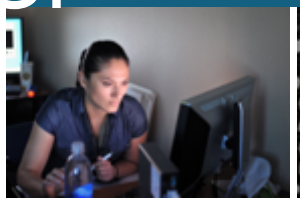
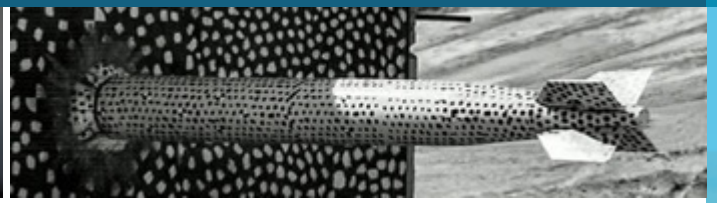
SAND2021-2459C

Center for Quantum Information and Control

Sandia National Laboratories

Signatures of missing donors in transport through atomically precise P donor chains in Si





March 2021

Mitchell Brickson (UNM/SNL), Quinn Campbell, Jeffrey Ivie, Justin Koepke, Peter Schultz, Richard Muller, Ezra Bussmann, Andrew Baczewski, Andrew Mounce, Shashank Misra

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Introduction: precision placement of donors

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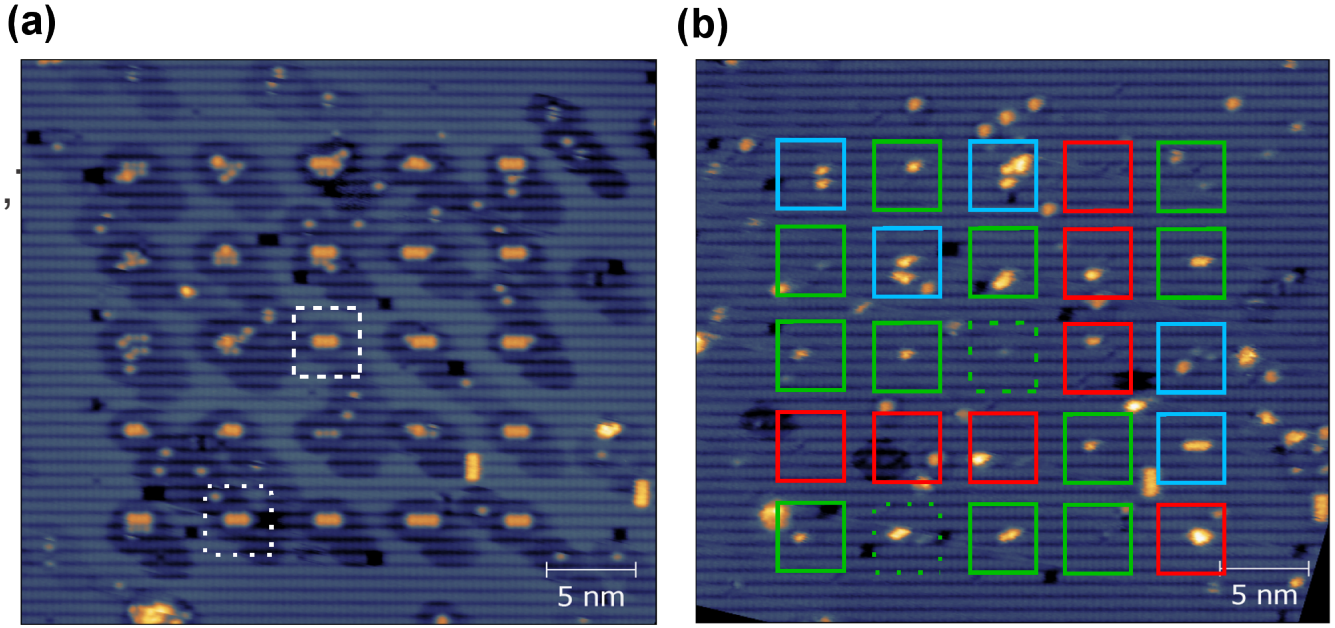
- Precision placement of donors has made a lot of progress recently:
  - Ion implantation: scanning probe ion aperature [1]
  - STM lithography: can place donors to within one lattice site [2]
- Metallic gates can be patterned nearby for electrical control.
- Opens many possibilities:
  - Single-atom transistors [3]
  - Donors as qubits [4]
  - Donors for analog quantum simulation [5,6,

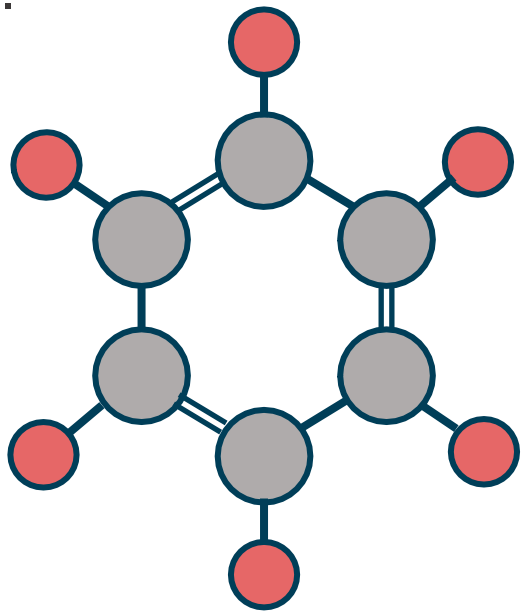


[8]

[1] A. M. Jakob et al., arXiv preprint: 2009.02892
[2] S. R. Schofield et al., vol. 91, 136104 (2003)
[3] M. Fuechsle et al., *Nature Nano*. Vol. 7, p. 242–246 (2012)
[4] J. J. Pla et al., Nature vol. 489, p. 541–545 (2012)
[5] N. H. Le et al., PRB 96, 245406 (2017)
[6] A. Dusko et al., NPJ Quant. Info., vol. 4, a. 1 (2018)
[7] E. Prati et al., Nature Nano. vol. 7, p. 443–447 (2012)

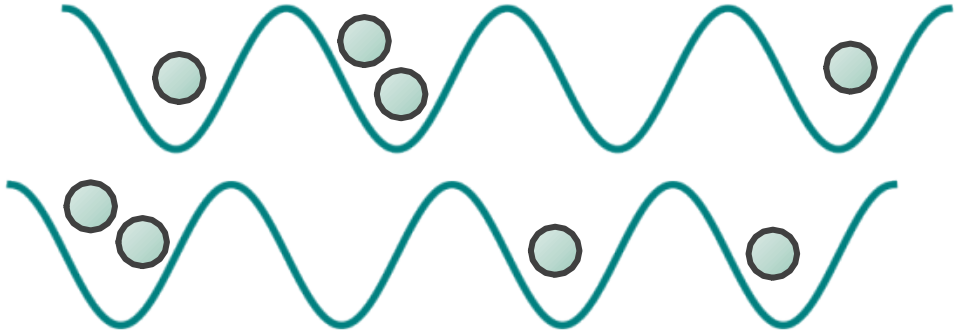
Introduction: analog quantum simulation

- Using one controllable quantum system to imitate and study a different interesting system.
- Example: atoms trapped in optical lattices to simulate 2D molecules. [9]
- No generic error correction schemes, so effects of errors need to be studied case-by-case.



Interesting system, e.g. molecule

$$\hat{H}_{mol} \leftarrow \hat{H}_{ctrl}(\lambda)$$



Controllable system, e.g. atoms in an optical lattice

[9] J. Arguello-Luengo, *PR Research*, vol. 2, 042013(R)

Analog quantum simulation with donors?

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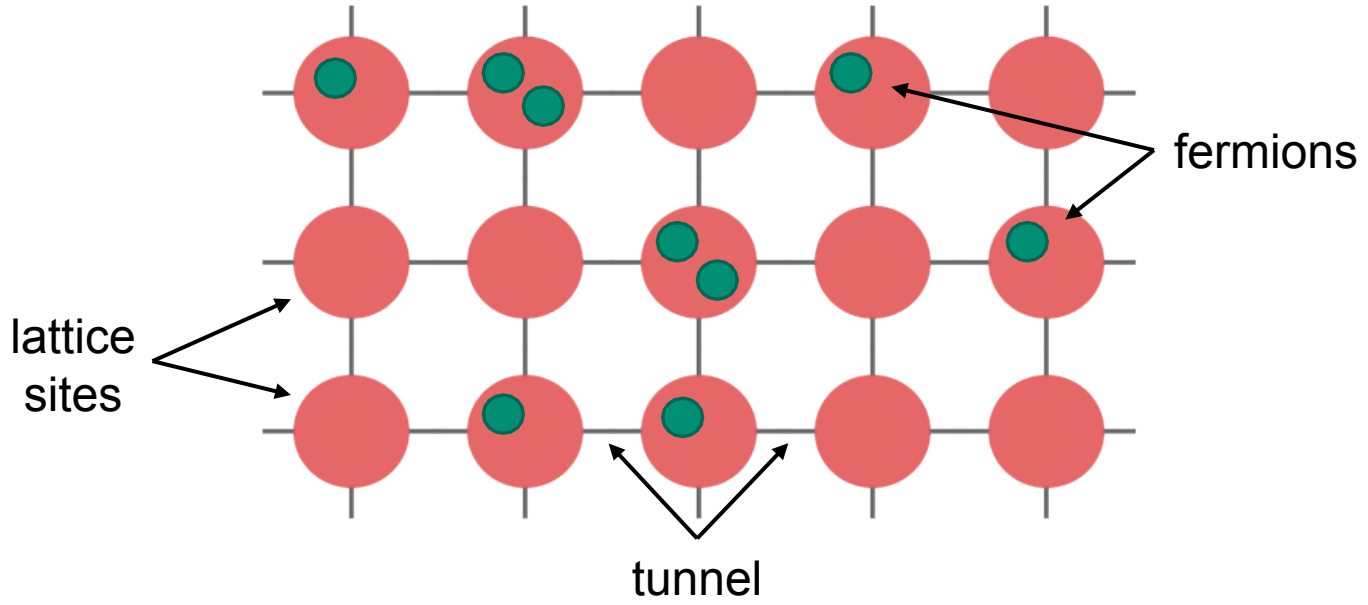
- Precision placement allows control of spacing between sites → control of tunnel coupling
- Ability to change voltages on nearby gates → control of on-site energies
- Ability to adjust nearby leads → effective control of chemical potential
- Errors from misplacing donors – donor placement isn't perfect, can significantly affect coupling
  - Le et al. [5] – found that transport in 2D arrays should remain intact
  - Dusko et al. [6] – found that charge/spin correlations are relatively unaffected on average

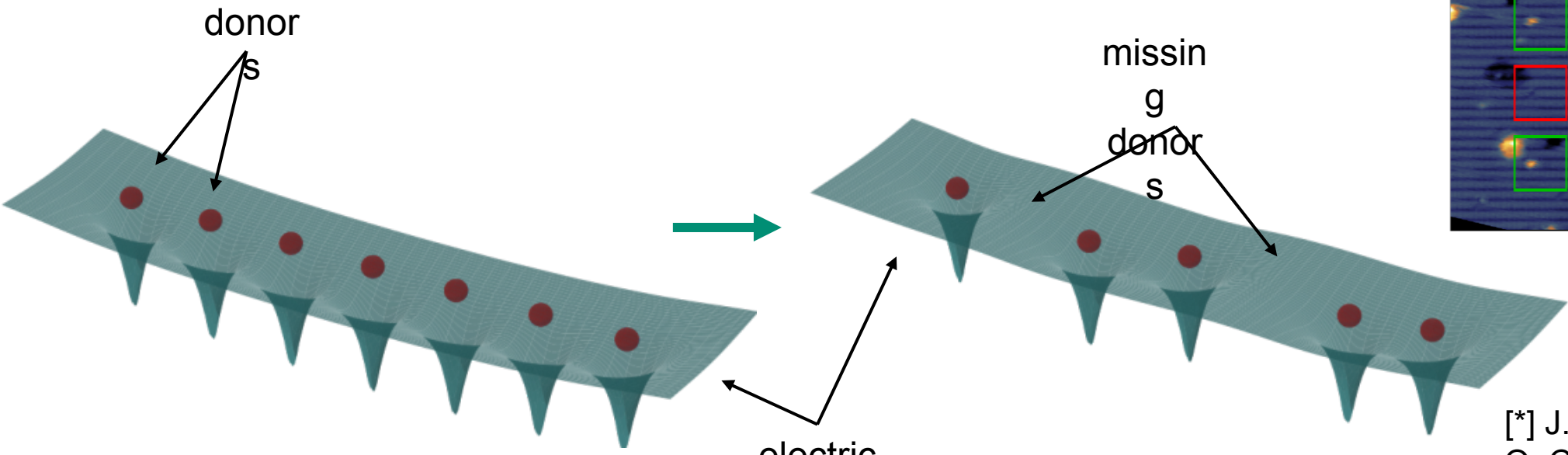
Can we build a Fermi-Hubbard model with STM lithography? →

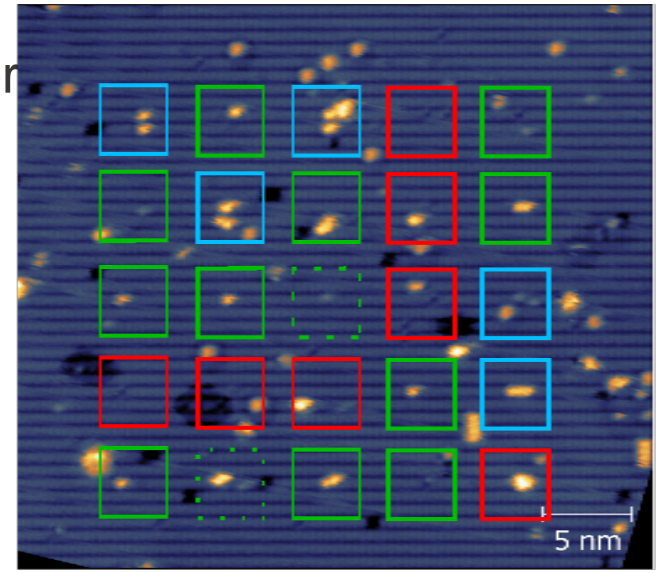


[5] N. H. Le et al., PRB 96, 245406 (2017)
[6] A. Dusko et al., NPJ Quant. Info., vol. 4, a. 1 (2018)

Stronger disorder: missing donors

- Yet unconsidered type of disorder: missing donors.
  - Experiments and kinetic modeling [*] suggest ~1/3 of donors might not be placed at all in STM lithography.
- How much will this affect target dynamics? Can this be seen in transpor





[8]

[8] J. A. Ivie et al., arXiv posting coming soon

[*] J. Ivie, talk B55.00004, Q. Campbell, talk E29.00003,

Exploring the effects of missing donors

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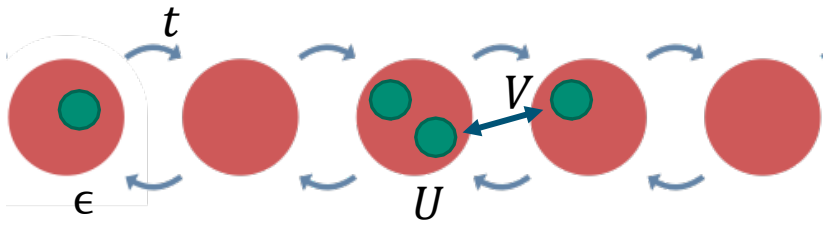
- Simple example Hamiltonian to target: extended 1-dimensional Fermi-Hubbard chain

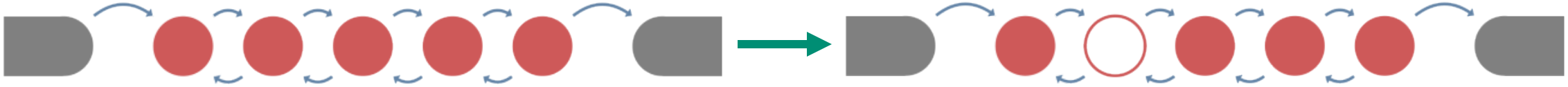
$$\hat{H} = \epsilon \sum_{j,\sigma} \hat{n}_{j\sigma} + U \sum_{j} \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} + t \sum_{j,\sigma} (\hat{c}^{\dagger}_{j\sigma}\hat{c}_{j+1,\sigma} + \hat{c}^{\dagger}_{j+1,\sigma}\hat{c}_{j\sigma}) + \sum_{j,k,\sigma,\tau} V_{jk}\hat{n}_{j\sigma}\hat{n}_{k\tau}$$

(numbers from effective mass theory [10,11])

- Short chains are easy to analyze.
- Standard model has an analytic solution in thermodynamic limit. [12]



- How do long-range interactions and missing sites affect transport?



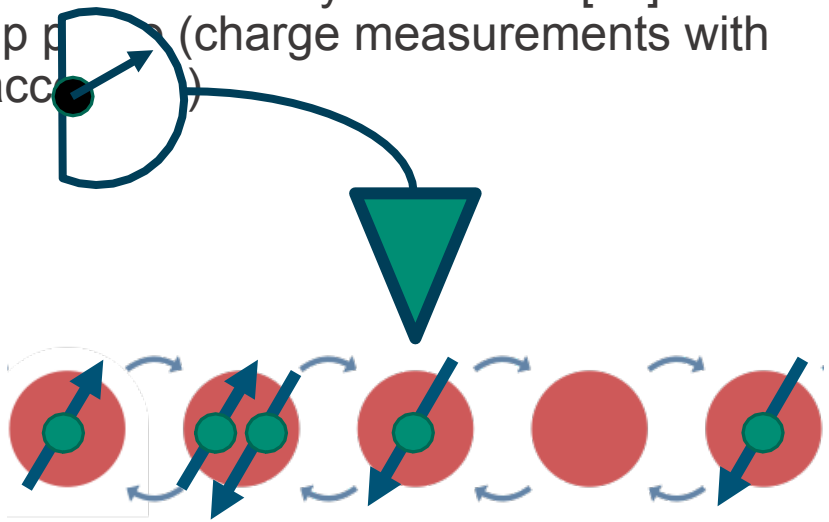
Intended donor chain

Placed donor chain

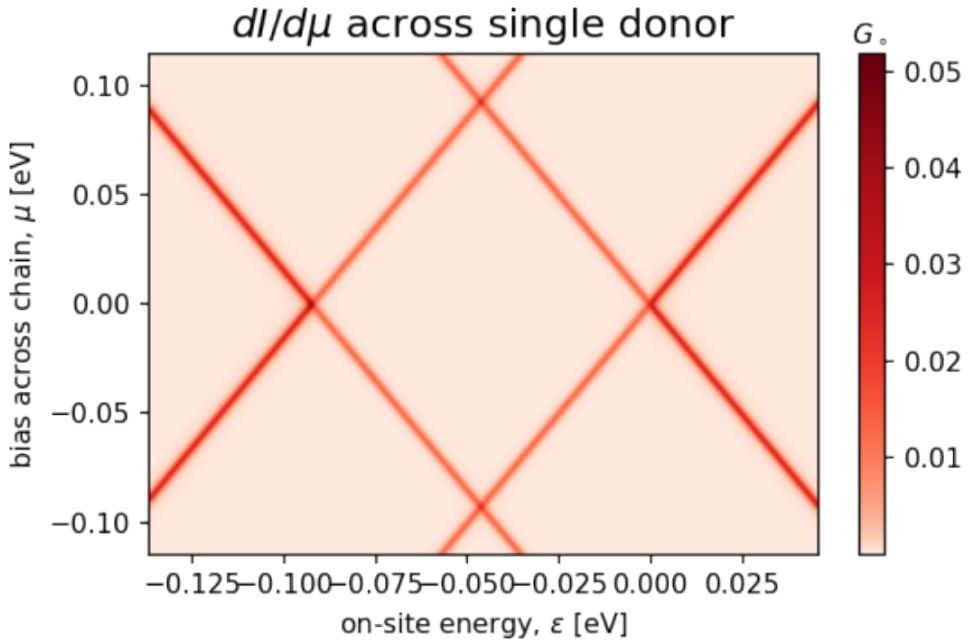
[10] B. Joecker et al., arXiv preprint: 2012.06293
[11] J. K. Gamble et al., *PRB* vol. 91, 235318 (2015)
[12] E. H. Lieb and F. Y. Wu, *PRL* vol. 20, 1445, (1968)

Measurements

- Charge/spin measurements of individual sites:
  - Pros: lot of information, correlations easy to see
  - Cons: very difficult to do
  - Demonstrated by Salfi et al. [13] with STM tip p… (charge measurements with acc…)



- Transport measurements:
  - Pros: comparatively easy to do, can determine model parameters
  - Cons: correlations not as clear, difficult to differentiate disorder and Mott physics
  - Demonstrated by Tan et al. [14], Fuechsle et al. [3], Prati et al. [7], etc.



[3] M. Fuechsle et al., *Nature Nano*. Vol. 7, p. 242–246 (2012)
[7] E. Prati et al., *Nature Nano*. vol. 7, p. 443–447 (2012)
[13] J. Salfi et al., *Nature Comm*. vol. 7, a. 11342 (2016)

Simulation of measurements

- Simulation of currents done using Green's function formalism
- Single-particle Green's function:

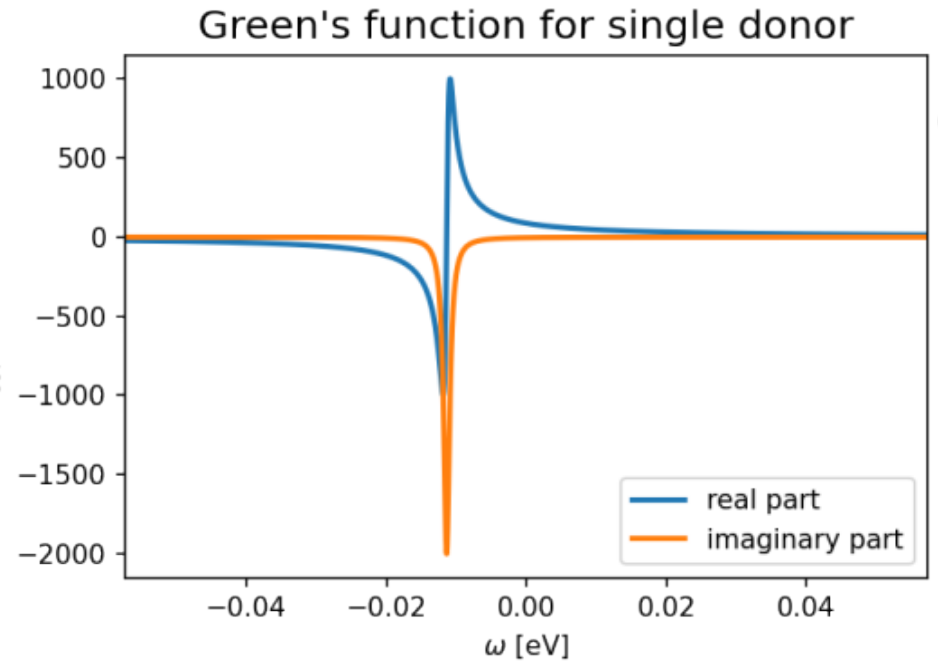
$$G_{jk\sigma}(\omega) = \sum_{\alpha} \left(\frac{\langle \psi_0 | \hat{c}_{j\sigma} | \psi_\alpha \rangle \langle \psi_\alpha | \hat{c}^{\dagger}_{k\sigma} | \psi_0 \rangle}{\omega - (E_\alpha - E_0)} + \frac{\langle \psi_\alpha | \hat{c}_{j\sigma} | \psi_0 \rangle \langle \psi_0 | \hat{c}^{\dagger}_{k\sigma} | \psi_\alpha \rangle}{\omega + (E_\alpha - E_0)} \right)$$

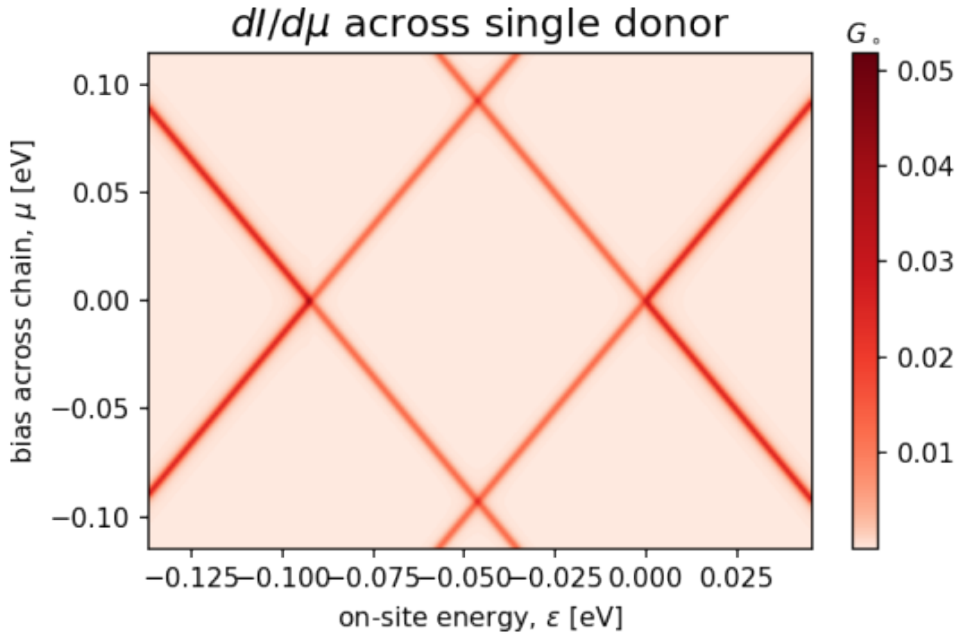
- Can be calculated exactly for small chains isolated from leads
- Effects of leads can then be approximated
- Current from lead L,

$$I_L = \frac{d}{dt} \langle \hat{n}_L \rangle$$

can be transformed w/ Green's functions into [15]

$$I_L = \int d\omega \, Tr\{\hat{\Sigma}^{<}_L \hat{G}^{A}_d + \hat{\Sigma}^{R}_L \hat{G}^{<}_d - \hat{\Sigma}^{<}_d \hat{G}^{A}_L - \hat{\Sigma}^{R}_d \hat{G}^{<}_L\}$$





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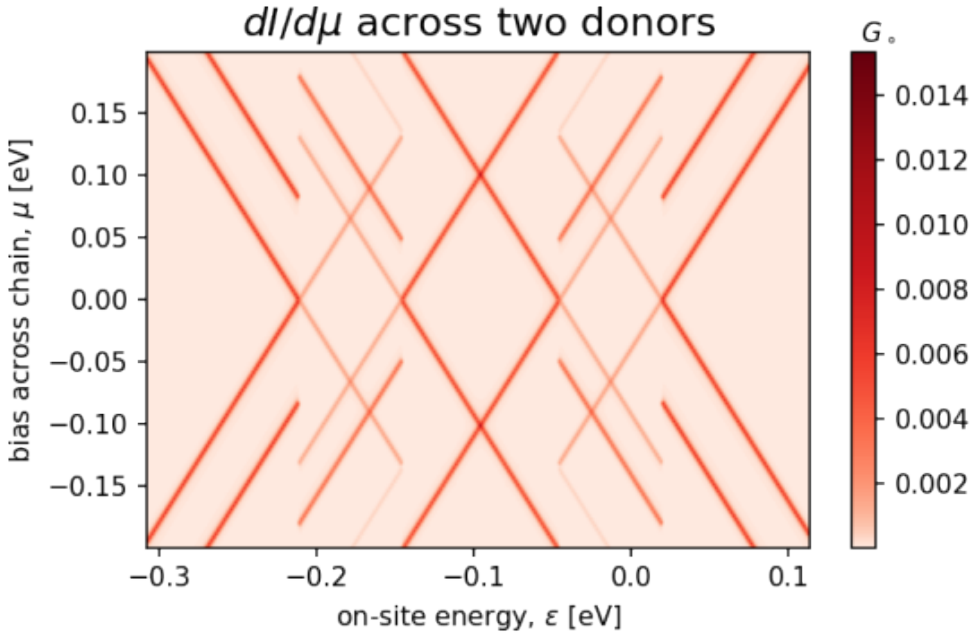
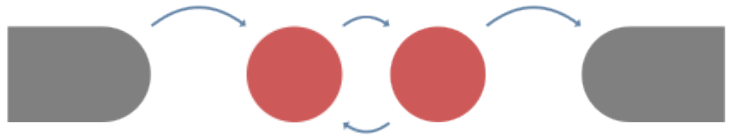
[15] Y. Meir, N. S. Wingreen, *PRL* vol. 68, 2512 (1992)

Example transport calculation: two-donor chain

- 2D bias spectrum calculated
  - On-site energies varied (e.g. by top gate)
  - Bias across chain varied
- Features:
  - Conductance peaks → charge transitions
  - Coulomb diamonds → charge states
- Here we have as many diamonds as possible charge states.
- How does this feature persist in longer chains with missing donors? What else can transport tell us?

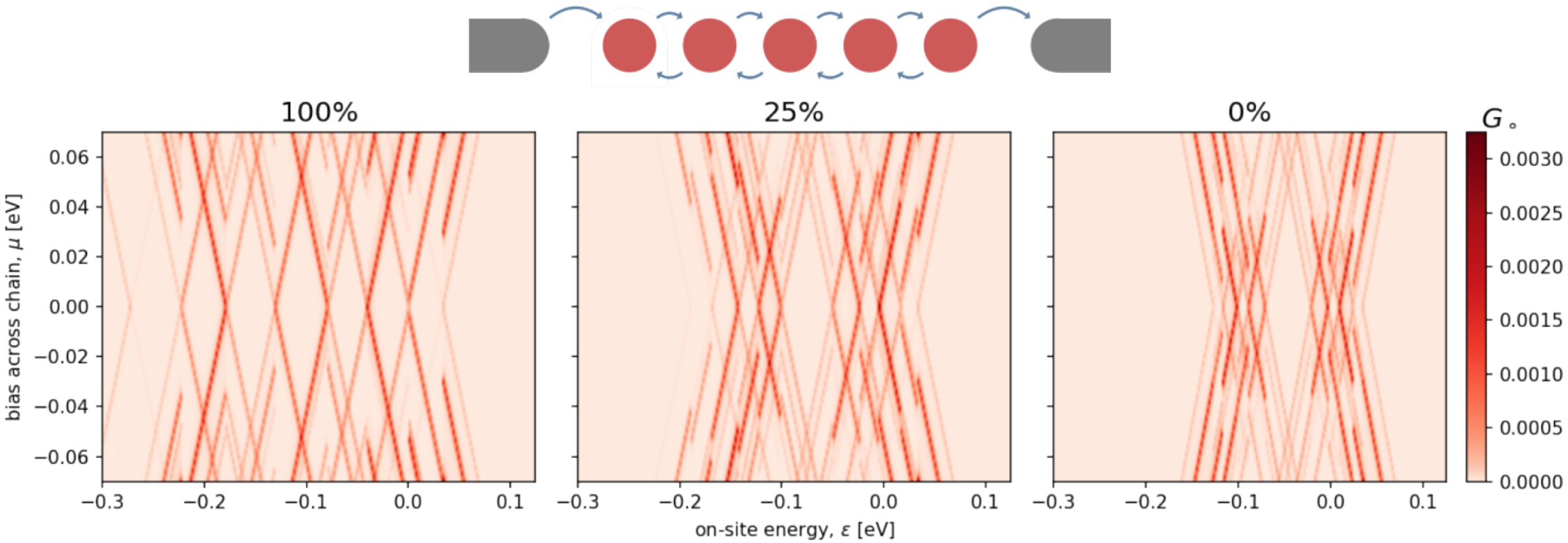




Long-range interactions spread out Coulomb diamonds

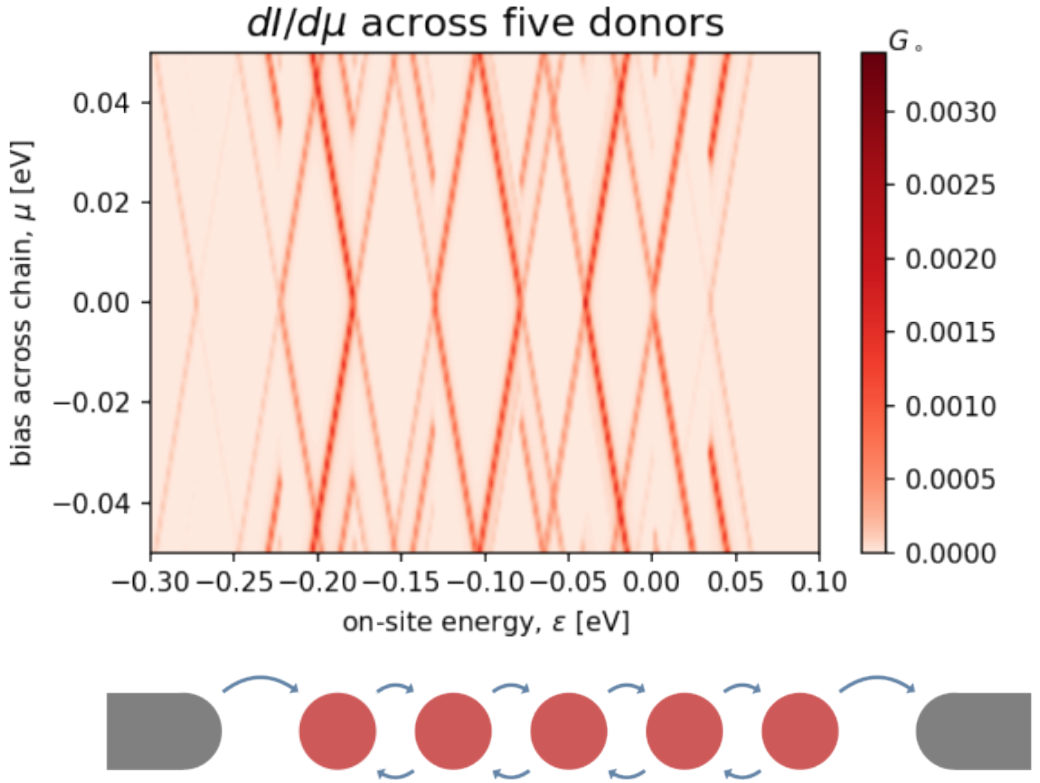
- Long-range interactions are critical in Si:P analog simulation. [6]
- How does transport change when we turn off these interactions?

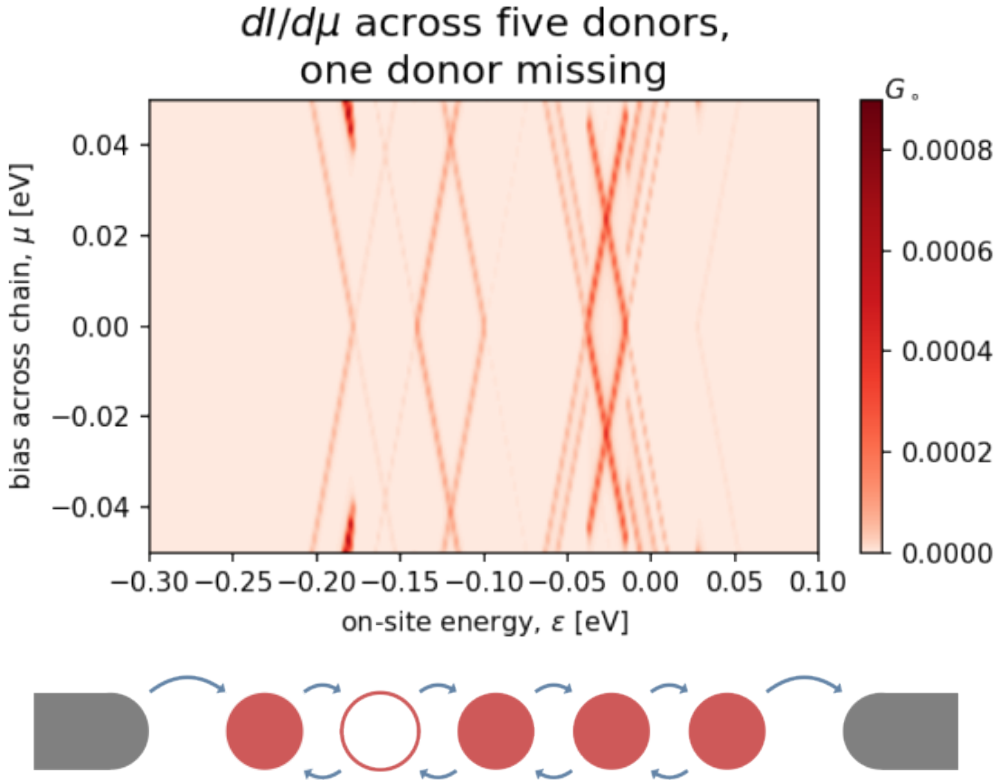
Example of 5 donor chain, 10 lattice sites apart:



Missing donors weaken transport signatures…

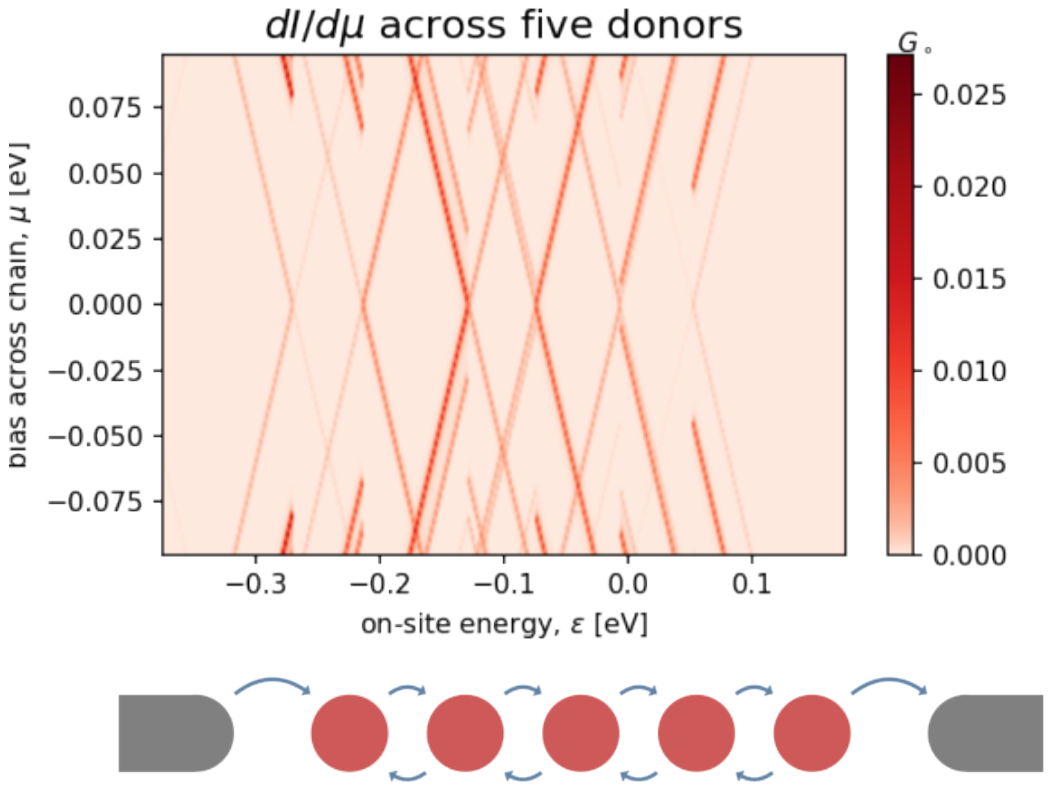
- Chains with donors 10 lattice sites apart: differential conductance peaks diminished
- For this spacing, the bulk limit has a spin-density wave: very sensitive to this disorder.

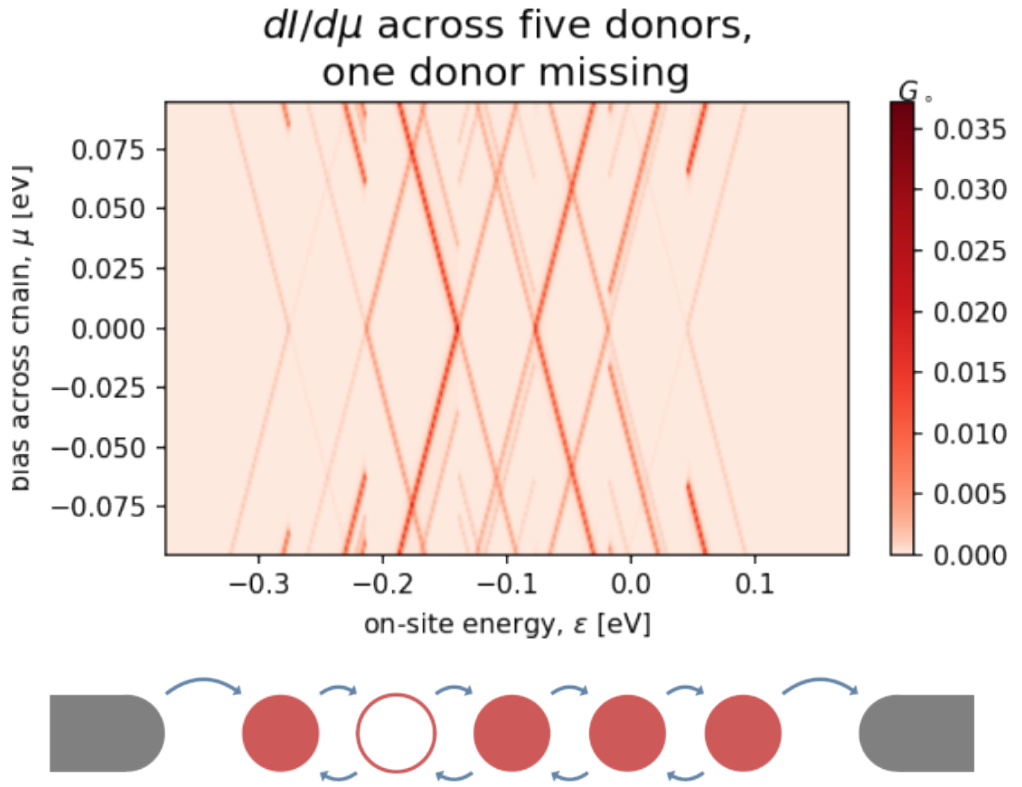




…unless the pitch is short enough

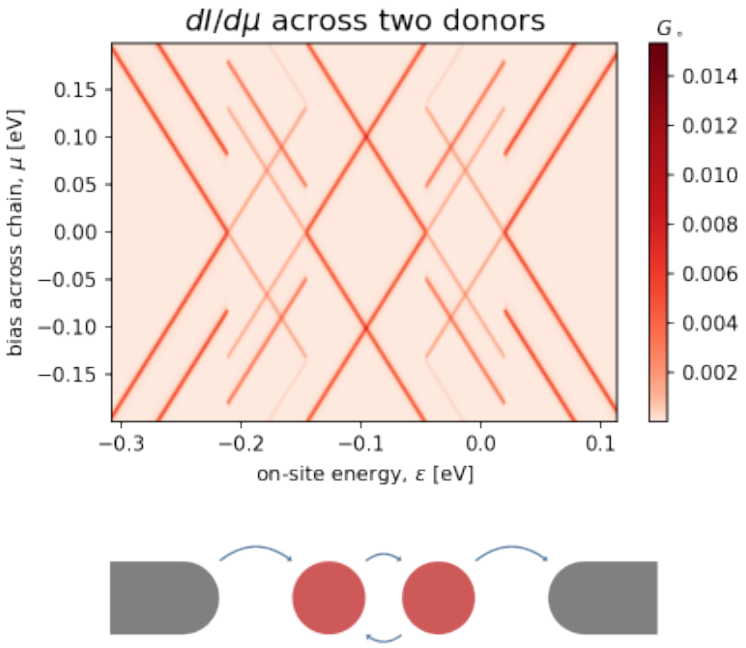
- Chains with donors 5 lattice sites apart: differential conductance peaks *grow*.
- For this spacing, the bulk limit has a charge density wave: less sensitive to this disorder.





Conclusions

- Precision placement of donors raises possibility of analog quantum simulation.
- Experimental imperfections require theoretical attention:
  - Variance in donor location: leaves average physics qualitatively similar
  - Incorporation statistics: unknown, explored here for 1D chain
- Focus on transport measurements:
  - Most accessible measurement.
  - Can give model parameters but be difficult to generally interpret.
- For 1D chain, qualitative effects depend on spacing of donor chain.
- Future work: what about 2D chains? Self-consistent electrostatics? Scattering states?



Thanks to my collaborators!

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Theory:

- Andrew Baczewski (advisor)
- Quinn Campbell
- Peter A. Schultz
- Richard Muller

Experiment:

- Jeffrey Ivie
- Justin Koepke
- Andrew Mounce
- Ezra Bussmann
- Shashank Misra

Citations

[1] A. M. Jakob et al., arXiv preprint: 2009.02892

[2] S. R. Schofield et al., vol. 91, 136104 (2003)

[3] M. Fuechsle et al., *Nature Nano*. vol. 7, p. 242–246 (2012)

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[5] N. H. Le et al., *PRB* 96, 245406 (2017)

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[8] J. A. Ivie et al., arXiv posting coming soon

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[14] K. Y. Tan et al., *Nano Lett.* 10, 1, 11–15 (2010)

[15] Y. Meir, N. S. Wingreen, *PRL* vol. 68, 2512 (1992)