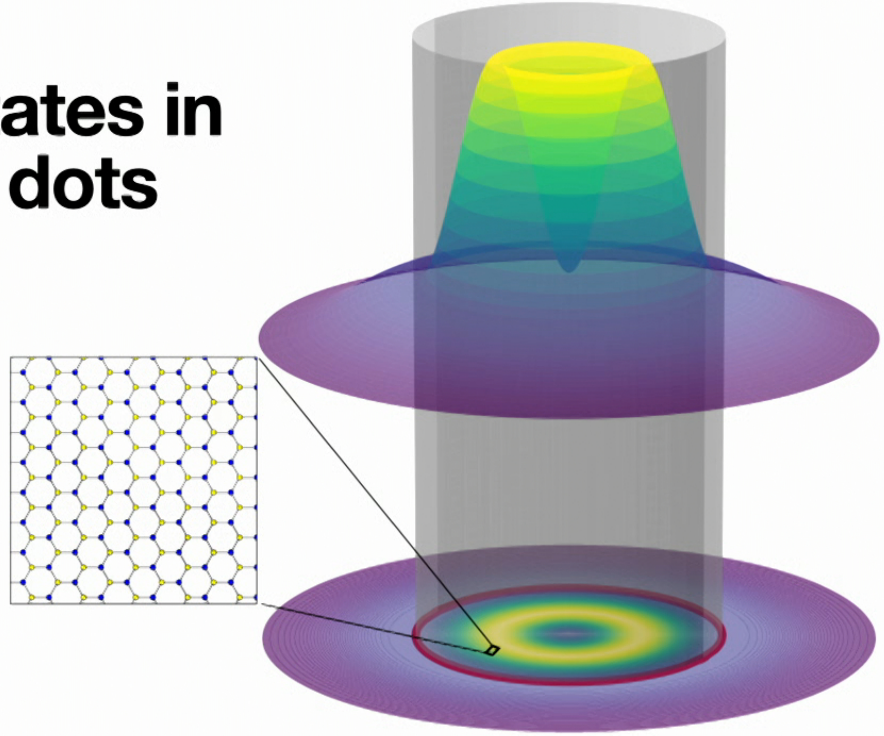
Part II: Automated reconstruction of bound states in bilayer graphene quantum dots

Jozef Bucko, Frank Schäfer, Chuyao Tong, Rebekka Garreis, Frantisek Herman, Annika Kurzmann, Klaus Ensslin, Thomas Ihn.

Part II: Automated reconstruction of bound states in bilayer graphene quantum dots



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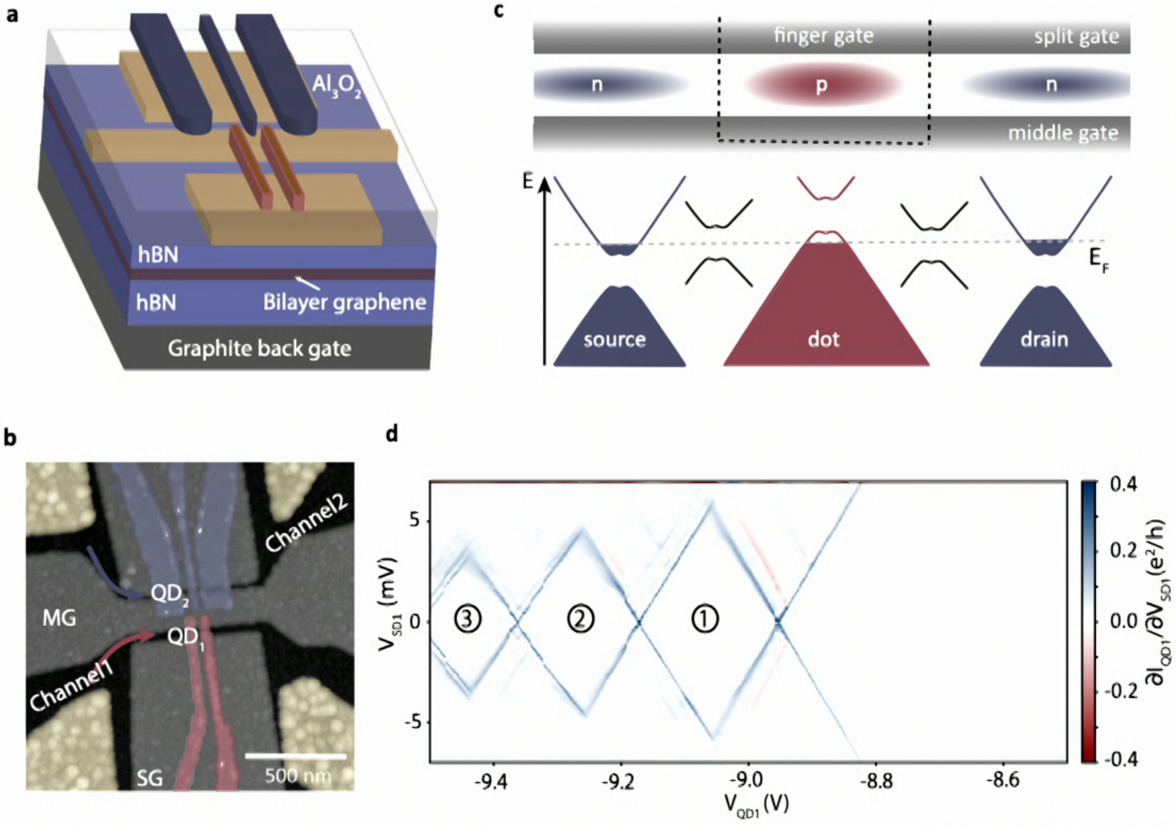
Bilayer Graphene Quantum Dots



Nano Lett. **2019, 19, 8, 5216-5221**

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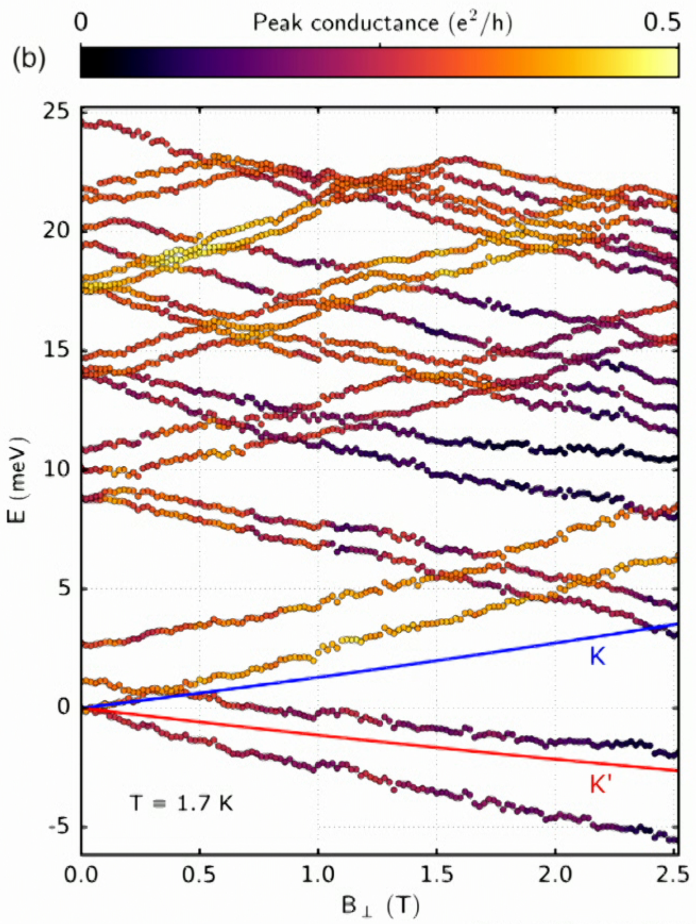

Phys. Rev. X **8**, 031023 (2018)

Is there a theory that fits this data?

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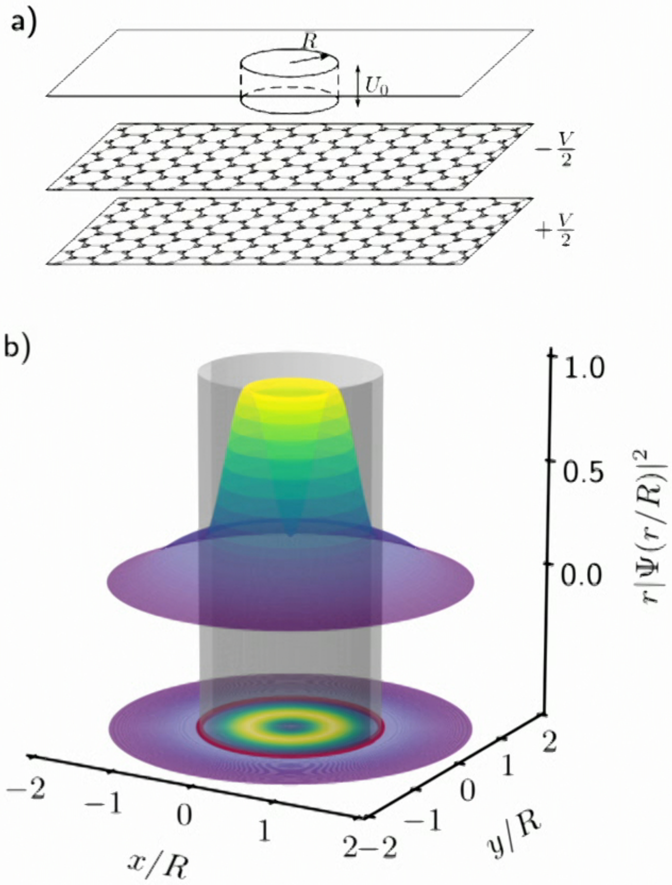

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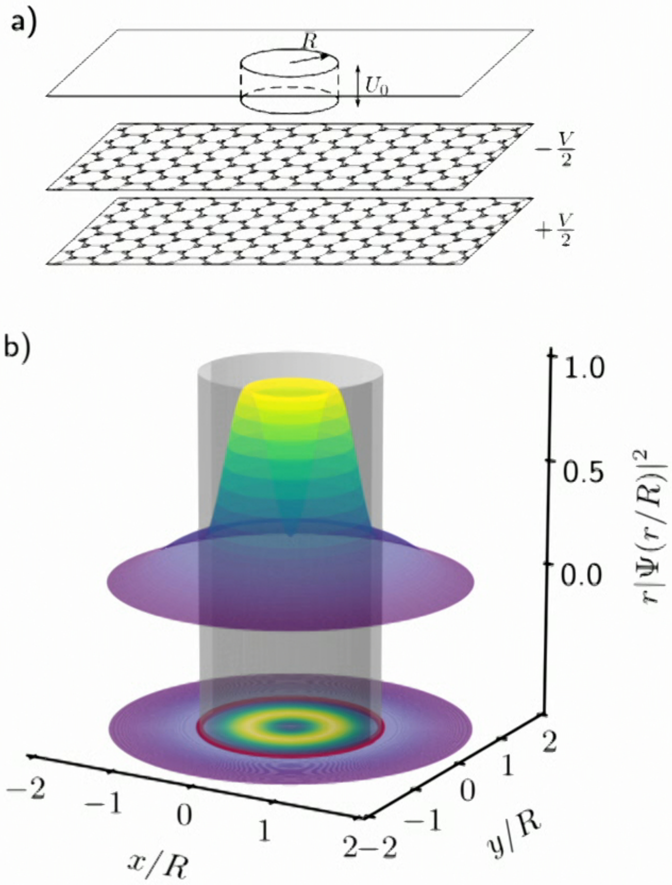
Confining potential

$$\mathcal{H} = \begin{pmatrix} \boxed{U(r)} + \frac{\tau V}{2} & p_x + ip_y & t_\perp & 0 \\ p_x - ip_y & U(r) + \frac{\tau V}{2} & 0 & 0 \\ t_\perp & 0 & U(r) - \frac{\tau V}{2} & p_x - ip_y \\ 0 & 0 & p_x + ip_y & U(r) - \frac{\tau V}{2} \end{pmatrix}$$

$$\Psi(r,\varphi) = \frac{e^{im\varphi}}{\sqrt{r}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i\varphi} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\varphi} \end{pmatrix} \Psi_1(r)$$

Physical Review B 79, 085407 (2009)



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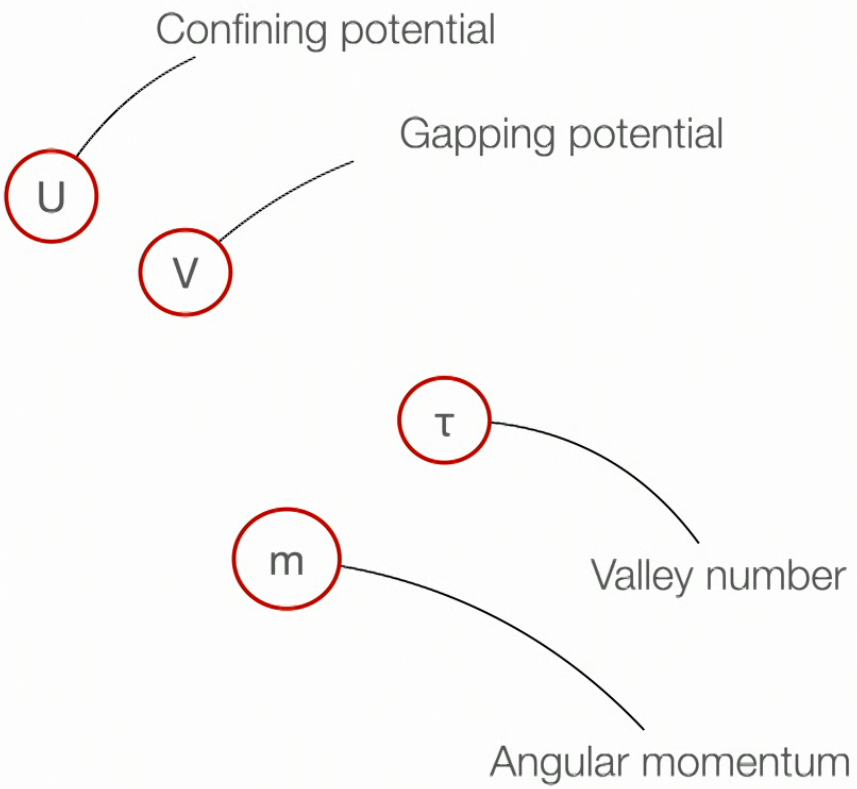
U — Confining potential

V — Gapping potential

τ — Valley number

m — Angular momentum

Goal: Find the parameters that best fit the experimental data



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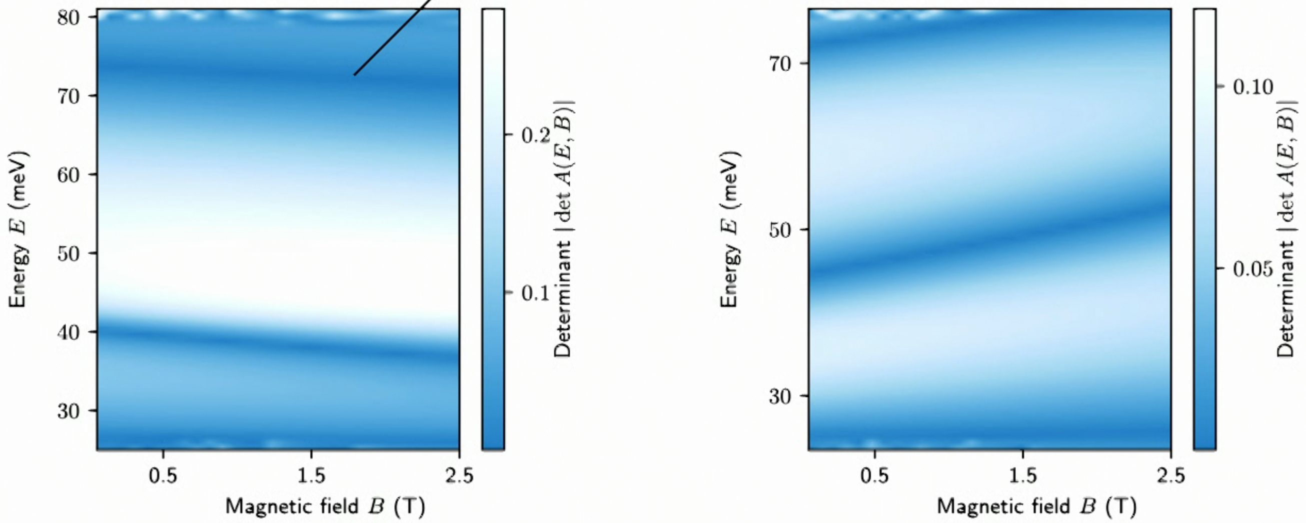
Theory detour: Determinants



measurable energies

{U, V, m, τ}

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t-SNE clustering: experiment

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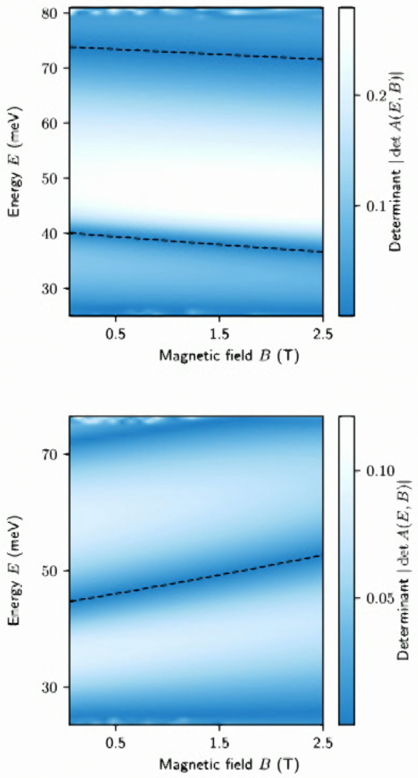

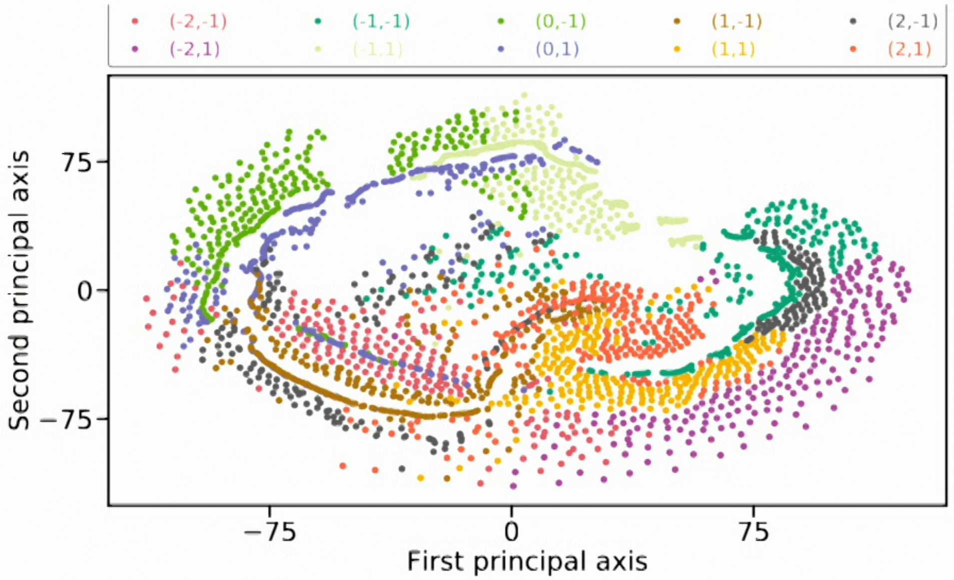

Bucko, J., Schäfer, F., Herman, F., Garreis, R, Tong, C, Kurzmann, A, Ian T., & **EG**. (2023). Automated reconstruction of bound states in bilayer graphene quantum dots. Physical Review Applied 19, 024015 (2023).

U-V landscape

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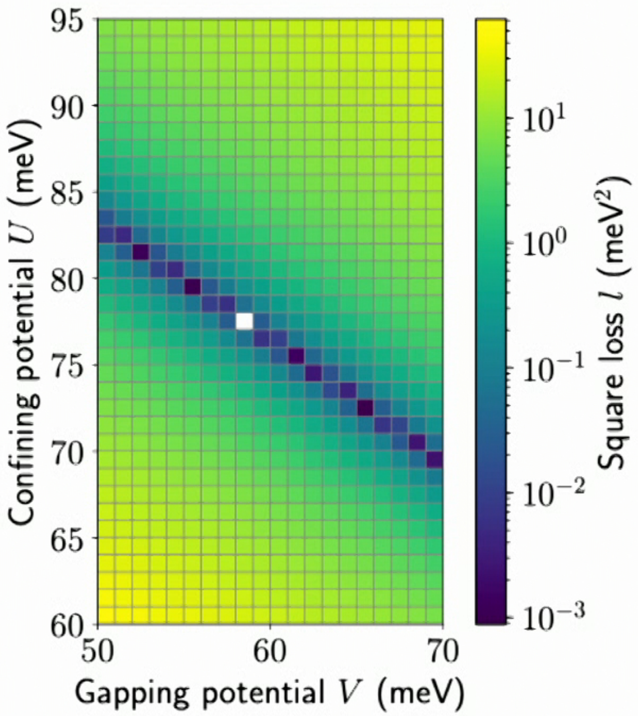
- lost cause for gradient methods
- global methods could fix this but extremely computationally expensive



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Hamiltonian driven random search

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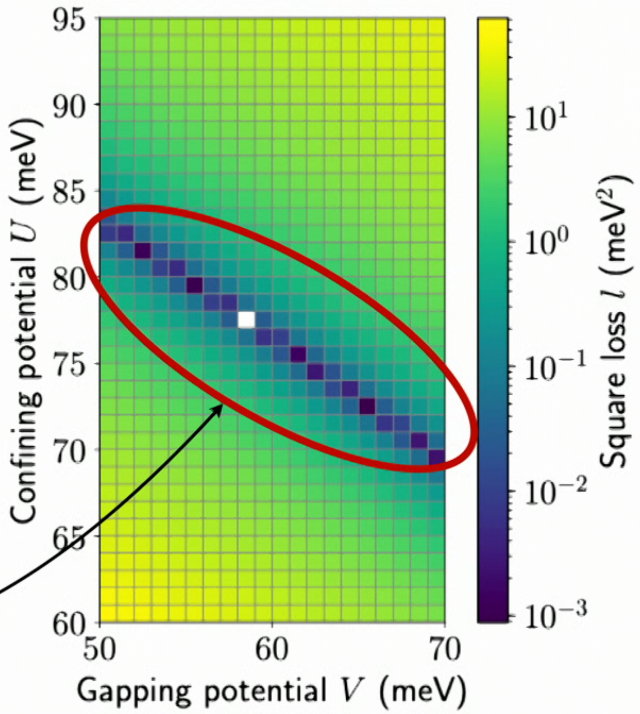
Step 1:

“Use the simple model to calculate gradients analytically and identify the valley"



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Hellmann-Feynman theorem

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$$\frac{dE}{dQ} = \left\langle \Psi \middle| \frac{dH}{dQ} \middle| \Psi \right\rangle \qquad Q \in \{U, V\}$$

$$\frac{\partial l_{m,\tau}(U,V)}{\partial Q} = \frac{\partial l_{m,\tau}(U,V)}{\partial E^{m,\tau}} \frac{\partial E^{m,\tau}}{\partial Q} =$$

$$\frac{1}{B_{\max}} \int_0^{B_{\max}} 2(E^{m,\tau} - E^{m,\tau}_{\mathrm{GT}}) \left\langle \Psi \middle| \frac{\partial H}{\partial Q} \middle| \Psi \right\rangle \mathrm{d}B.$$

H-F Theorem allows to calculate the gradients exactly!

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Precision on simulated data

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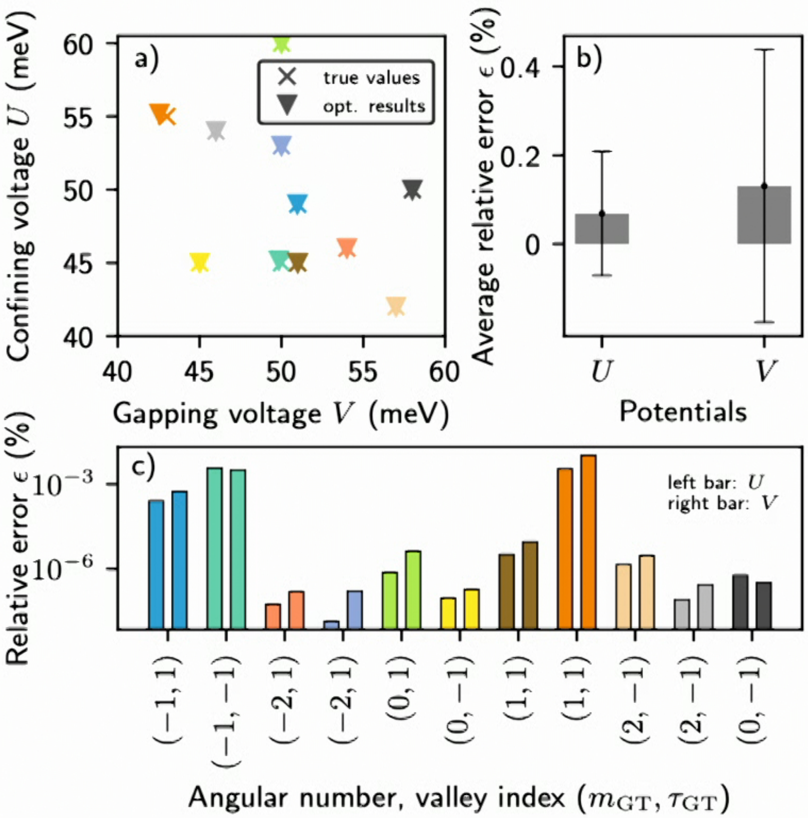
- **U/V fitting precision ~ 0.2 %**

- **m/τ found in 100% of cases**



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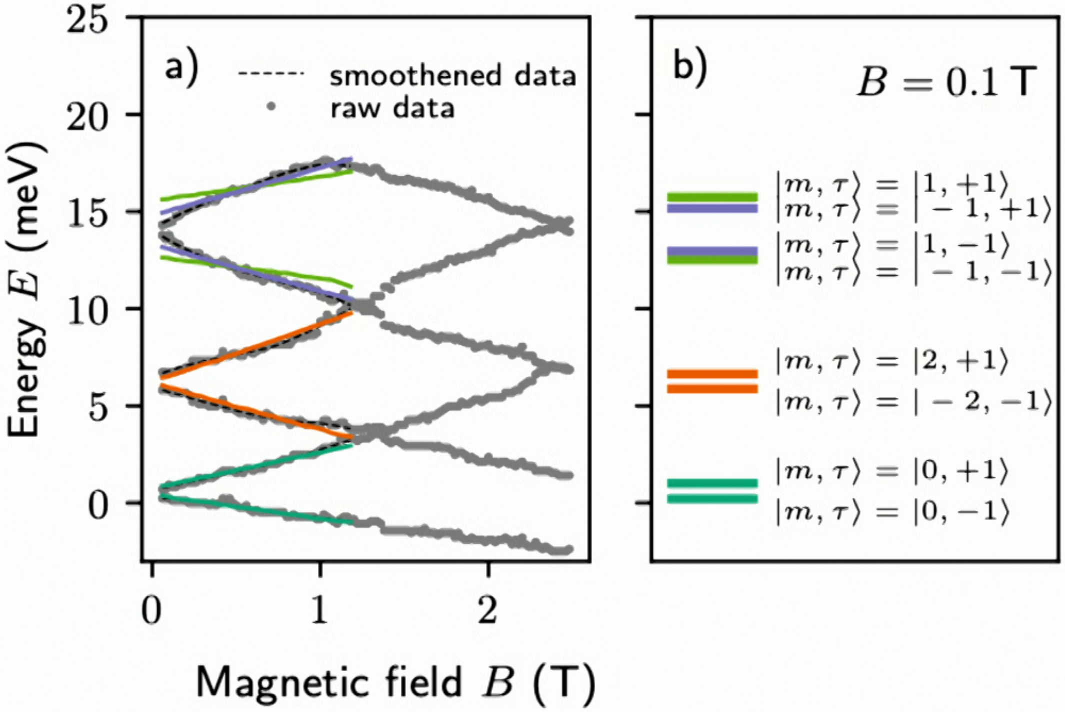
Precision on experimental data

DATASET 1



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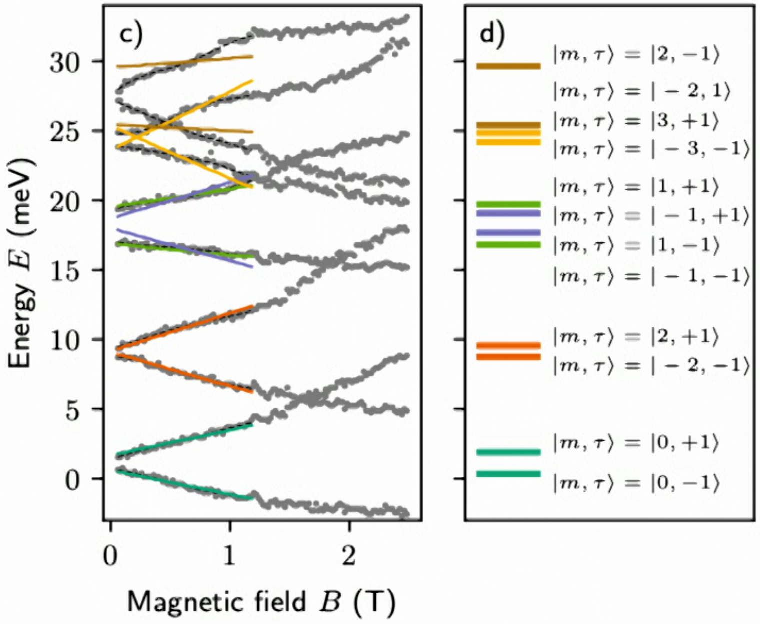
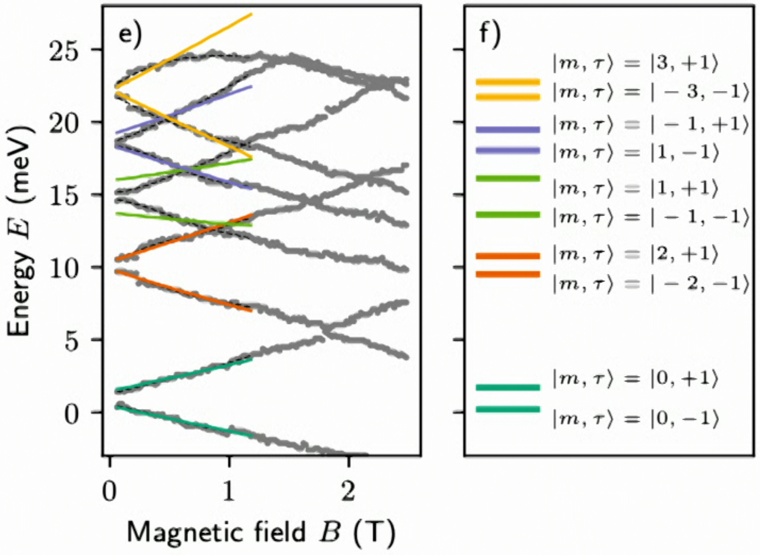
Precision on experimental data

DATASET 2



DATASET 3



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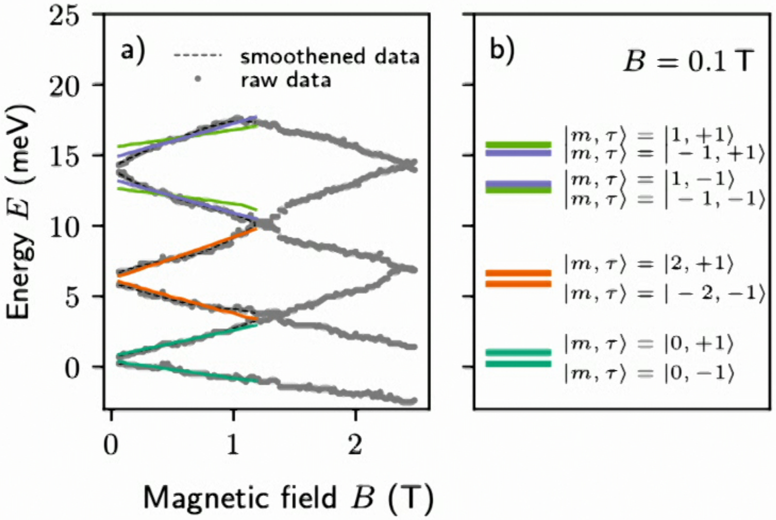
Part II Conclusion: Automated reconstruction of bound states in bilayer graphene quantum dots



We determined bound states in bilayer graphene quantum dots with best known fit to experimental data.

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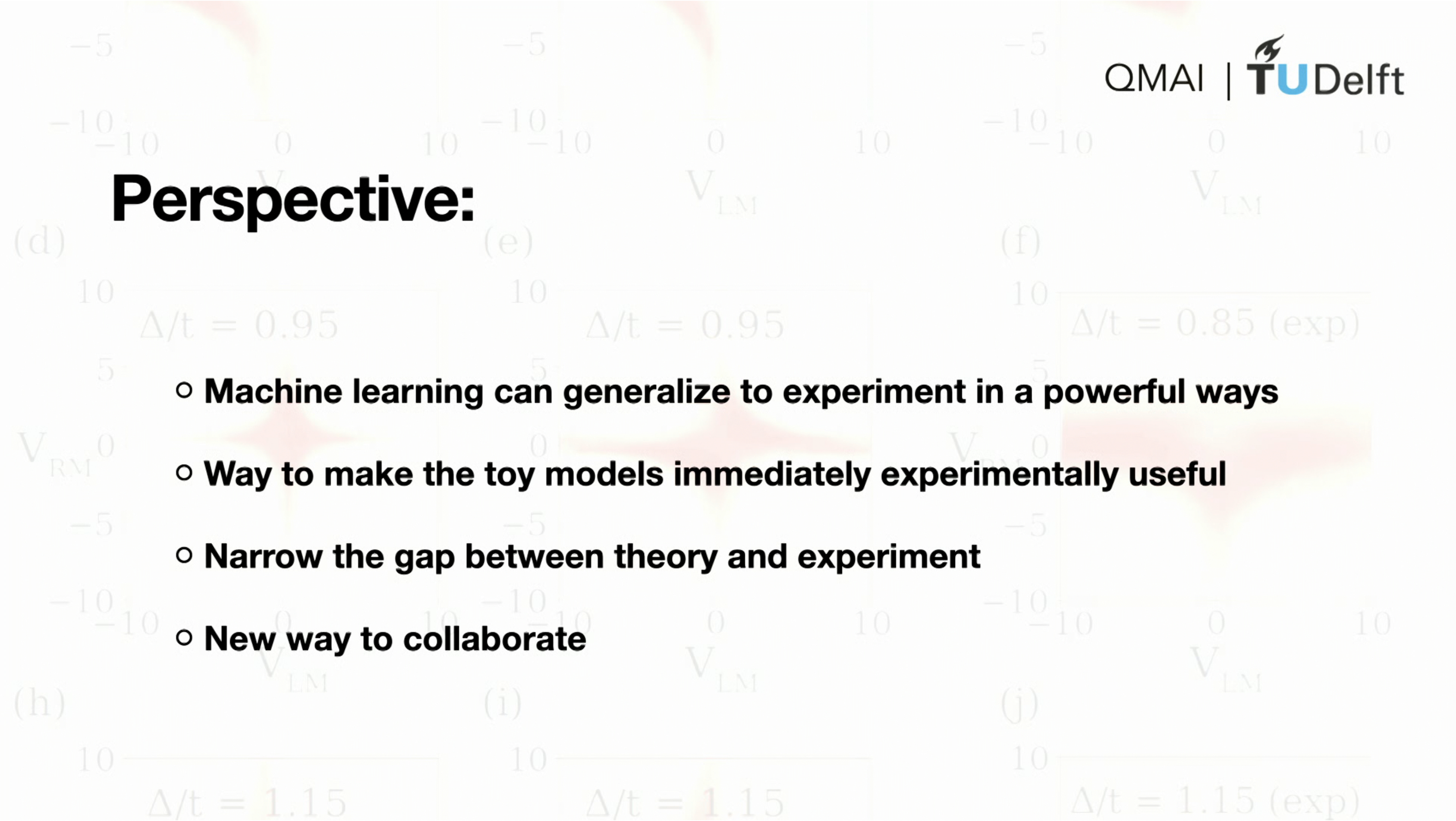
Perspective:



- Machine learning can generalize to experiment in a powerful ways
- Way to make the toy models immediately experimentally useful
- Narrow the gap between theory and experiment
- New way to collaborate

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THE END

QUANTUM FLAGSHIP

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