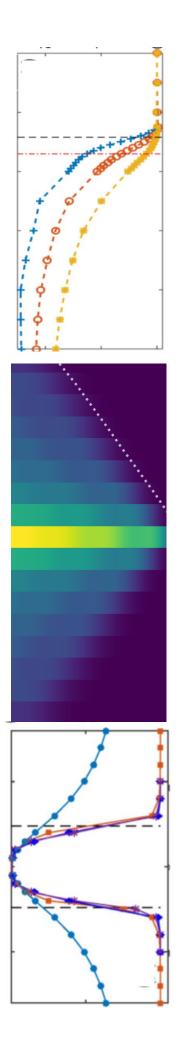




Singapore University of Technology and Design

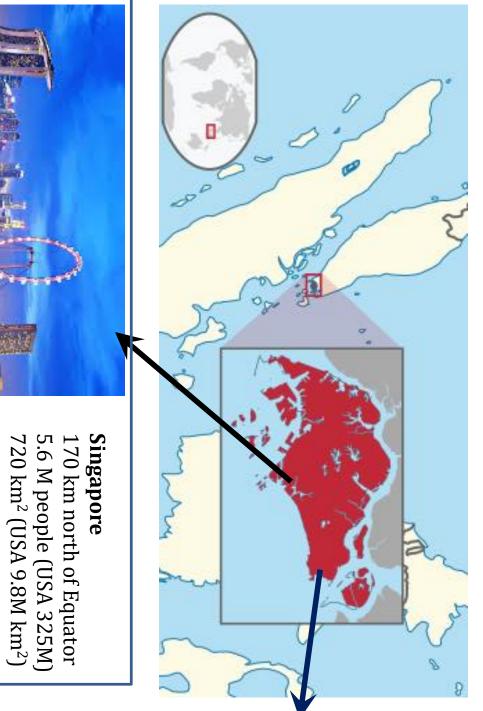
Dario Poletti





Many-body open quantum systems: about baths and transport

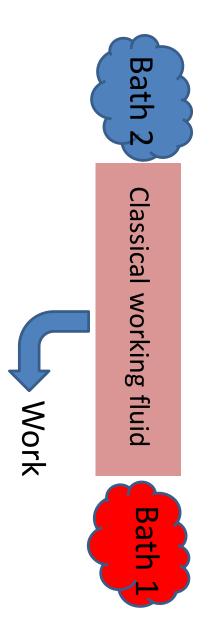
Thermodynamics of Quantum Systems

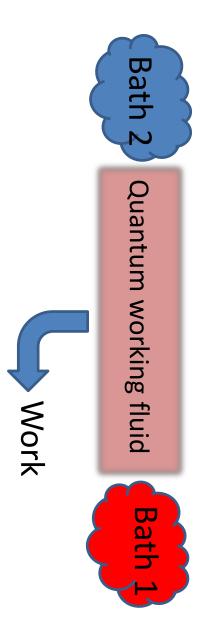


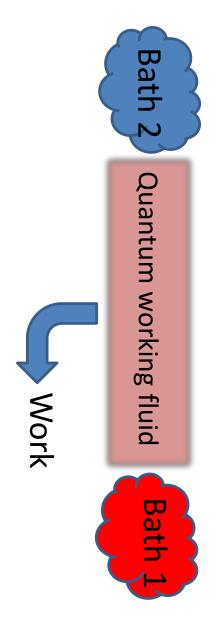


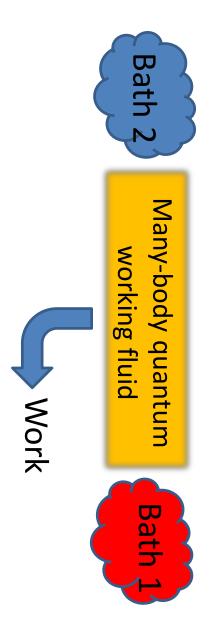
13% Malay 9% Indian 74% Chinese





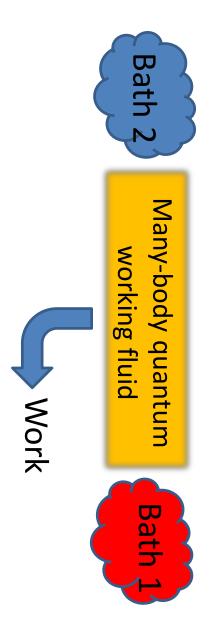




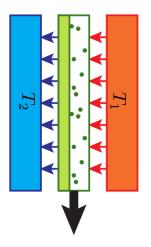








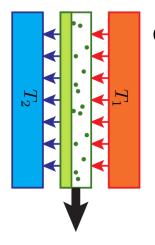
Phase transitions and latent heat in working fluid



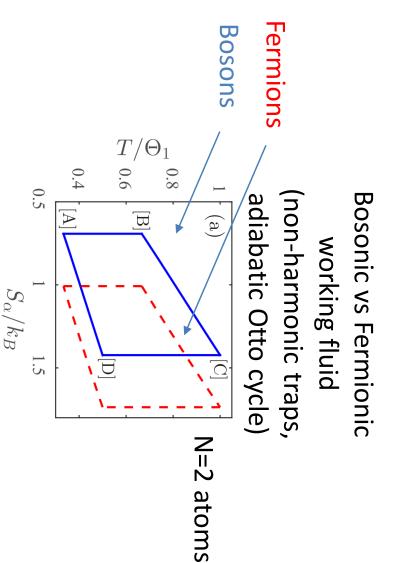
Campisi, Fazio, Nat. Comm. (2016)



Phase transitions and latent heat in working fluid



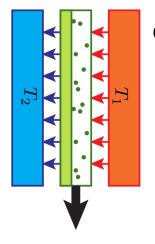
Campisi, Fazio, Nat. Comm. (2016)



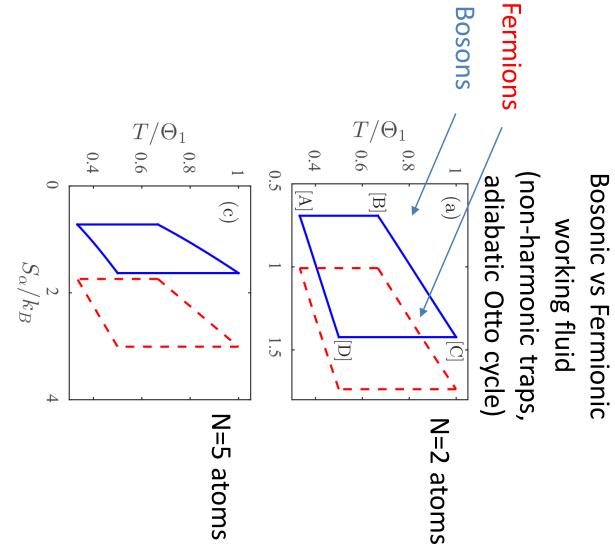
Zheng, Poletti, PRE (2015)



Phase transitions and latent heat in working fluid



Campisi, Fazio, Nat. Comm. (2016)

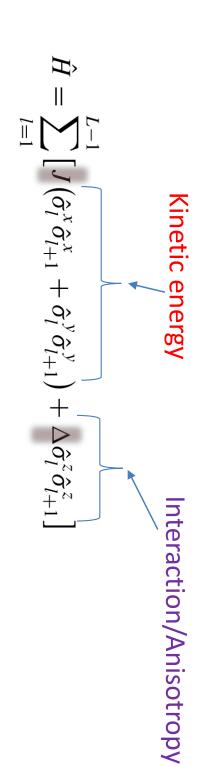


Zheng, Poletti, PRE (2015)

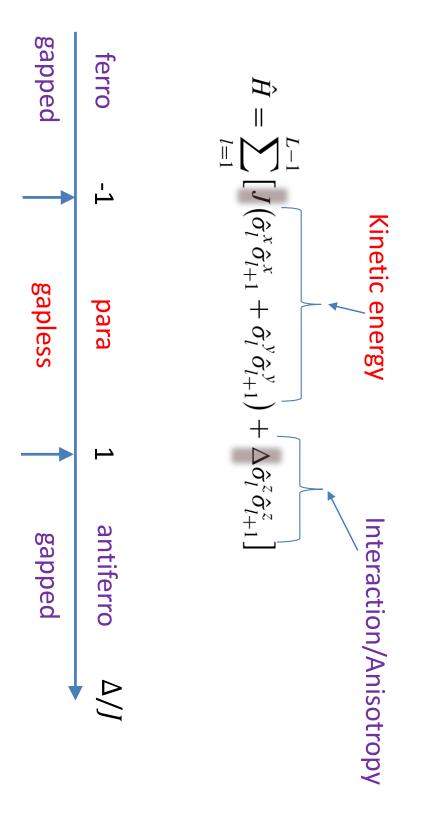
XXZ model

$$\hat{H} = \sum_{l=1}^{L-1} \left[J \left(\hat{\sigma}_l^x \hat{\sigma}_{l+1}^x + \hat{\sigma}_l^y \hat{\sigma}_{l+1}^y \right) + \Delta \hat{\sigma}_l^z \hat{\sigma}_{l+1}^z \right]$$

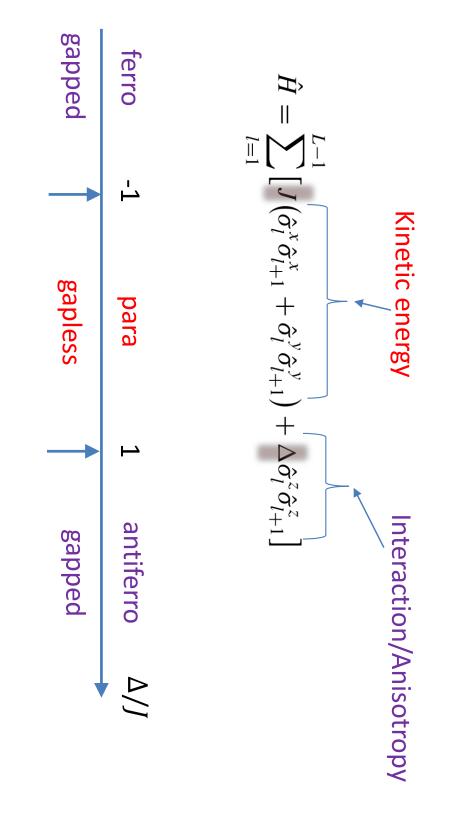
XXZ model



XXZ model

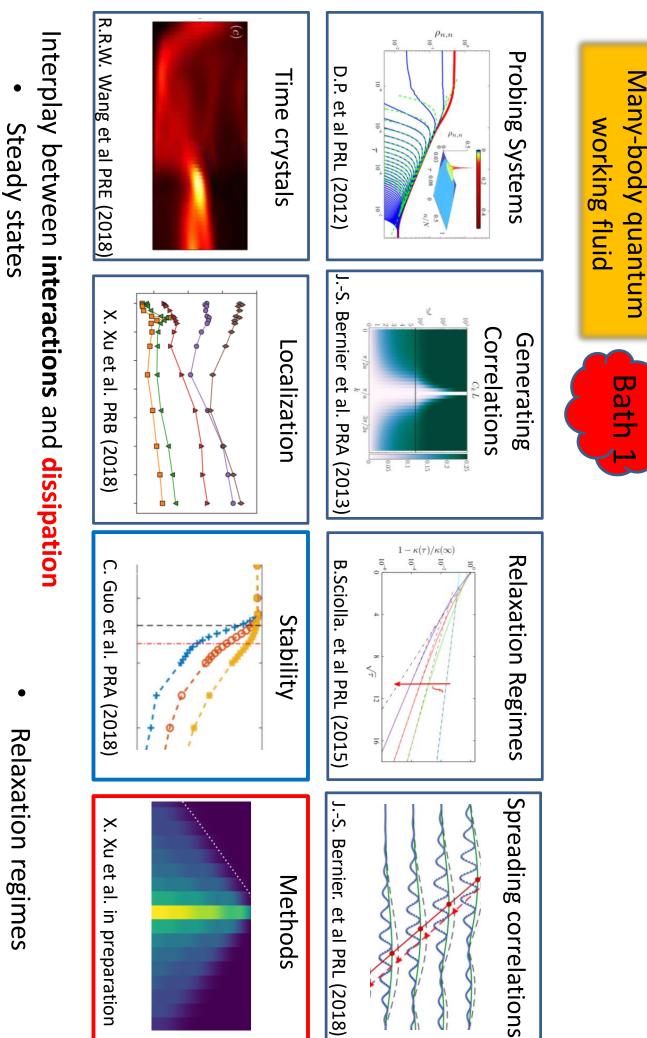


XXZ model



1D systems -> much more easily strongly correlated, tools





Out-of-equilibrium phase transitions Transient correlations

- Propagation correlations

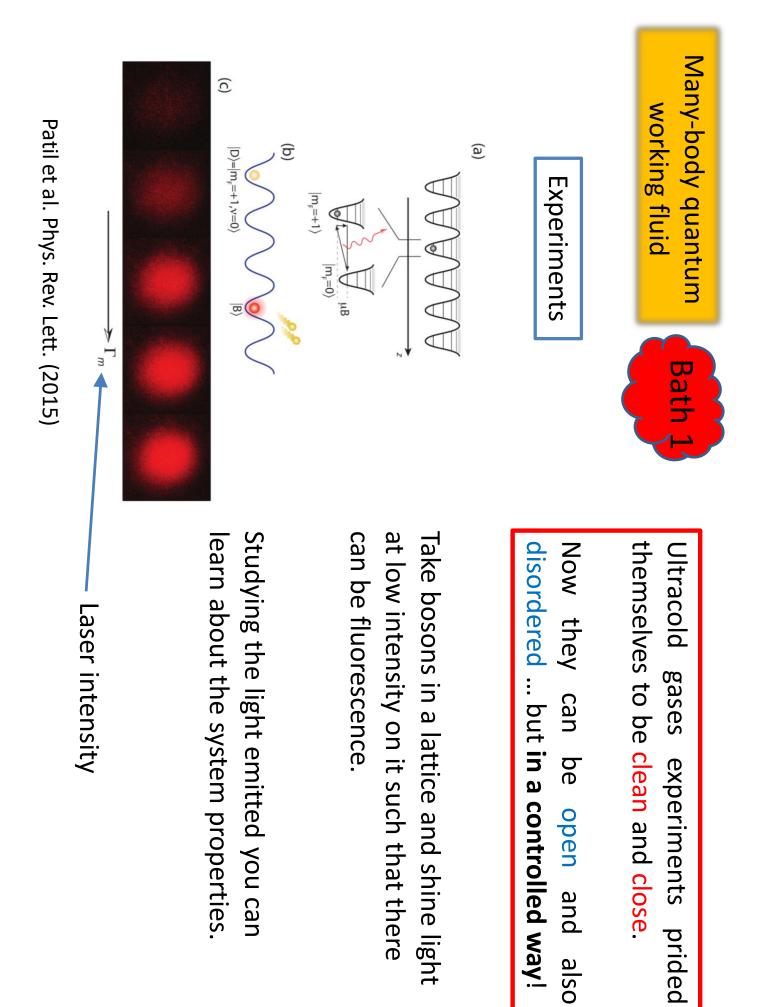
Methods

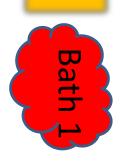


Experiments

Ultracold gases experiments prided themselves to be clean and close.

Now they can be open and also disordered ... but in a controlled way!

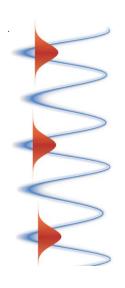




Experiments

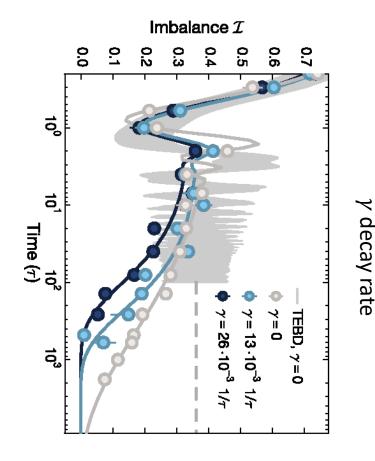
Take a strongly interacting disordered Hubbard model. It is many-body localized -> the population imbalance I between nearest sites stays large.

But once dephasing is applied the Imbalance will decay.

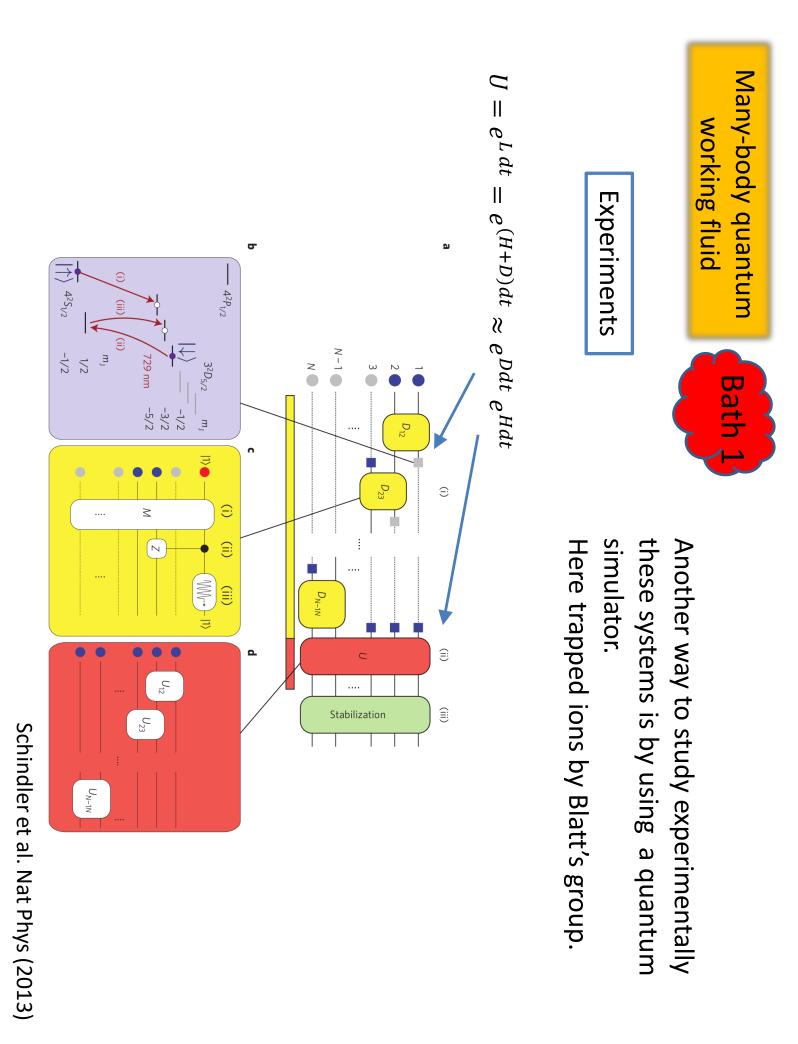


Ultracold gases experiments prided themselves to be clean and close.

Now they can be open and also disordered ... but in a controlled way!



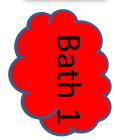
Luschen et al. Phys. Rev. X (2017)





Strategies to study manybody open quantum systems (which cannot be diagonalized)





Large (small) baths

- Couple the many-body system to another many-body system
- Represent the bath's harmonic oscillators as a chain

Local Lindblad master equations

Local jump operators (with or without unraveling)





Large (small) baths

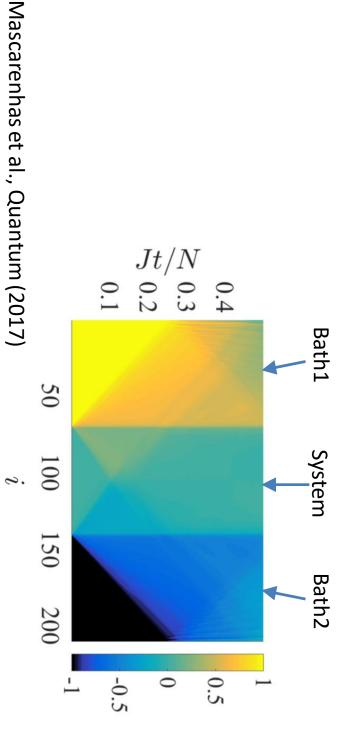
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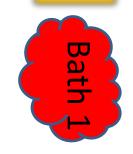
Large (small) baths

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Mascarenhas et al. Znidaric et al. Biella et al. Balachandran et al. Ponomarev et al.

:

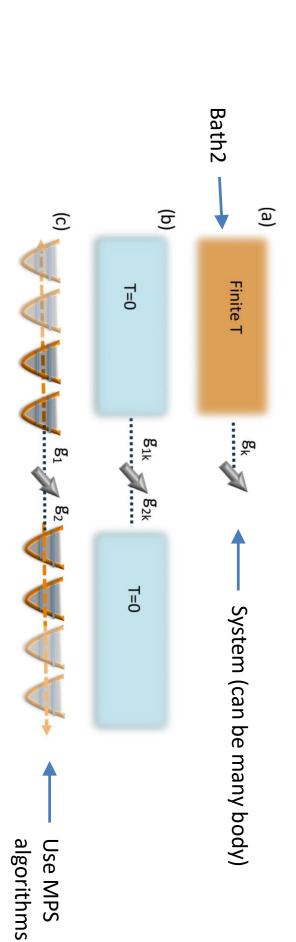


Strategies to study manybody open quantum systems (which cannot be diagonalized)

Large (small) baths

- Couple the many-body system to another many-body system
- Represent the bath's harmonic oscillators as a chain

Thermofield transformation + star to chain mapping



de Vega and Banuls, PRA (2015)





Local Lindblad master equations

Local jump operators (with or without unraveling)





Local Lindblad master equations

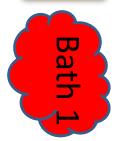
Local jump operators (with or without unraveling)

$$egin{aligned} &rac{d\hat{
ho}}{dt} = \mathcal{L}[\hat{
ho}] = -rac{i}{\hbar}[\hat{H},\hat{
ho}] + \mathcal{D}[\hat{
ho}] \ &rac{M^2-1}{\sum} \gamma_{kl}(t) \left[V_k arrho V_l^\dagger - rac{1}{2} \{ V_l^\dagger V_k, arrho \}
ight] \end{aligned}$$

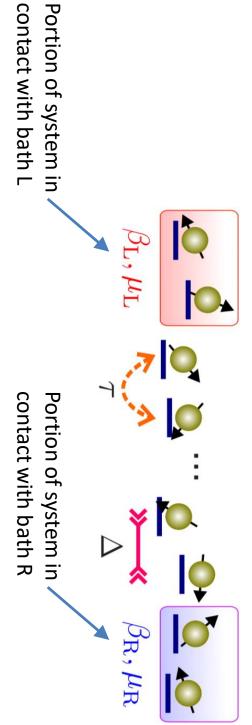
where V_k is local (most of the time single site).

 $l,k{=}1$





most promising is Local Lindblad master equations can be done in different ways. One of the



Prosen, Znidaric JStatMech (2009) MendozaArenas et al (2018)

Gelman et al., J. Chem. Phys. (2004) Torrontegui, Kosloff NJP (2016)



Another possibility is to use the method of surrogate Hamiltonian

Prosen, Znidaric JStatMech (2009) MendozaArenas et al (2018)

most promising is contact with bath L Portion of system in C $[\mathcal{D}_{\mathrm{L}}, \mu]$ contact with bath R Portion of system in $\beta_{
m R}, \mu_{
m R}$

Local Lindblad master equations can be done in different ways. One of the

Many-body quantum

Bath :

working fluid





which deserves to be studied further. How to effectively model baths for many-body quantum systems is something





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second law. master equations have been shown to result in apparent violations of the And remember that one needs to be careful, because single site local Lindblad

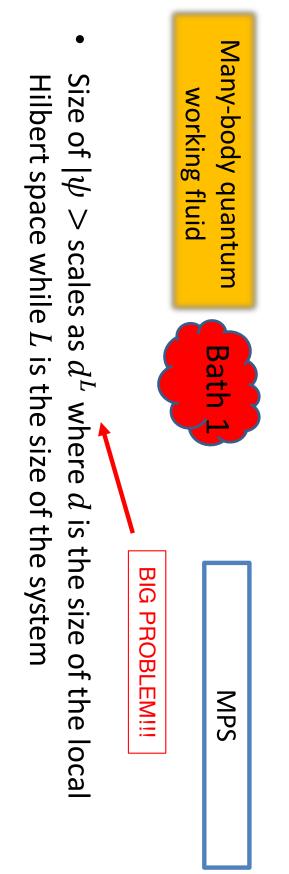
Levy, Kosloff, EPL (2014)

2 second law before this ... a little discussion on Matrix Product States and Operators 1 We show here one of the two approaches that we have been exploring. master equations have been shown to result in apparent violations of the And remember that one needs to be careful, because single site local Lindblad which deserves to be studied further. How to effectively model baths for many-body quantum systems is something Redfield master equation Thermofield transformation de Vega and Banuls, PRA (2015) Guo et al. PRA (2018) Redfield, J Res Dev (1957) Levy, Kosloff, EPL (2014)

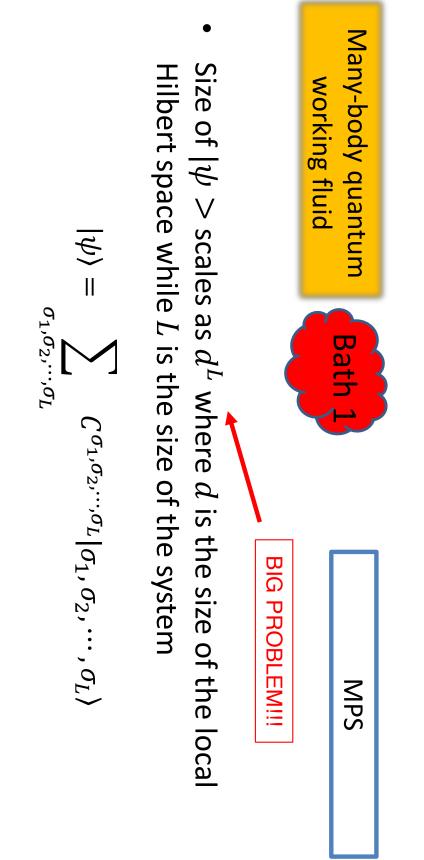
Many-body quantum

Bath 1

working fluid



 $|\psi\rangle =$ $\sigma_1, \sigma_2, \cdots, \sigma_L$ $C^{\sigma_1,\sigma_2,\cdots,\sigma_L}|\sigma_1,\sigma_2,\cdots,\sigma_L
angle$



tensors Rewrite $|\psi\rangle$ as the product of a series of 3-dimensional

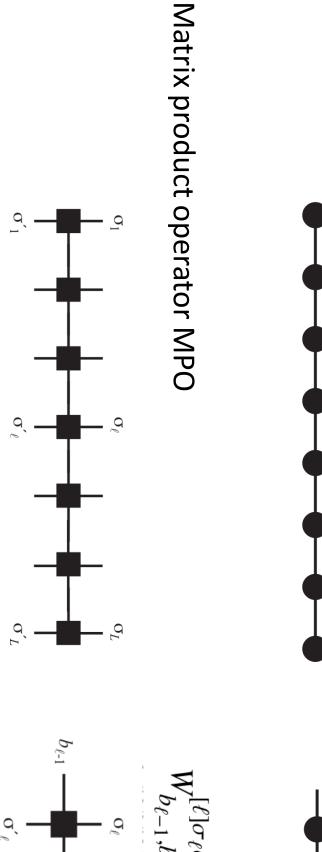
$$c_{\sigma_1,\dots,\sigma_L} = \sum_{\substack{a_1,a_2,\dots,a_{L+1}}} M_{a_1,a_2}^{\sigma_1} \frac{M_{a_2,a_3}^{\sigma_2}}{\dots M_{a_L,a_{L+1}}^{\sigma_L}} \dots M_{a_L,a_{L+1}}^{\sigma_L}$$

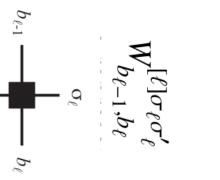
Now it scales polynomially with system size $\, dD^2L$

U. Schollwock, Ann. Phys. 326, 96 (2011)

Standard tool for 1dimensional quantum many body systems!











 $M^{\sigma_2}_{a_2,a_3}$

 $M_{a_1,a_2}^{\sigma_1} M_{a_2,a_3}^{\sigma_2} \cdots M_{a_L,a_{L+1}}^{\sigma_L}$

 σ_L

<u>q</u>

MPS

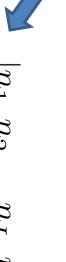


MPS

For the simulation we map the density operator to a state $\left|\hat{
ho}
ight
angle$ by the manning

by the mapping

 $|n_1, n_2 \dots n_L \rangle \langle n'_1, n'_2 \dots n'_L |$



 $|n_1, n_2 \dots n_L, n'_1, n'_2 \dots n'_L \rangle$

example with dephasing $+\gamma\sum_{j}\left(\hat{n}_{j}\right)$ $=\mathcal{L} \hat{\rho}\rangle\rangle$	$rac{d \hat ho angle}{dt}=-rac{\mathrm{i}}{\hbar}\left(\hat{H}\otimes1 ight)$	The evolution is then given by	$ n_1, n_2 \dots n_L \rangle \langle n_1', n_2' \dots n_L' $	For the simulation we map the density operator to a by the mapping	Many-body quantum working fluid
$\hat{n}_j \otimes \hat{n}_j - rac{1}{2} (\hat{n}_j^2 \otimes 1 + 1 \otimes \hat{n}_j^2) ig) \hat{ ho} angle$	 	$ n_1, n_2 \dots n_L, n_1', n_2' \dots n_L'\rangle$		erator to a state $ ho angle angle$	MPS

Verstraete et al., PRL.(2004)

$$|\hat{\rho}\rangle\rangle = \sum_{\{n_j, n'_k\}} M_1 \dots M_i \dots M_L | n_1, n_2 \dots n_L, n'_1, n'_2 \dots n'_L \rangle\rangle$$
Verstraete et al., PRL (2)

And we use matrix product states (or exact diagonalization) with number conservation in bra and ket

$$\begin{split} \frac{d|\hat{\rho}\rangle\!\!\rangle}{dt} &= -\frac{\mathrm{i}}{\hbar} \left(\hat{H} \otimes \mathbf{1} - \mathbf{1} \otimes \hat{H}^{\mathsf{t}} \right) |\hat{\rho}\rangle\!\!\rangle \\ &+ \gamma \sum_{j} \left(\hat{n}_{j} \otimes \hat{n}_{j} - \frac{1}{2} (\hat{n}_{j}^{2} \otimes \mathbf{1} + \mathbf{1} \otimes \hat{n}_{j}^{2}) \right) |\hat{\rho}\rangle\!\!\rangle \\ \text{example with dephasing} &= \mathcal{L}|\hat{\rho}\rangle\!\!\rangle \end{split}$$

Bath 1

Many-body quantum

working fluid

For the simulation we map the density operator to a state $\left|\hat{
ho}
ight
angle$ by the manning

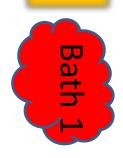
by the mapping

$$|n_1, n_2 \dots n_L \rangle \langle n'_1, n'_2 \dots n'_L \rangle$$

The evolution is then given by

 $|n_1, n_2 \cdots n_L, n'_1, n'_2 \cdots n'_L \rangle$

MPS



MPS

Using stochastic trajectories is of course also possible.

Daley, Adv. Phys. (2014)

density matrix). accurate evolution is less for stochastic evolution of for purification (evolution of the However it is dynamics dependent whether the needed bond dimension D for an

Bonnes, Lauchli, arXiv:1411.4831

Both methods are used.



Redfield with MPS



X. Xu SUTD



C. Guo SUTD/ZISTI

Luxembourg

J. Thingna



+ D.P.



 $H_{\rm tot} = H_S + H_B + \gamma S \otimes B$



 $H_{\rm tot} = H_S + H_B + \gamma S \otimes B$

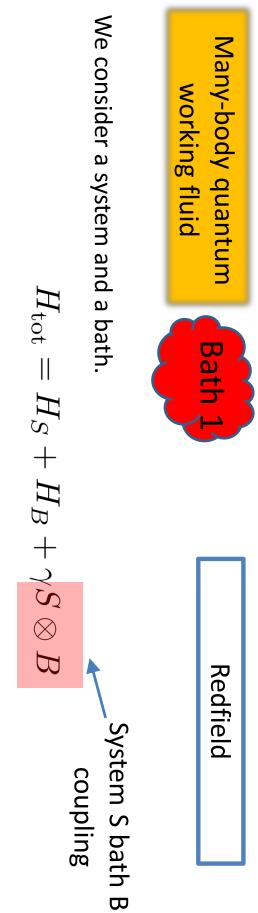
Consider weak coupling, γ small, Born-Markov approximation $\rho_{\rm tot} \approx \rho(t) \otimes \rho_B$

It is possible to write a second-order master equation in this form

$$\frac{\partial \rho(t)}{\partial t} = -i \left[H_{\rm S}, \rho(t) \right] - \mathcal{R}^t \left[\rho(t) \right]$$

$$\begin{array}{c} \mbox{Many-body quantum} \mbox{Werking fluid} \mbox{Hath} \mbox{Redfield} \mbox{Redfield} \mbox{System and a bath.} \mbox{We consider a system and a bath.} \mbox{H}_{tot} = H_S + H_B + \gamma \underline{S \otimes B} \mbox{System S bath B} \mbox{Coupling, } y \mbox{ small, Born-Markov approximation} \mbox{$\rho_{tot} \approx \rho(t) \otimes \rho_B$} \mbox{Consider weak coupling, } y \mbox{ small, Born-Markov approximation} \mbox{$\rho_{tot} \approx \rho(t) \otimes \rho_B$} \mbox{It is possible to write a second-order master equation in this form} \mbox{$\frac{\partial \rho(t)}{\partial t} = -i[H_S, \rho(t)] - \mathcal{R}^t[\rho(t)] \mbox{ρ_B} \mbox{$Mhere} \mbox{$\mathcal{R}^t[\cdot] = [S, \mathbb{S}(t) \cdot] + [\cdot \mathbb{S}^\dagger(t), S] \mbox{γ}} \mbox{γ} \mbox{γ} \mbox{$Mhere} \mbox{$\mathcal{R}^t[\cdot] = [S, \mathbb{S}(t) \cdot] + [\cdot \mathbb{S}^\dagger(t), S] \mbox{γ}} \mbox{γ} \mbox{Σ} \mbox{γ} \mb$$

and
$$\mathbb{S}(t) = \int_0^t \tilde{S}(-\tau) C(\tau) d\tau$$
 with $\tilde{S}(\tau) = e^{iH_S\tau} S e^{-iH_S\tau}$
and $\tilde{C}(\tau) = \operatorname{tr}(e^{iH_B\tau} B e^{-iH_B\tau} B \rho_B)$
Bath 2-time correlations



Consider weak coupling, γ small, Born-Markov approximation $\rho_{\rm tot} \approx \rho(t) \otimes \rho_B$

It is possible to write a second-order master equation in this form

$$\frac{\partial \rho \left(t \right)}{\partial t} = -\operatorname{i} \left[H_{\mathrm{S}}, \rho \left(t \right) \right] - \mathcal{R}^{t} \left[\rho(t) \right]$$

Where
$$\mathcal{R}^{t}[\cdot] = [S, \mathbb{S}(t) \cdot] + [\cdot \mathbb{S}^{\dagger}(t), S]$$

Solved usually by exact

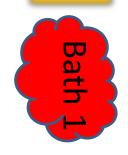
system Hamiltonian!

diagonalization of

many-body systems

Quickly difficult for

Where
$$\mathcal{R}^{t}[\cdot] = [S, \mathbb{S}(t) \cdot] + [\cdot \mathbb{S}^{\dagger}(t), S]$$



Redfield with MPS



Redfield with MPS

We now show how to study large(r) system with Redfield and MPS

We consider the system coupled to the bath only in the centre of the chain

$$S = \mathbf{1} \bigotimes \cdots \bigotimes \mathbf{1} \bigotimes \sigma_0^x \bigotimes \mathbf{1} \bigotimes \cdots \bigotimes \mathbf{1}$$

This can be seen as an MPO which we then evolves in time



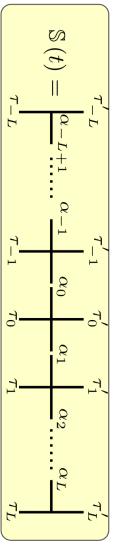
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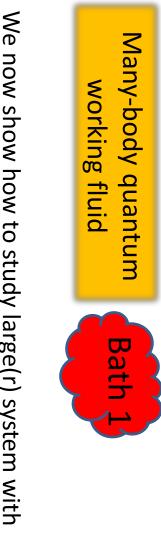
$$S = \mathbf{1} \bigotimes \cdots \bigotimes \mathbf{1} \bigotimes \sigma_0^x \bigotimes \mathbf{1} \bigotimes \cdots \bigotimes \mathbf{1}$$

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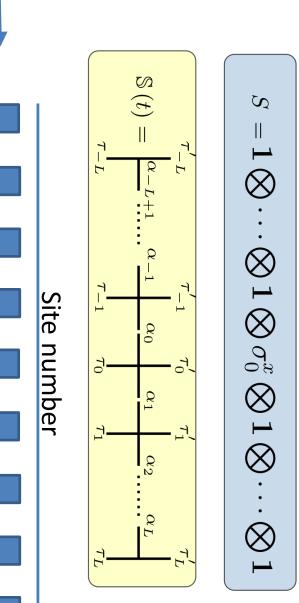
Trotterized evolution and convolution with bath correlations

 $\tilde{S}(\tau) = \mathrm{e}^{\mathrm{i}H_{\mathrm{S}}\tau}S\mathrm{e}^{-\mathrm{i}H_{\mathrm{S}}\tau}$ $\mathbb{S}\left(t\right) = \int_{0}^{\cdot} \tilde{S}\left(-\tau\right) C\left(\tau\right) d\tau$

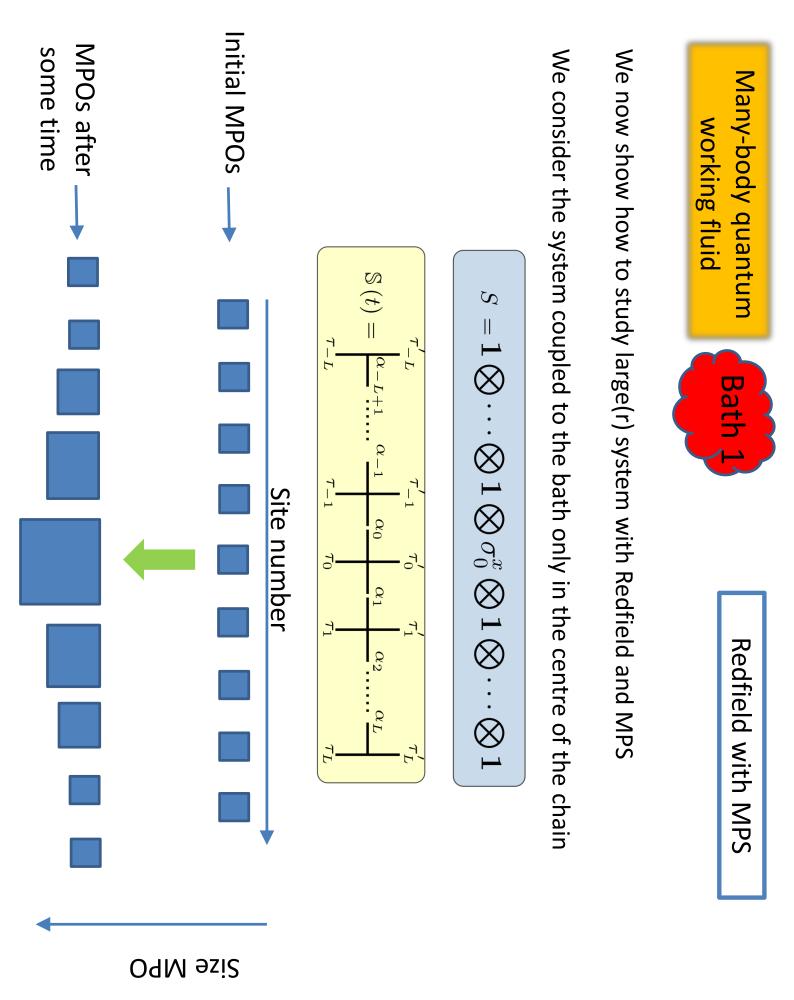


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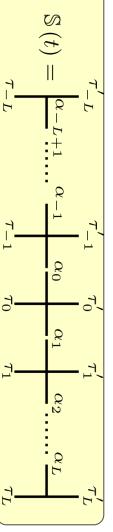


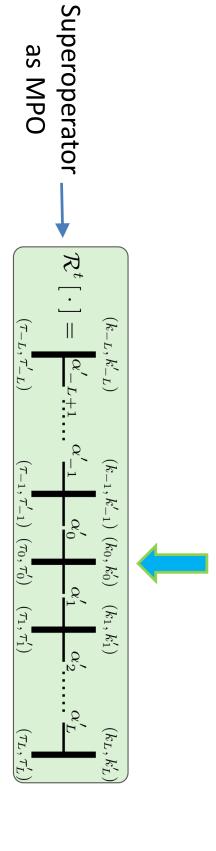


We now show how to study large(r) system with Redfield and MPS

We consider the system coupled to the bath only in the centre of the chain



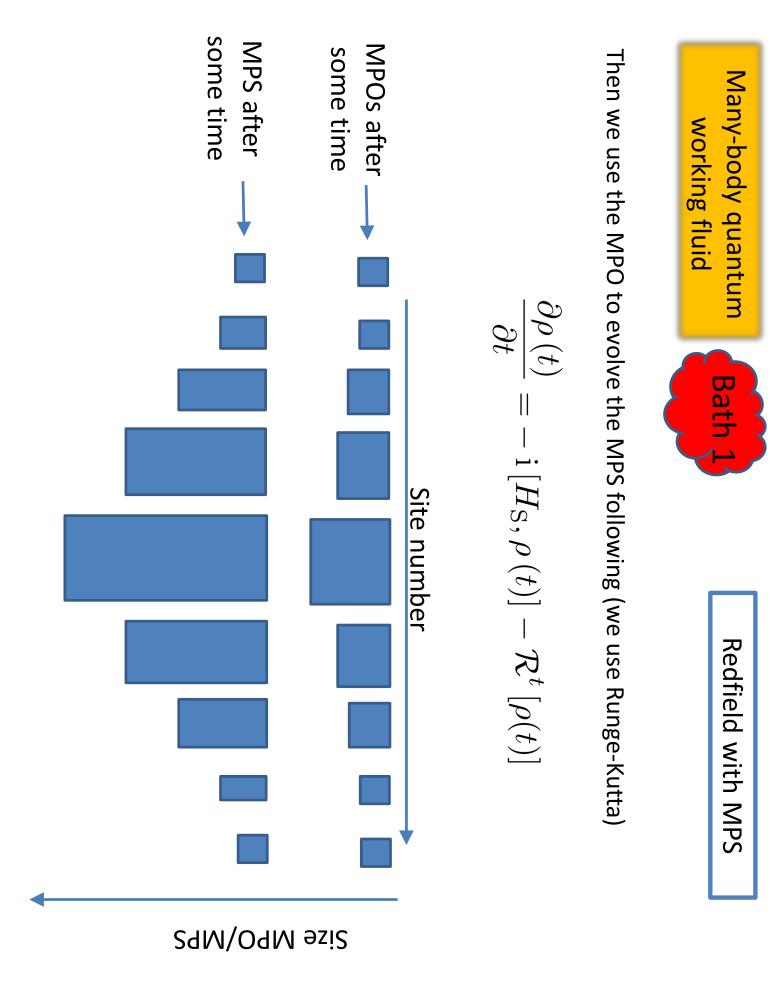






Then we use the MPO to evolve the MPS following (we use Runge-Kutta)

$$\frac{\partial \rho(t)}{\partial t} = -i \left[H_{\rm S}, \rho(t) \right] - \mathcal{R}^t \left[\rho(t) \right]$$



$$\begin{array}{ll} \mbox{Many-body quantum} & \mbox{Mat we got} & \mbox{Mat we got} & \mbox{Mat we got} & \mbox{Hat we got} & \mbox{Hat } &$$

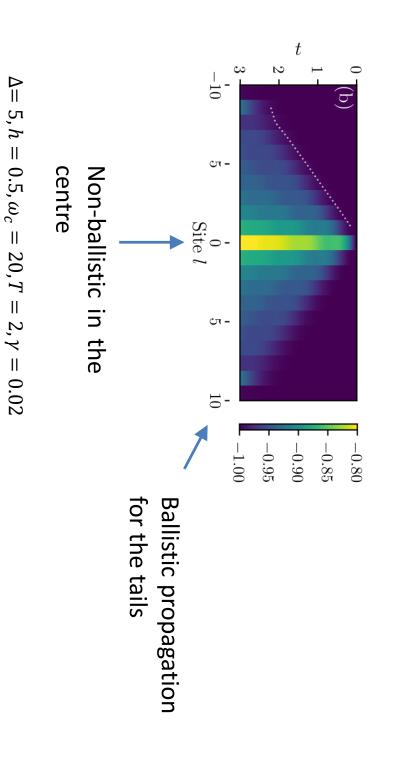




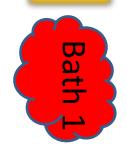
What we got

Let us look at the local magnetization versus time for different positions



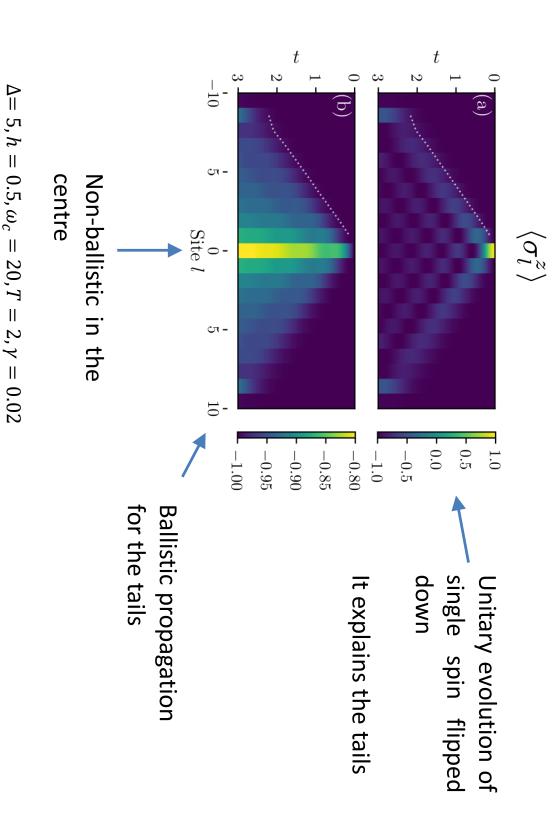




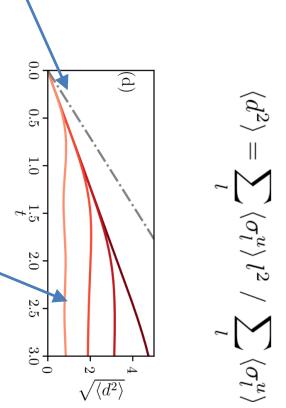


What we got

Let us look at the local magnetization versus time for different positions



5, 9, 13 and 21 spins Dissipative evolution for



how the perturbation due to the bath propagates in the system.

To study the evolution we look at

$$\langle d^2 \rangle = \sum \langle \sigma_l^u \rangle l^2 / \sum \langle \sigma_l^u \rangle$$

$$\left\langle d^2 \right\rangle = \sum_l \left\langle \sigma^u_l \right\rangle l^2 \ / \ \sum_l \left\langle \sigma^u_l \right\rangle$$

$$\langle d^2
angle = \sum_l \left< \sigma_l^u \right> l^2 \ / \ \sum_l \left< \sigma_l^u \right>$$

$$\langle d^2
angle = \sum_l \left< \sigma_l^u \right> l^2 / \sum_l \left< \sigma_l^u \right>$$

$$\langle d^2 \rangle = \sum_l \left< \sigma_l^u \right> l^2 \ / \ \sum_l \left< \sigma_l^u \right>$$

$$\langle d^2
angle = \sum_l \langle \sigma^u_l \rangle \, l^2 \, / \, \sum_l \langle \sigma^u_l \rangle$$

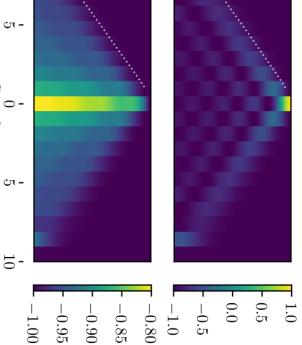
$$\left\langle d^2 \right\rangle = \sum_{l} \left\langle \sigma^u_l \right\rangle l^2 \ / \ \sum_{l} \left\langle \sigma^u_l \right\rangle$$

$$\langle d^2 \rangle = \sum \langle \sigma_l^u \rangle l^2 / \sum \langle \sigma_l^u \rangle$$

$$\left\langle d^{2}
ight
angle =\sum_{l}\left\langle \sigma_{l}^{u}
ight
angle l^{2}$$
 / $\sum_{l}\left\langle \sigma_{l}^{u}
ight
angle$

$$\langle d^2
angle = \sum_l \left< \sigma^u_l \right> l^2$$
 ,

$$-0.0 \\ -0.5 \\ -0.80 \\ -0.90 \\ -0.95$$



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 $\langle \sigma_l^z
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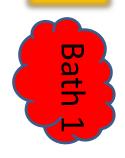






Many-body quantum

What we got



What we got

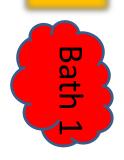
We compare Redfield to master equations in Lindblad limit

1) Singular coupling limit

$$\mathcal{T}(au) pprox 2\gamma T\delta(au)$$

 Local Hamiltonian neglect couplings between sites Wichterich et al. PRE (2007)





What we got

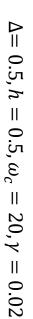
We compare Redfield to master equations in Lindblad limit

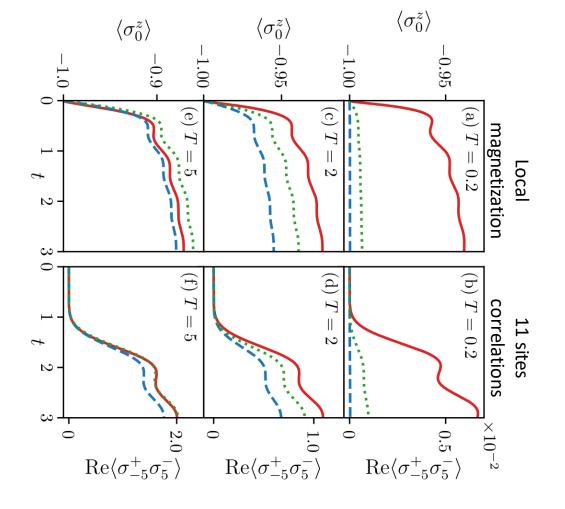
1) Singular coupling limit

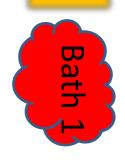
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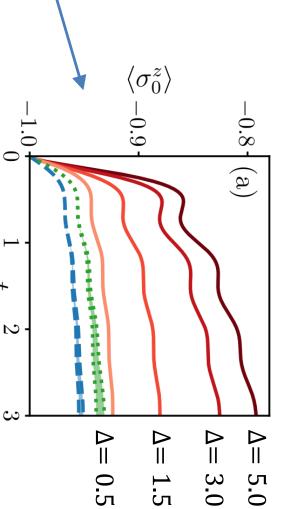
1) Singular coupling limit

$$\mathcal{C}(\tau) \approx 2\gamma T \delta(\tau)$$

Different interactions

 Local Hamiltonian neglect couplings between sites Wichterich et al. PRE (2007)

Both approaches which give Lindblad evolutions struggle to capture the dependence on the interaction





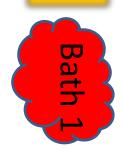
Conclusions

Many-body quantum systems can be a useful working fluid

Important to model properly baths for them

We showed how to use the Redfield master equation for large systems

regimes. We showed that thanks to this master equation we can explore a much broader set of



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Outlook

Steady states with Redfield and MPS? Time-dependence?

:





Rectification



V. Balachandran





E. Pereira



Physical Review Letters 120, 200603 (2018)



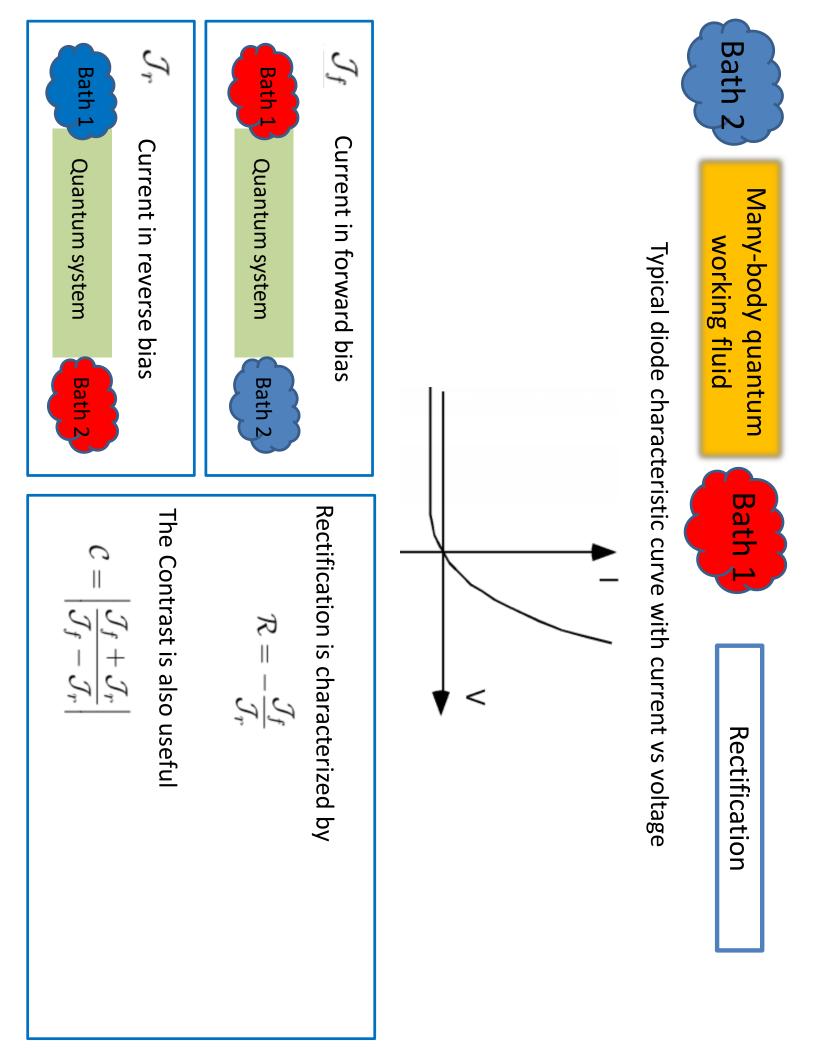
G. Benenti

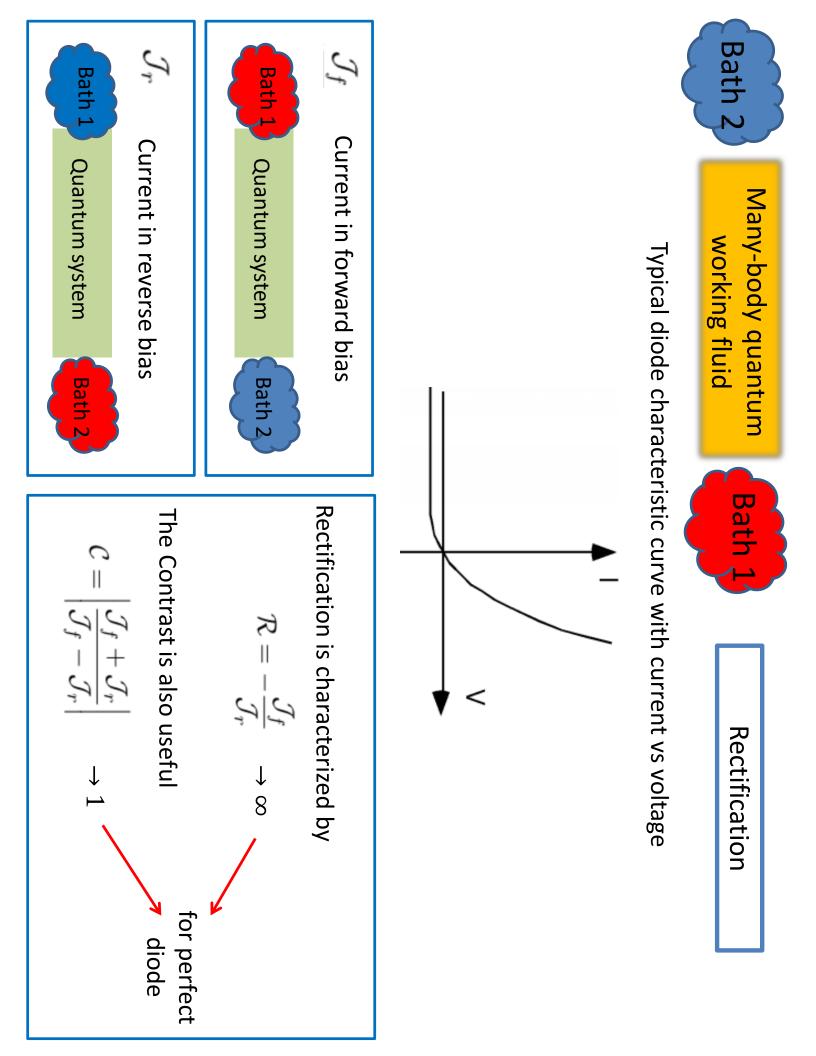


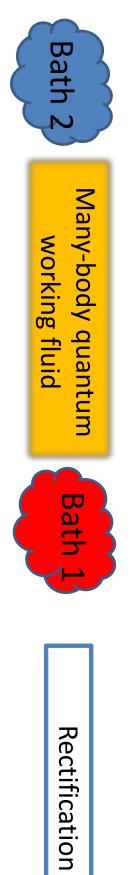
G. Casati



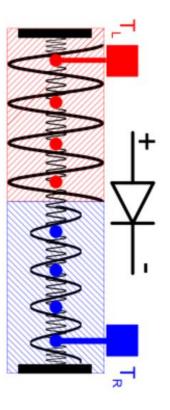
+ D.P.



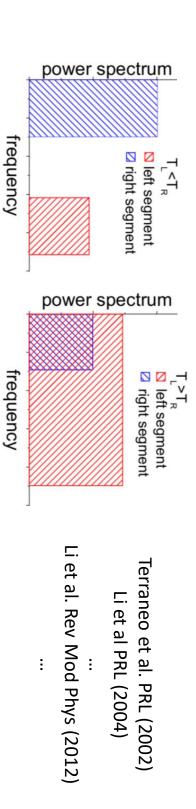


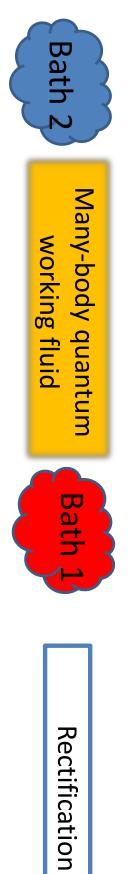


broken. Consider a classical chain of particles with **nonlinear** couplings and reflection symmetry

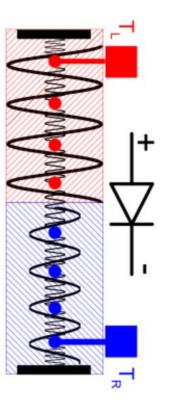


These ingredients allow a diode to function.

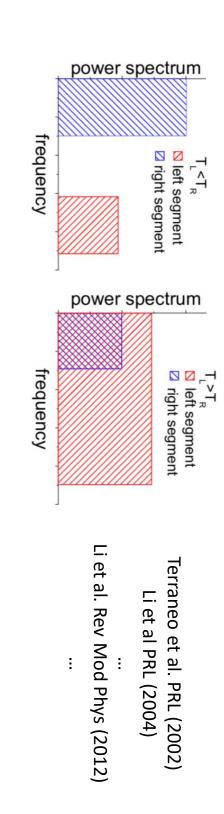




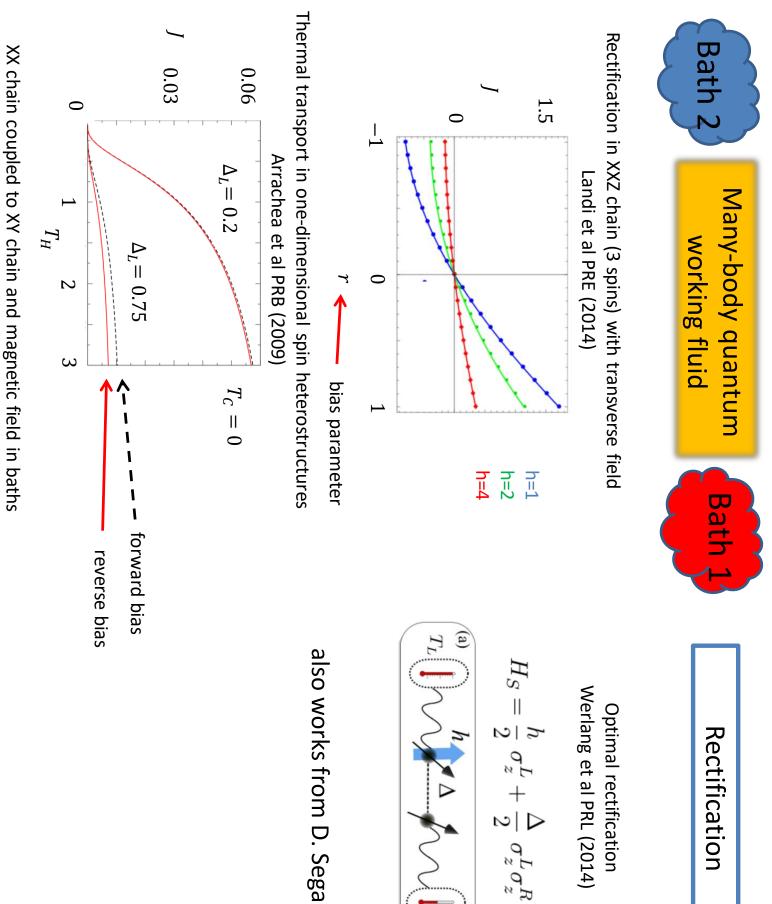
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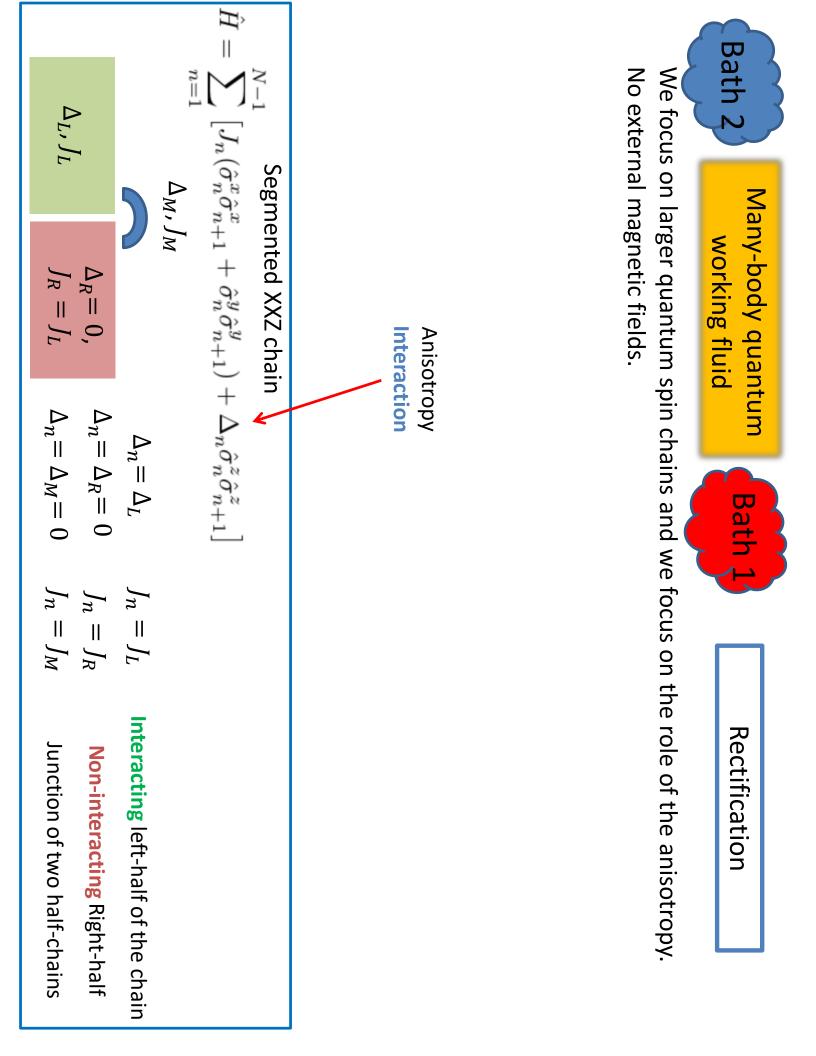


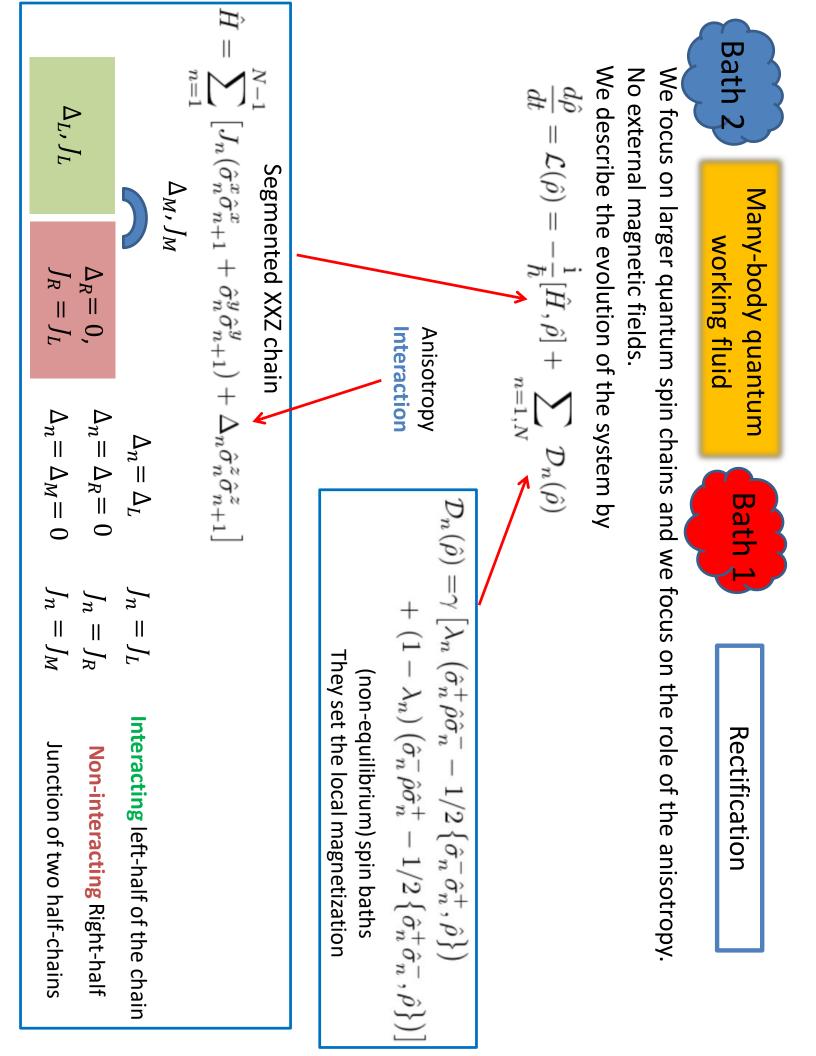
It is natural to try to understand what happens in the quantum regime **nonlinear** → strongly interacting

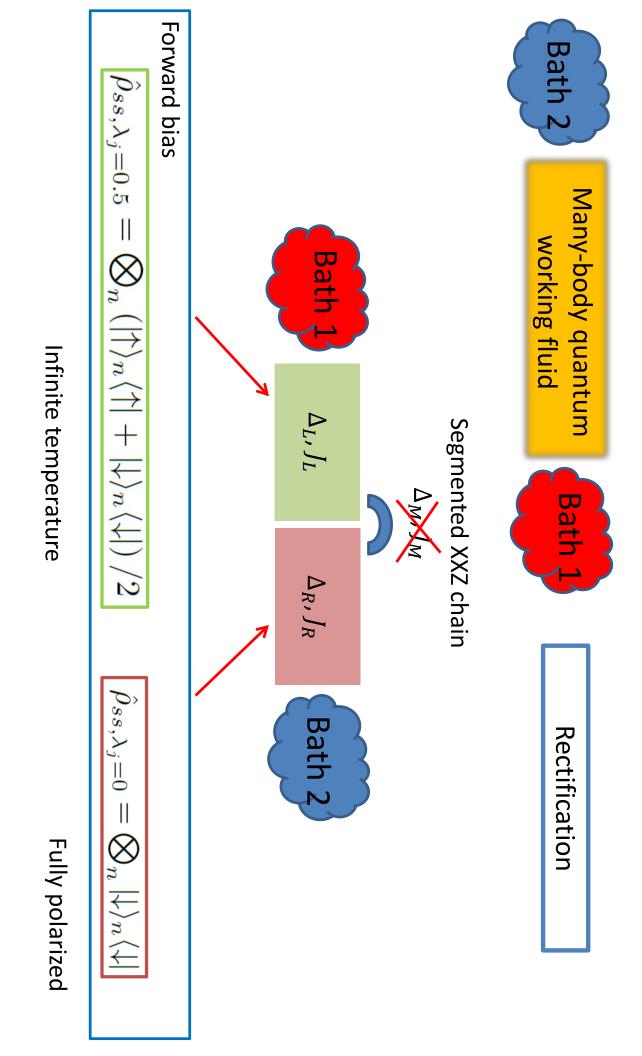


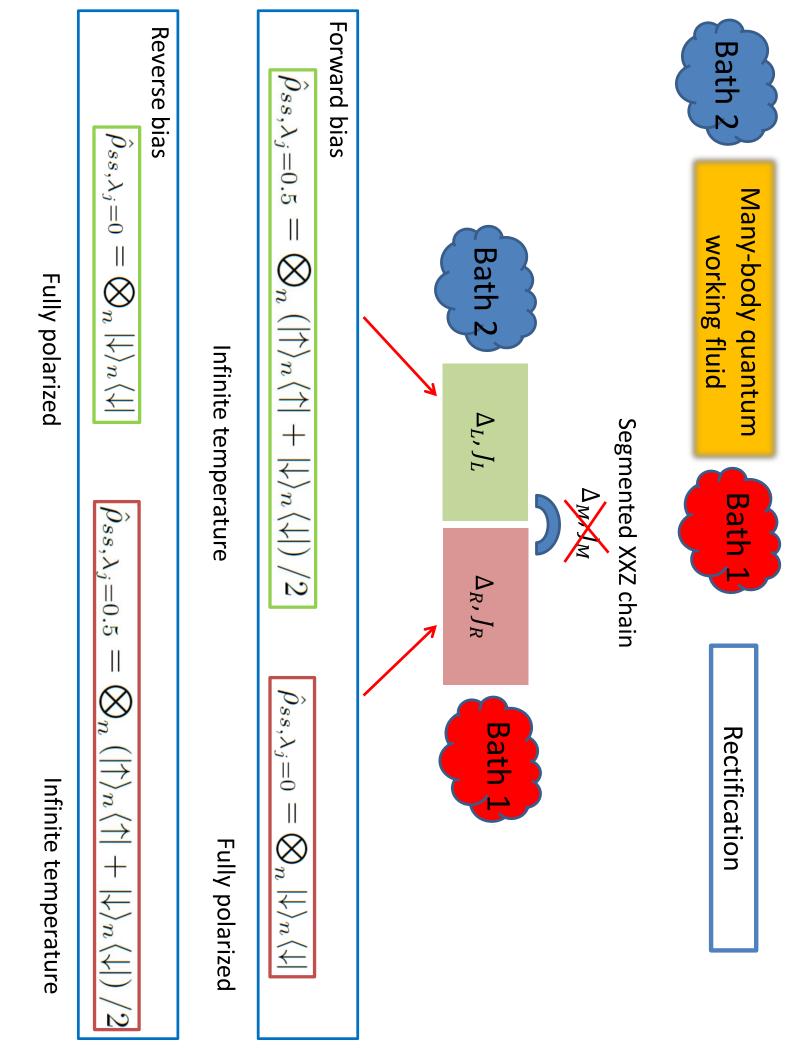
also works from D. Segal, A. Dhar ...

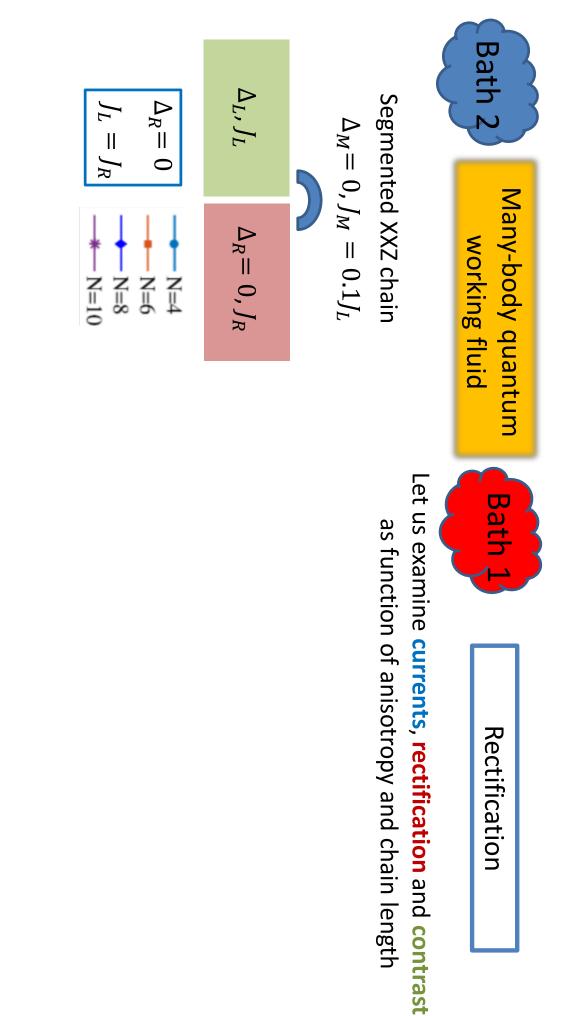
 T_R



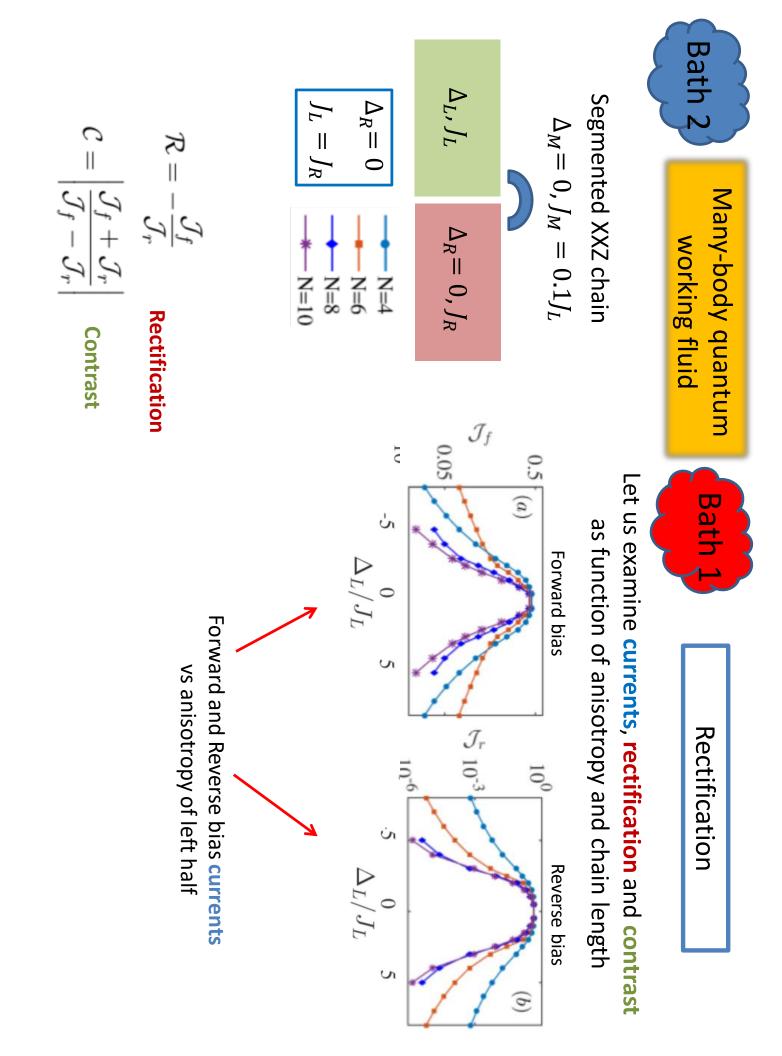


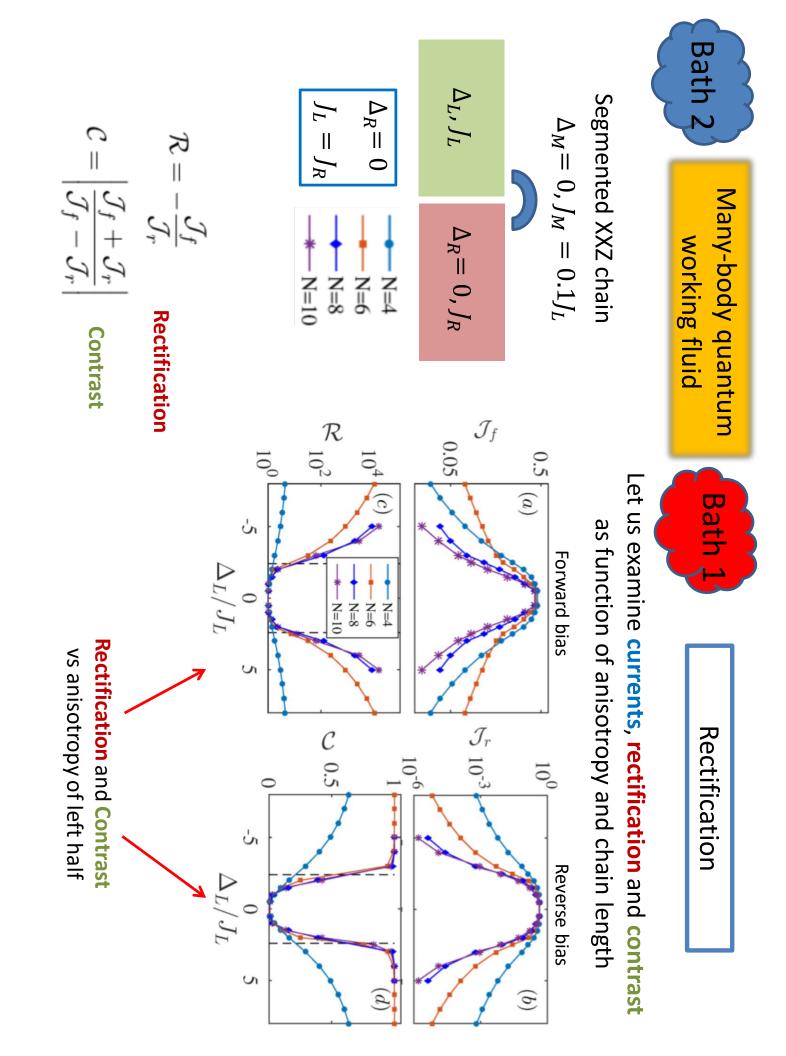


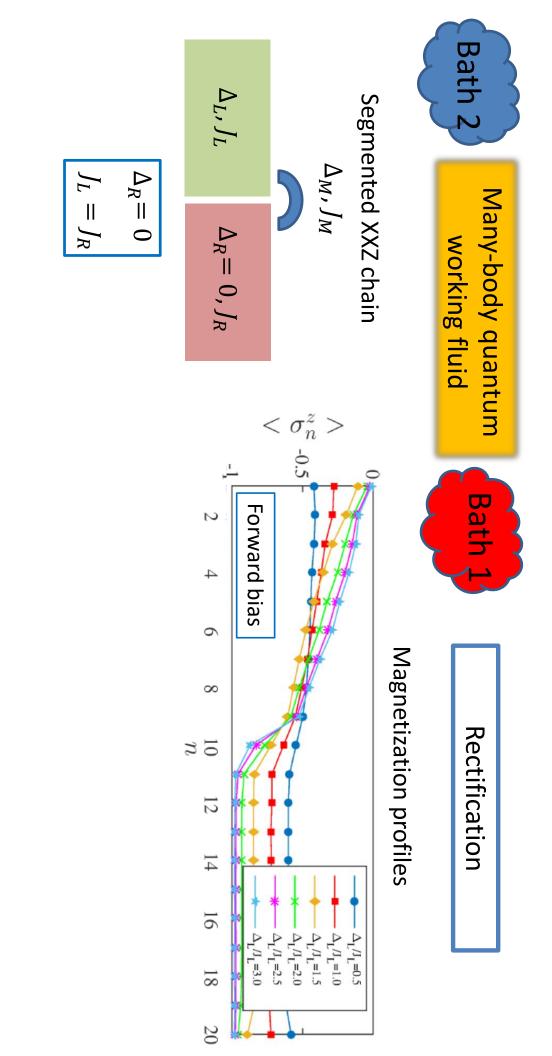


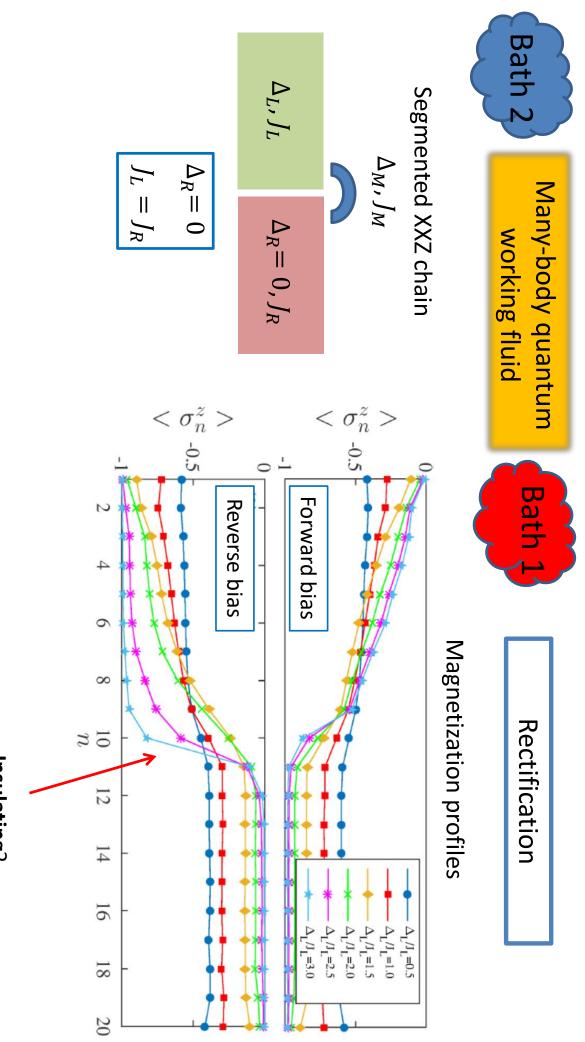


 $\mathcal{C} = \left| rac{\mathcal{J}_f + \mathcal{J}_r}{\mathcal{J}_f - \mathcal{J}_r}
ight|$ $\mathcal{R} =$ \mathcal{L}_{r} Rectification Contrast

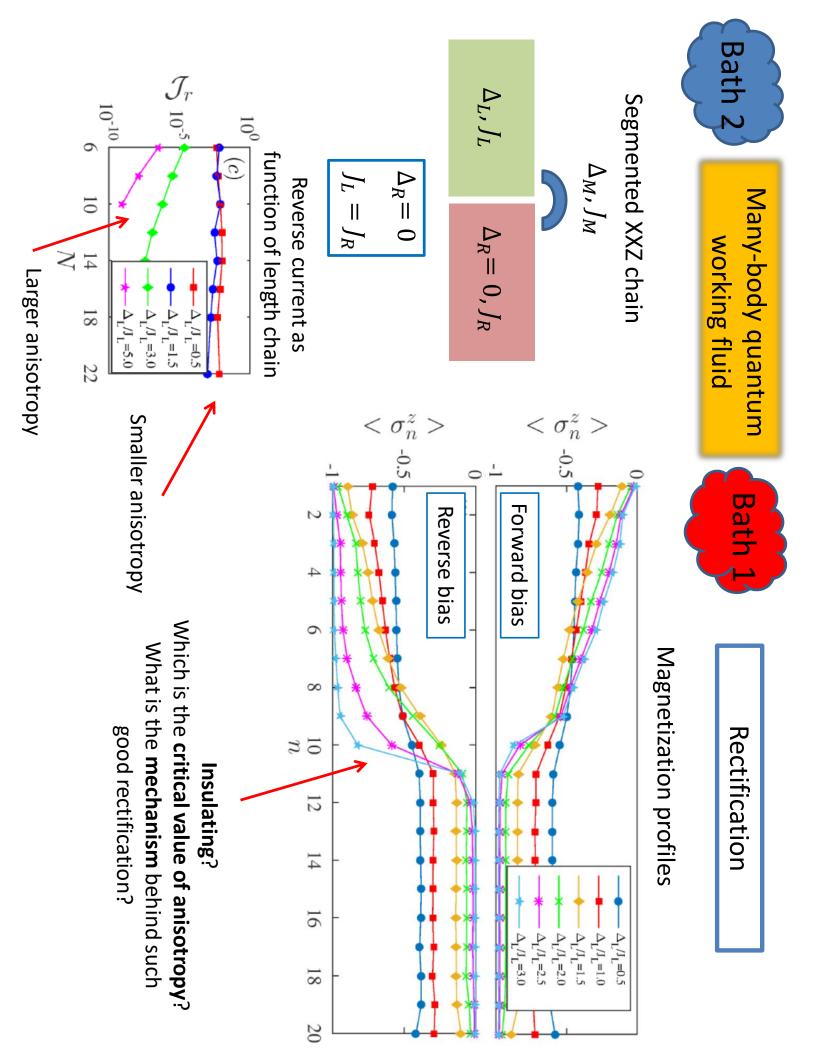


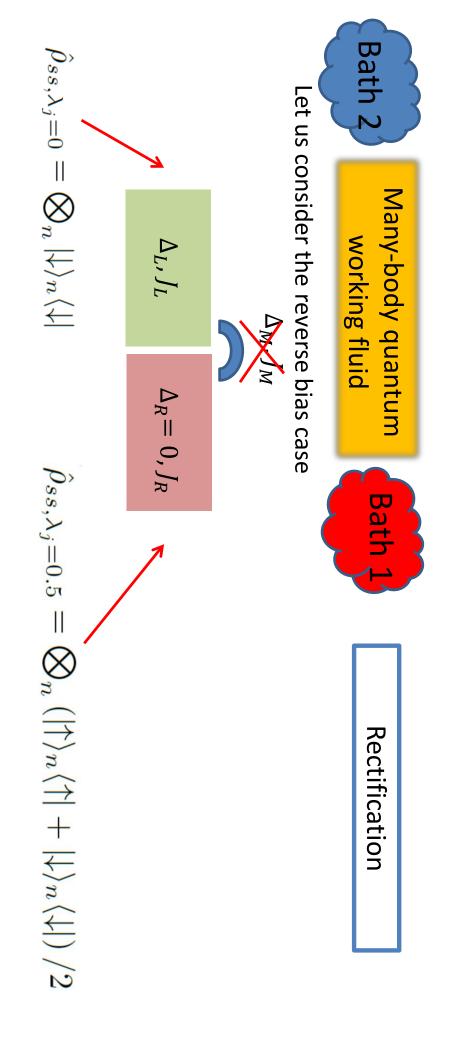


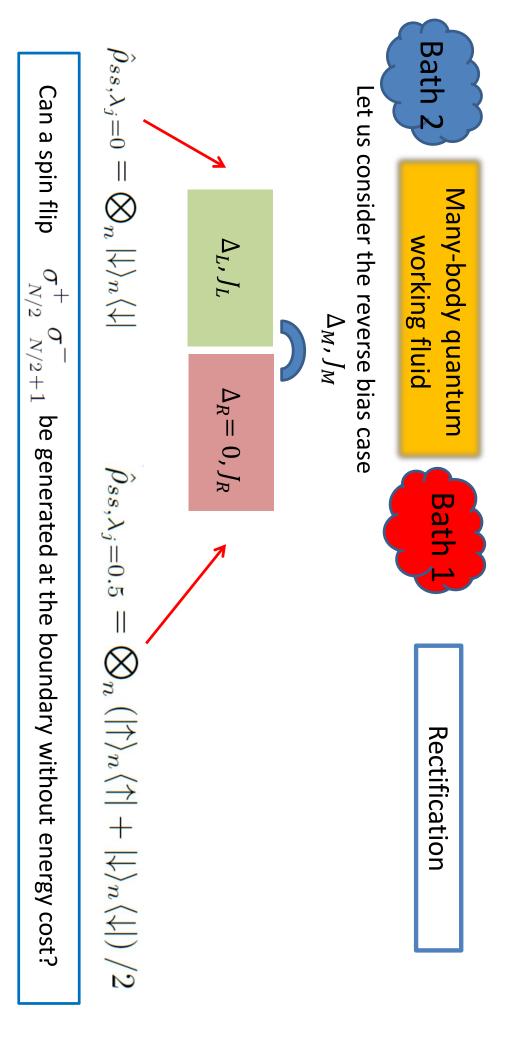


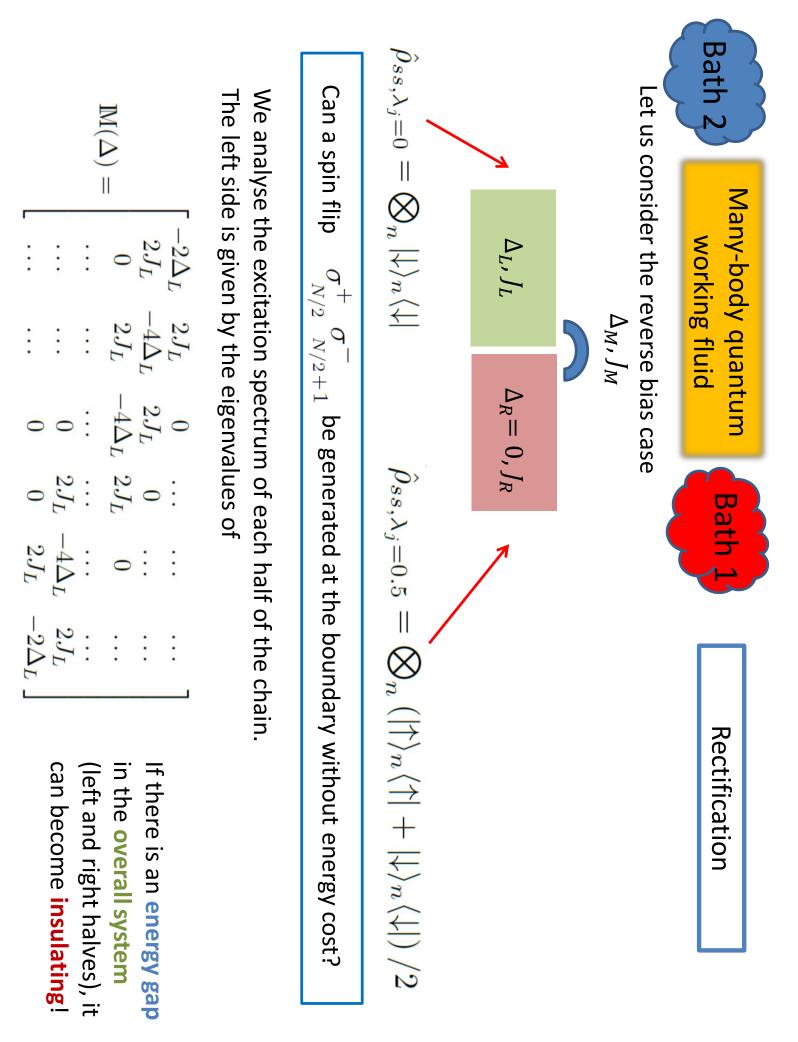


Insulating? Which is the critical value of anisotropy? What is the mechanism behind such good rectification?

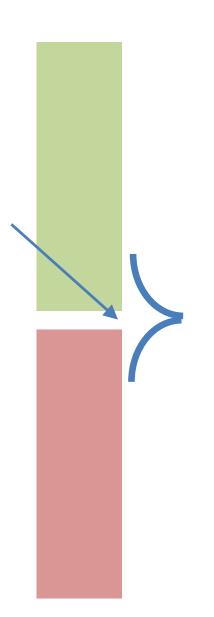


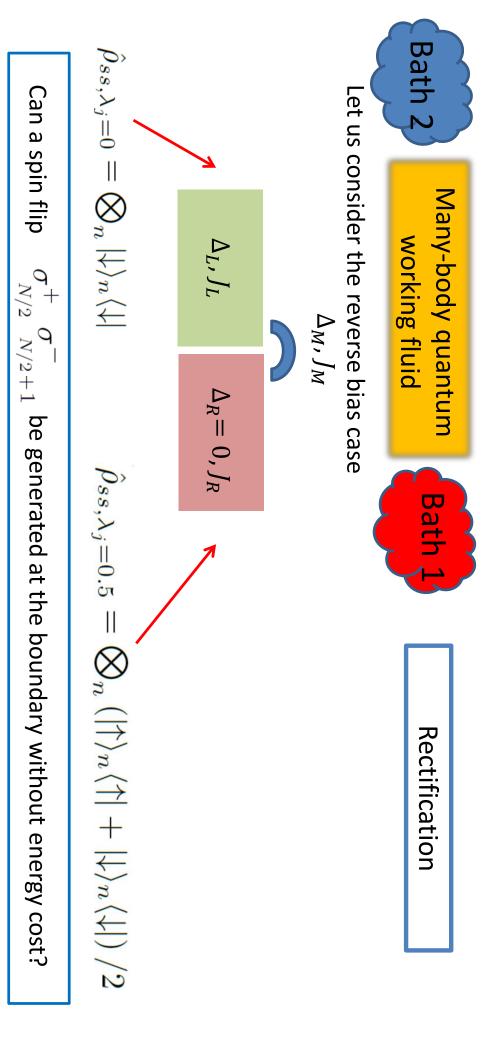


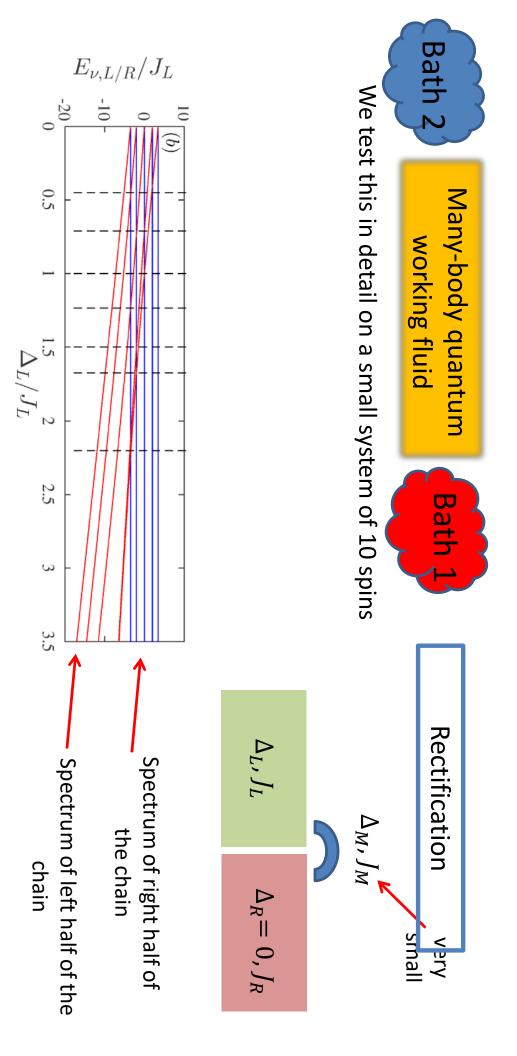


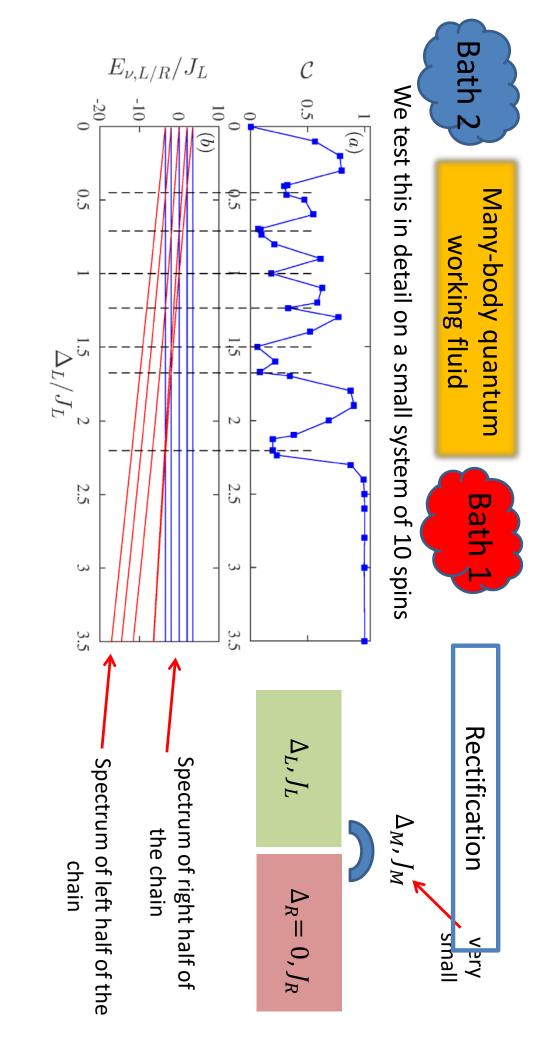


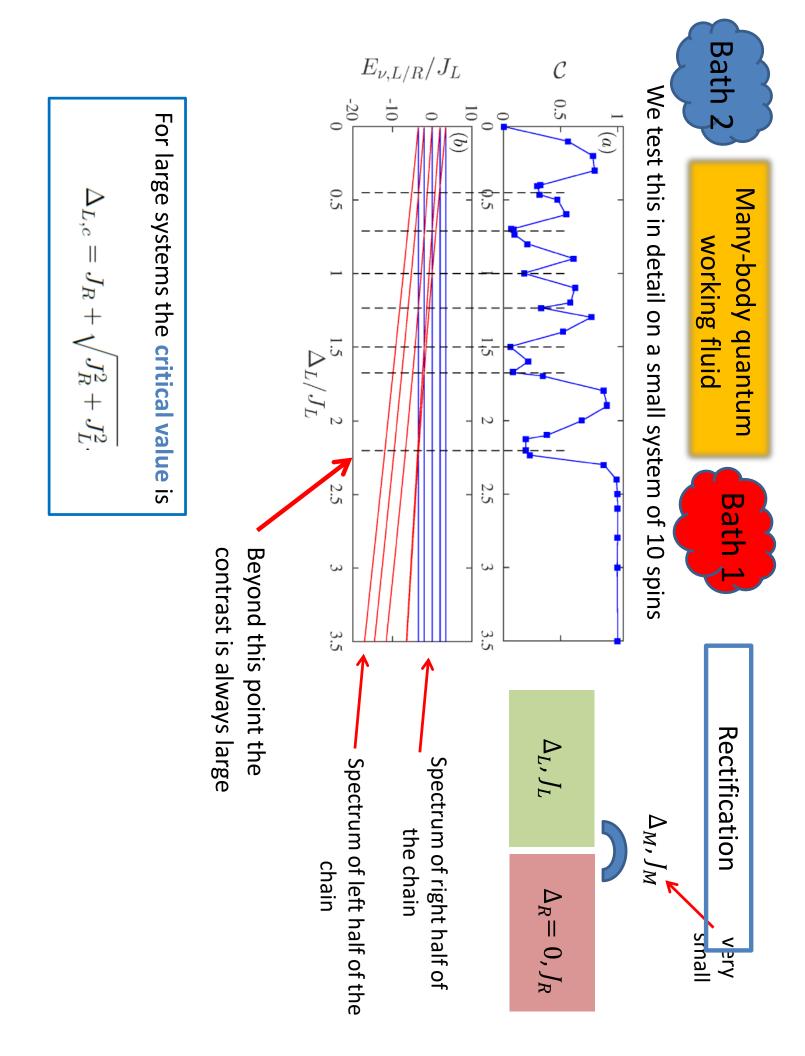
Excitations are gapped and localized at the boundary: but only in reverse bias

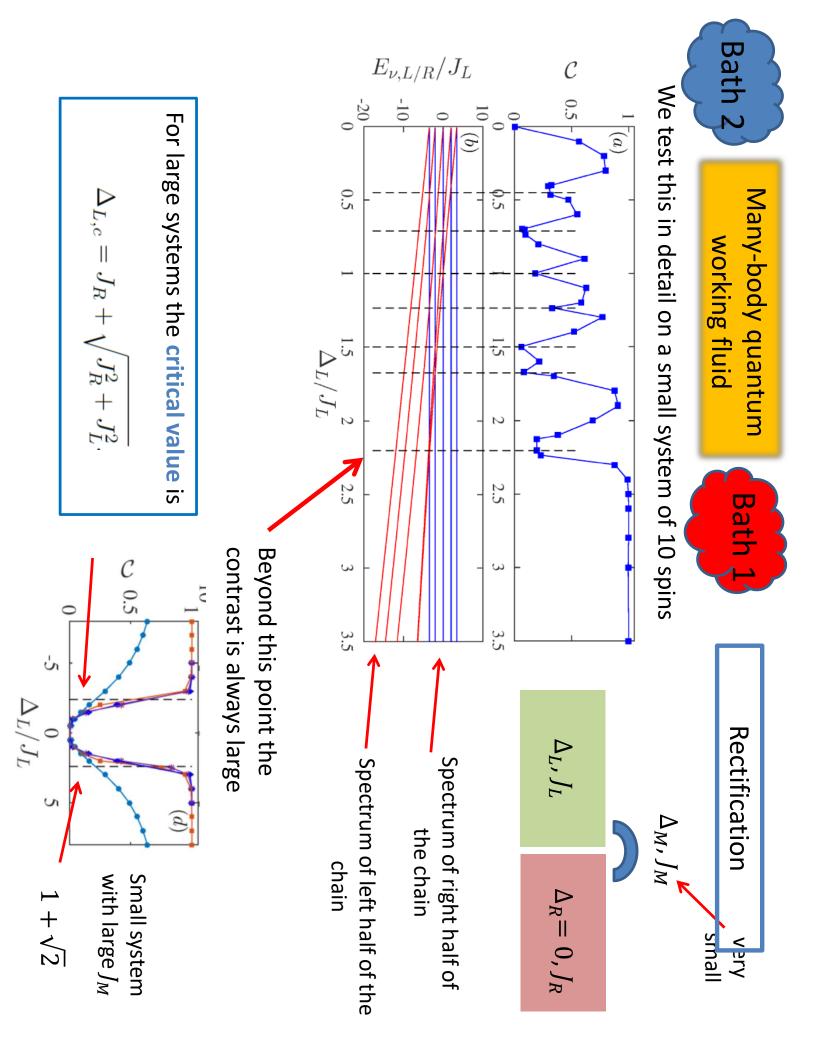


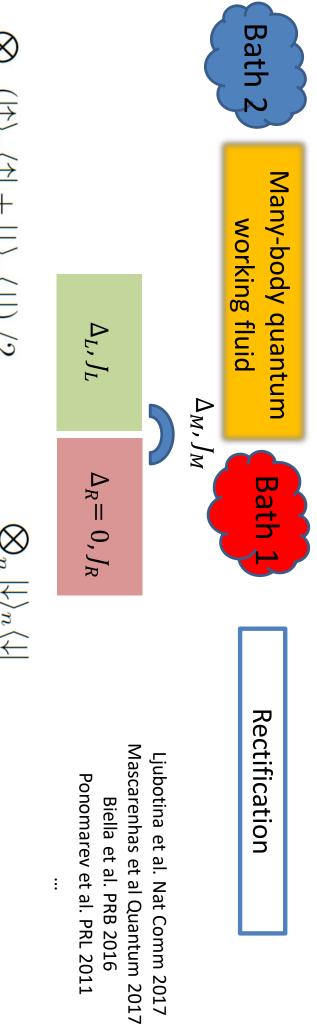








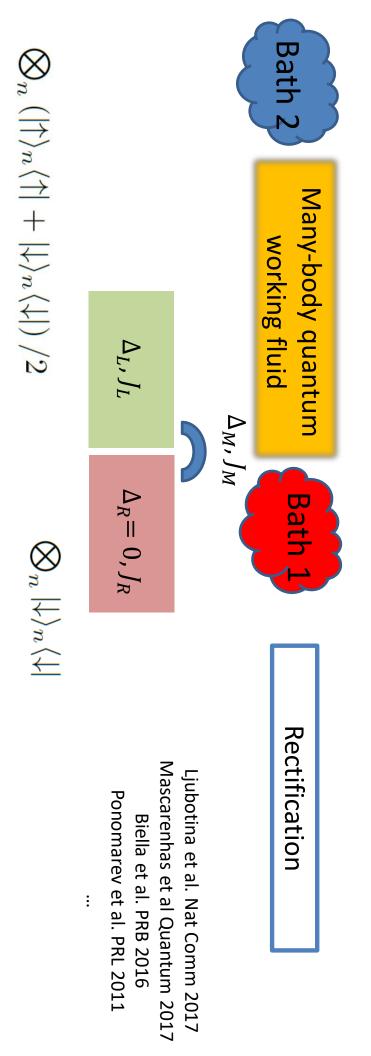




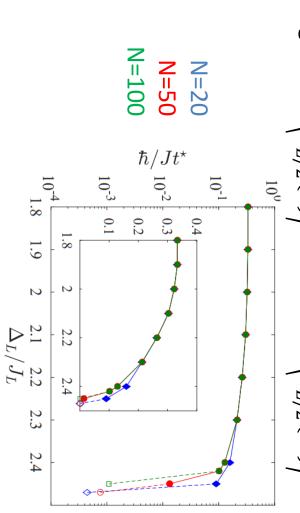
$$\bigotimes_n (|\uparrow\rangle_n \langle \uparrow| + |\downarrow\rangle_n \langle \downarrow|) / 2$$

$$\bigotimes_n |\downarrow\rangle_n\langle$$

change from $\langle \sigma_{L/2}^{Z}(0) \rangle = -1$ to $\langle \sigma_{L/2}^{Z}(t^*) \rangle = -0.99$ We then connect them and measure the time t^* it takes for the spin at the interface to We prepare two long chains in either the infinite temperature state or fully polarized state.



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 $1/t^*$ decreases abruptly as Δ_L/J_L approaches $1 + \sqrt{2}$



Rectification

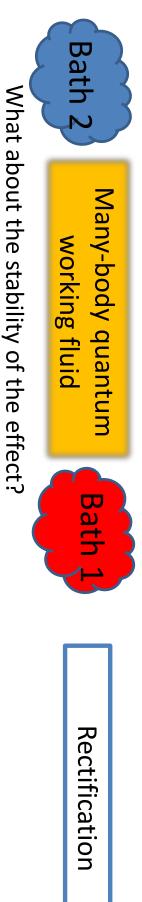
possible to rectify currents but in the thermodynamic limit the system is We have found that thanks to the interplay between baths and interactions not only it is

- diffusive in forward bias
- Insulating in reverse bias

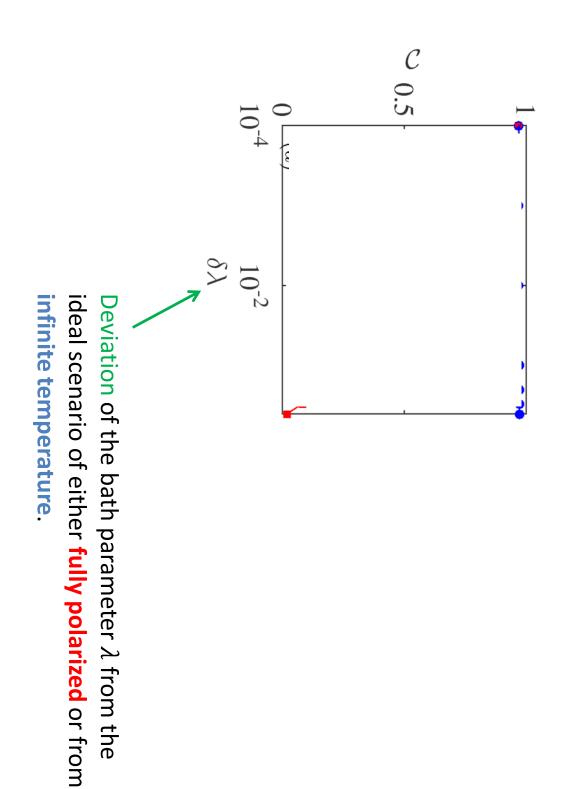
when the interaction exceeds

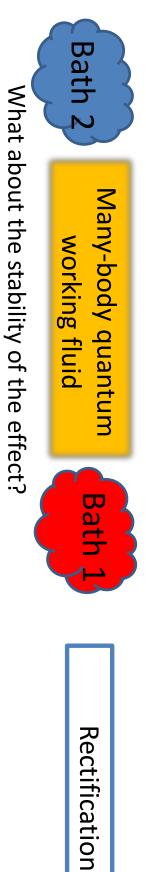
$$\Delta_{L,c} = J_R + \sqrt{J_R^2 + J_L^2}.$$

resulting in a perfect diode

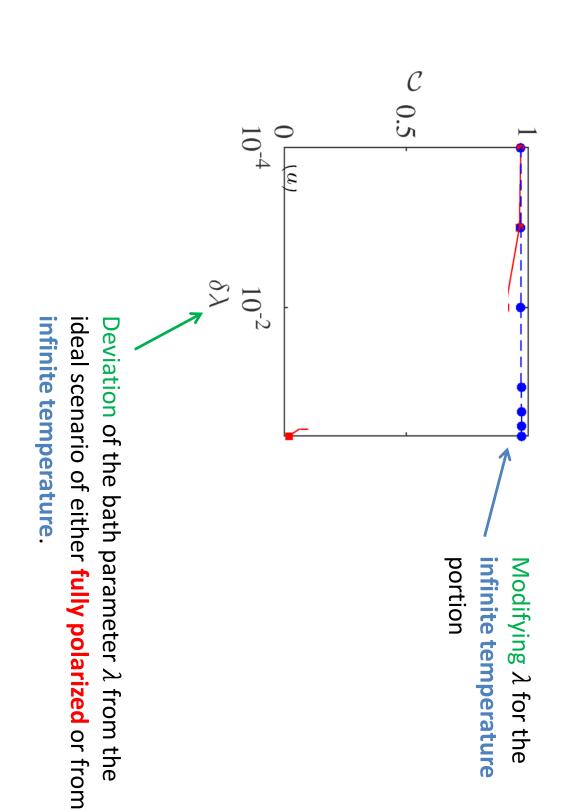


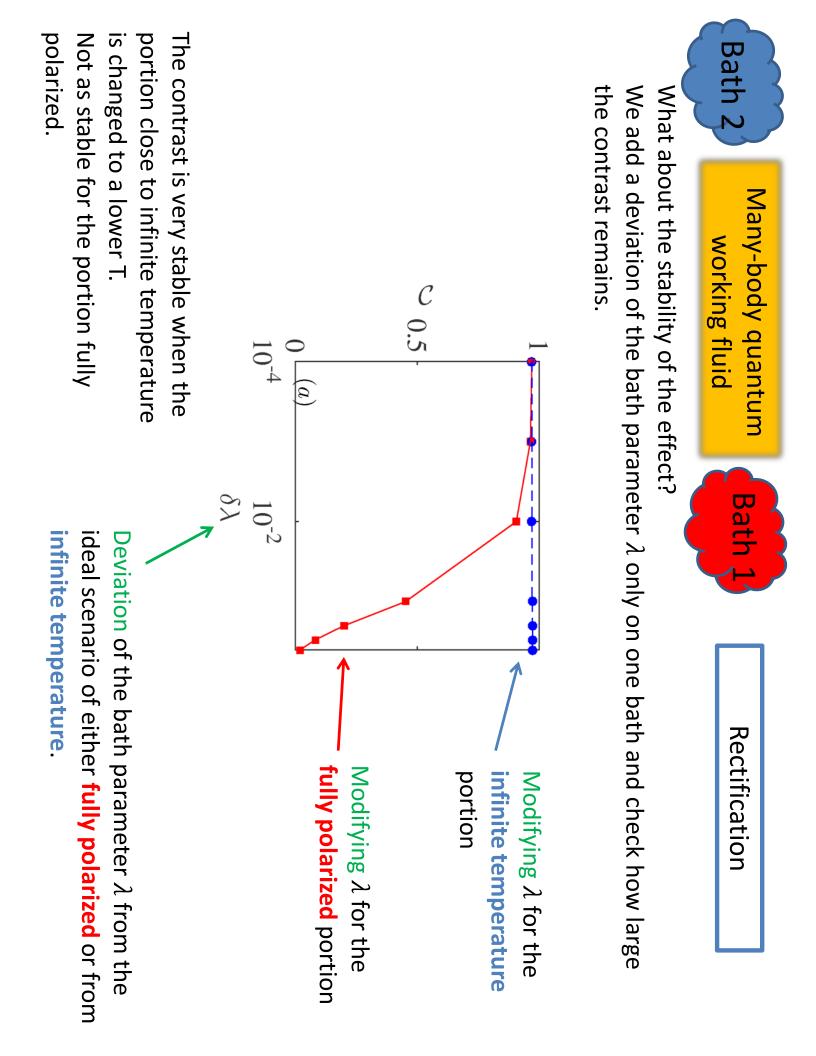
the contrast remains. We add a deviation of the bath parameter λ only on one bath and check how large





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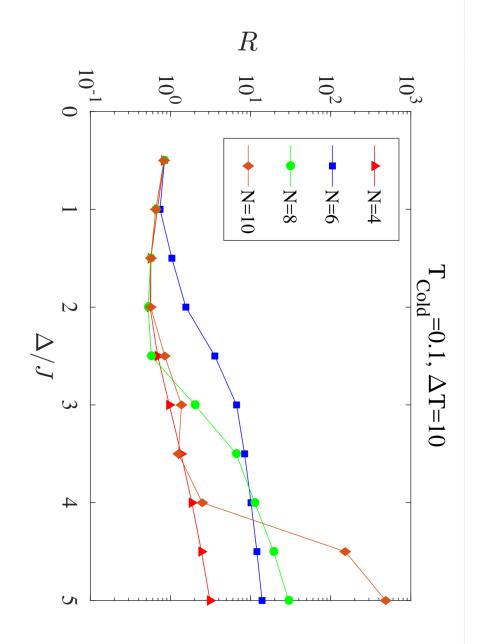
What about thermal baths?



Rectification

What about thermal baths?

we still see strong rectification as the anisotropy Δ increases. We use global Lindblad baths, for which we do exact diagonalization, and



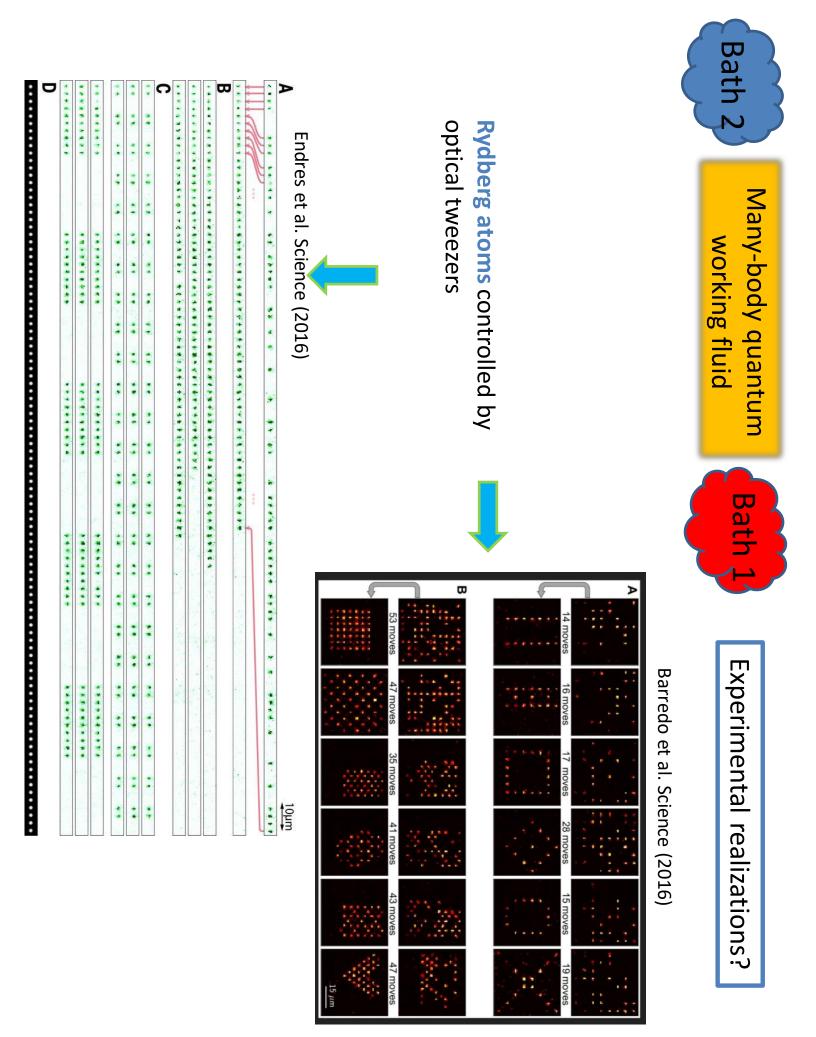


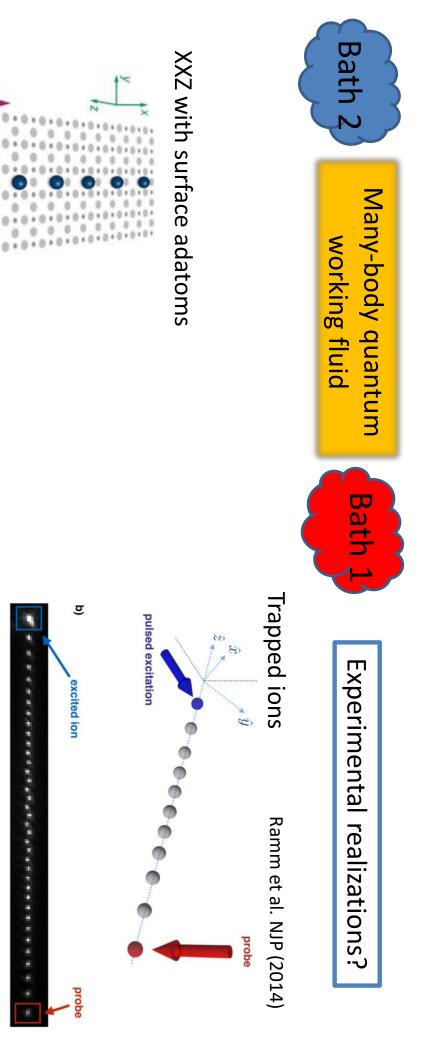
Many-body quantum working fluid

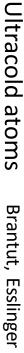


Experimental realizations?

Solid state: difficult to find materials with such large anisotropy and of course difficult to grow them on top of others.







Transverse field

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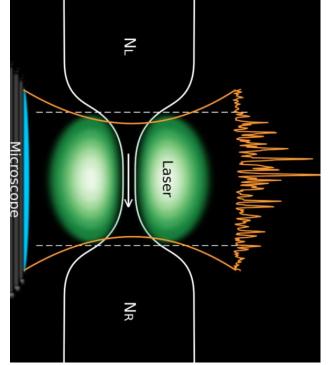
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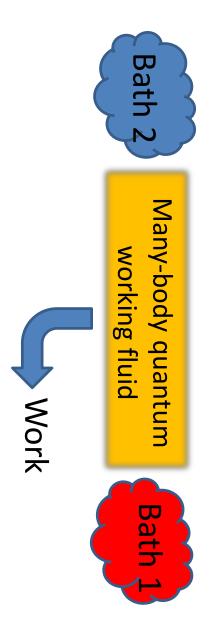
Nat. Phys. (2016)

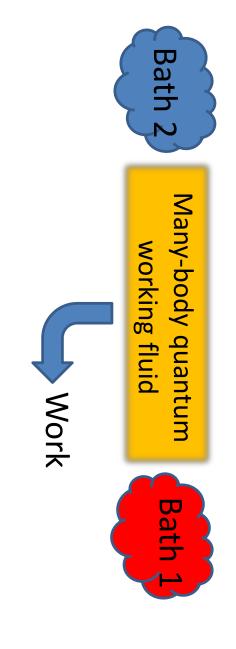
Toskovic et al.

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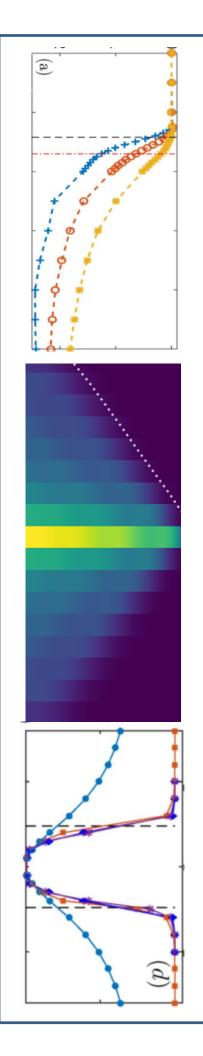
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Well ... this will be for another time



CONCLUSIONS

- Many-body open quantum systems are the best!
- Emerging properties
- Phase transitions
- •
- Implementation of Redfield
- Perfect diode

OUTLOOK

- We need to understand them better
- We need to find ways to understand them better!
- Extract work
- •



SUTD-MIT INTERNATIONAL DESIGN CENTRE (IDC)



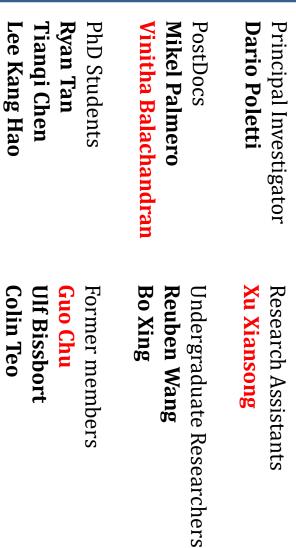




Financial support

Yuanjian Zheng

Thank you!





(a)

