Title: Modelling bubble nucleation in finite temperature Bose gases

Speakers:

Collection: Quantum Simulators of Fundamental Physics

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Modelling bubble nucleation in finite-temperature Bose gases

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Joint Quantum Centre

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Collaborators:

- Kate Brown
- Ian Moss

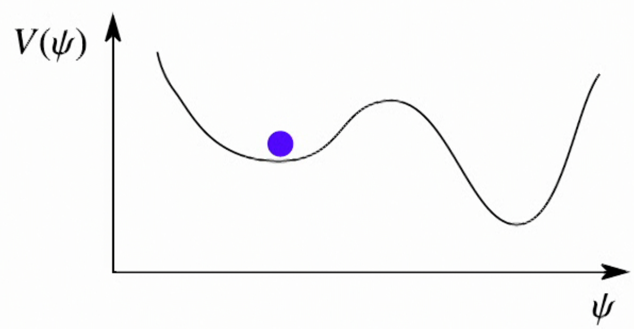
- Andrew Groszek (UQ)

QSimFP Workshop: Perimeter institute

08 June 2023

Basic question(s)

- What if the vacuum decay experiments (see previous talks!) aren't at zero temperature?
  - supercooled system in metastable state
  - unavoidable (can't reach T=0)
  - still of interest as an early universe analogue
  - interesting in itself to study bubble nucleation and dynamics in the presence of thermal dissipation



Contents

- Finite-temperature modelling of BECs
- Modelling continuous phase transitions
- Matching experiments quantitatively

- Applications to bubble nucleation

- Outlook
  - Full stochastic projected GPE
  - Bubble wall dynamics

Finite-temperature models

Gross-Pitaevskii equation (GPE)

Finite-temperature models

Gross-Pitaevskii equation (GPE)

	Perturbative approaches: *Deterministic*	Perturbative approaches: *Stochastic*	System + bath approach: *Stochastic*
Static thermal cloud	HFB, Popov, number-conserving, Etc.	Langevin-like stochastic GPE (SGPE) ↔	‘Simple growth’ stochastic projected GPE (SPGPE) ‘Full’ SPGPE
Dynamic thermal cloud		Zaremba-Nikuni-Griffin (ZNG) Stochastic GPE coupled to quantum Boltzmann	

The ‘classic’ route to the GPE

- Number-conserving, perturbative theory:

$$\hat{\Psi}(\mathbf{r},t) = \hat{a}_0\psi(\mathbf{r},t) + \delta\hat{\Psi}(\mathbf{r},t)$$

Small, neglect

- Into Heisenberg equation yields GPE

$$i\partial_t\psi = \left[-\frac{1}{2}\nabla^2 + |\psi|^2 - \lambda\right]\psi$$

- Interpretation: ψ describes the single highly occupied mode of the single particle density matrix

$$\langle\hat{\Psi}^\dagger(\mathbf{r}',t)\hat{\Psi}(\mathbf{r},t)\rangle$$

The 'classical field' route to the GPE (1)

- Bosons in a box

$$\hat{\Psi}(\mathbf{r},t) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{|\mathbf{k}|<k_{\mathrm{cut}}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{|\mathbf{k}|\geq k_{\mathrm{cut}}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\approx \sum_{|\mathbf{k}|<k_{\mathrm{cut}}} \alpha_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{\Psi}_I(\mathbf{r},t)$$

Mode occupations $\langle \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} \rangle > 1$

Replace $\hat{a}_{\mathbf{k}} \rightarrow \alpha_{\mathbf{k}}$

Assume incoherent particles

Describe by single-particle Wigner function $W_1(\mathbf{r},\mathbf{k},t)$

The ‘classical field’ route to the GPE (2)

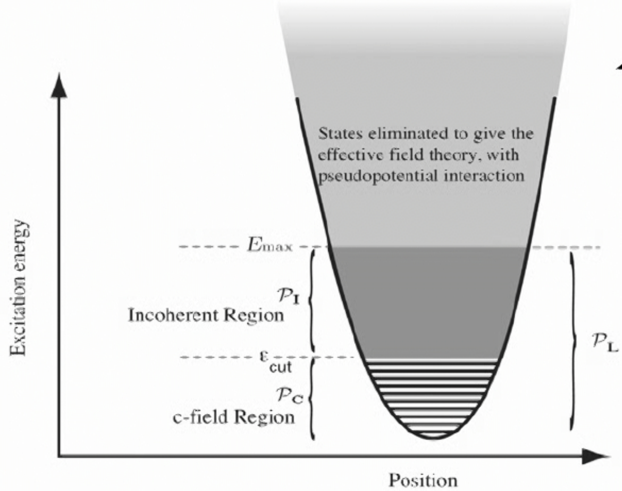
- Throw away incoherent part yields *PGPE*:

$$i\partial_t = \mathcal{P}\left\{\left[-\frac{1}{2}\nabla^2 + |\psi|^2 - 1\right]\psi\right\}$$

- We gained a *projector*. If using Fourier pseudospectral methods, this corresponds to *dealiasing*.
- Our *interpretation* changes:
- Eigenvectors of $\langle\psi^*(\mathbf{r}', t)\psi(\mathbf{r}, t)\rangle$ over appropriate ensemble approximate the many substantially occupied eigenvectors of $\langle\hat{\Psi}^\dagger(\mathbf{r}', t)\hat{\Psi}(\mathbf{r}, t)\rangle$

The SPGPE approach (1)

- Develop theory in terms of multimode Wigner function, *then solve trajectories*
- Coherent dynamics of c-field region described by PGPE
- Incoherent region treated as grand canonical thermal bath: μ, T
- Coupling adds noise and damping terms to PGPE dynamics



[Blakie, Bradley *et al*., Adv. Phys. 57, 363 (2008)]

Stochastic, Projected, Gross-Pitaevskii Equation

The SPGPE approach (2)

[Rooney, Blakie, Bradley, PRE **89** 013302 (2014)]

$$(S)d\psi(\mathbf{r},t) = d\psi|_H + d\psi|_\gamma + (S)d\psi|_\varepsilon,$$

$$d\psi|_H = \mathcal{P}\{-i(\mathcal{L}-\mu)\psi\, dt\},$$

Hamiltonian evolution

$$d\psi|_\gamma = \mathcal{P}\{-\gamma(\mathcal{L}-\mu)\psi\, dt + dW_\gamma(\mathbf{r},t)\},$$

Particle exchange with reservoir

$$(S)d\psi|_\varepsilon = \mathcal{P}\{-iV_\varepsilon(\mathbf{r},t)\psi\, dt + i\psi\, dW_\varepsilon(\mathbf{r},t)\},$$

Number-conserving scattering processes

(S): Stratonovich form

Single-component shown for simplicity. Spinor and multicomponent form known.

‘Simple’ growth SPGPE

- First two terms only: particle exchange with reservoir, grand canonical
  - The ‘obvious’ Langevin form – fluctuation-dissipation relation
  - Projector ensures noise is defined in principled way

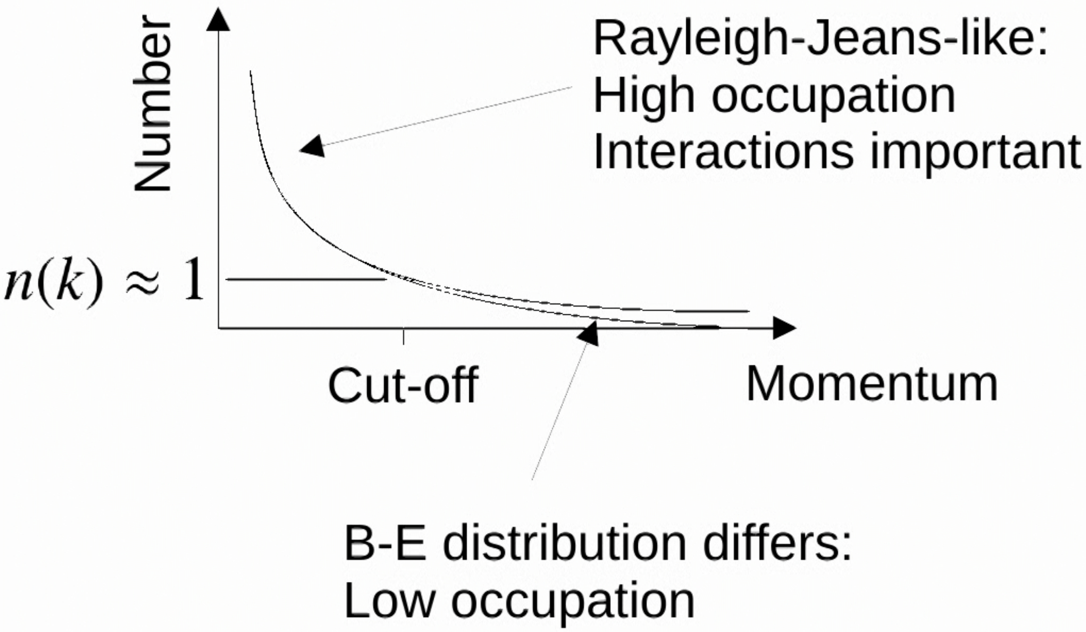
$$
\begin{aligned}
d\psi &= d\psi|_H + d\psi|_\gamma \\
&= \mathcal{P}\{-(i+\gamma)(\mathcal{L}-\mu)\psi\, dt + dW_\gamma(\mathbf{r},t)\}
\end{aligned}
$$

$$
\langle dW_\gamma^*(\mathbf{r},t) dW_\gamma(\mathbf{r}',t)\rangle = 2\gamma T \delta_{\mathrm{C}}(\mathbf{r},\mathbf{r}')dt
$$

δ_C: delta function in the projected space

Where to put the cut-off

- Critical behaviour at the BEC phase transition (BKT transition in 2D) is driven by interactions of the long-wavelength, highly-occupied modes

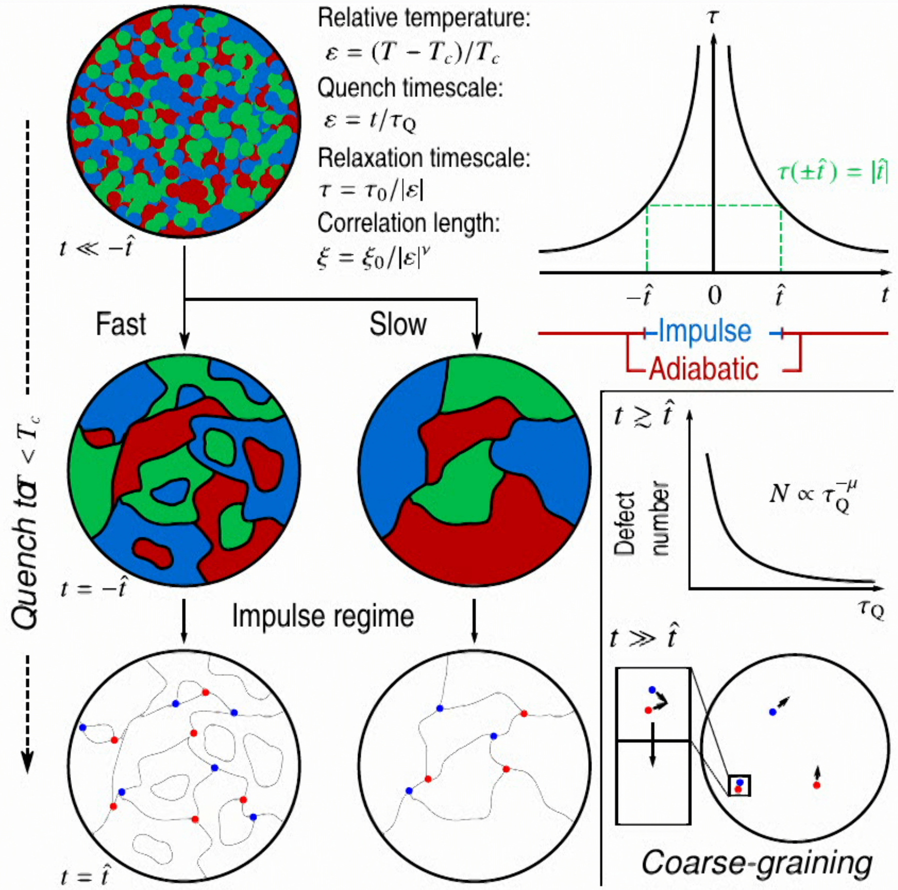


This idea used, outside of the (S,P)GPE formalism, to calculate BKT transition temperature by Prokof'ev and Svistunov

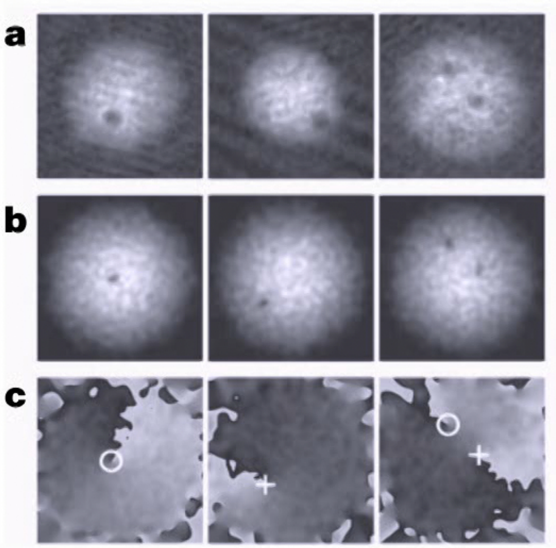
[Prokof'ev, Ruebenacker, Svistunov PRL **87** 270402 (2001)]

Previous non-equilibrium application: KZM

- Kibble-Zurek mechanism
- Cross 2nd order phase transition in finite time
- Expect power law scaling of defect number
- For cold atoms, good candidate for stochastic / c-field models

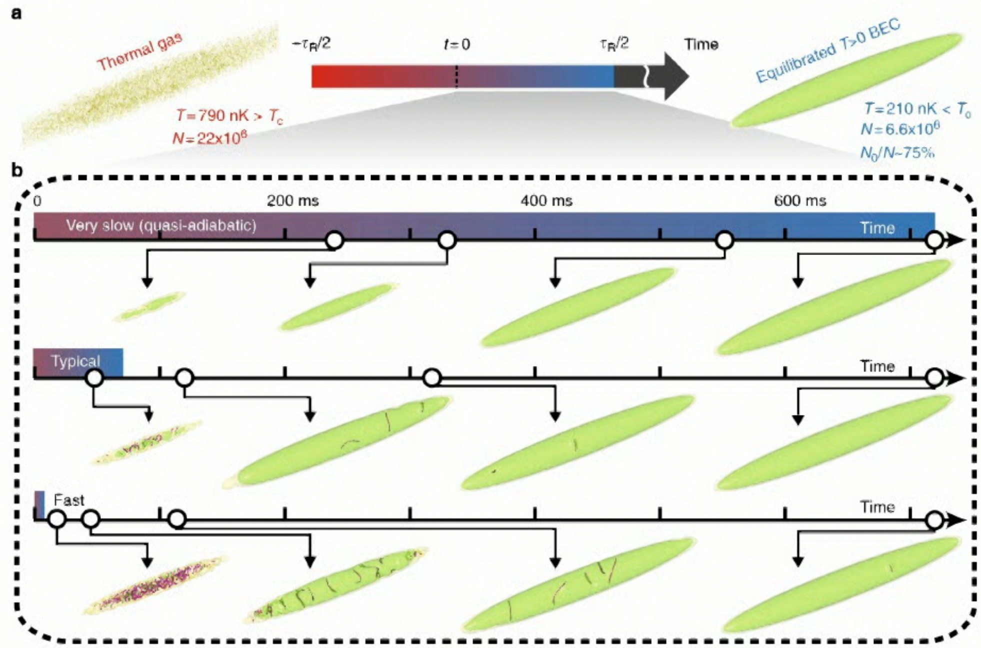


KZM: success story for stochastic / c-field



[Weiler, Neely, Scherer, Davis, Bradley, Anderson, *Nature* **455** 948 (2008)]

Measure correlations instead: Navon, Gaunt, Smith, Hadzibabic, *Science* **347** 167 (2015)

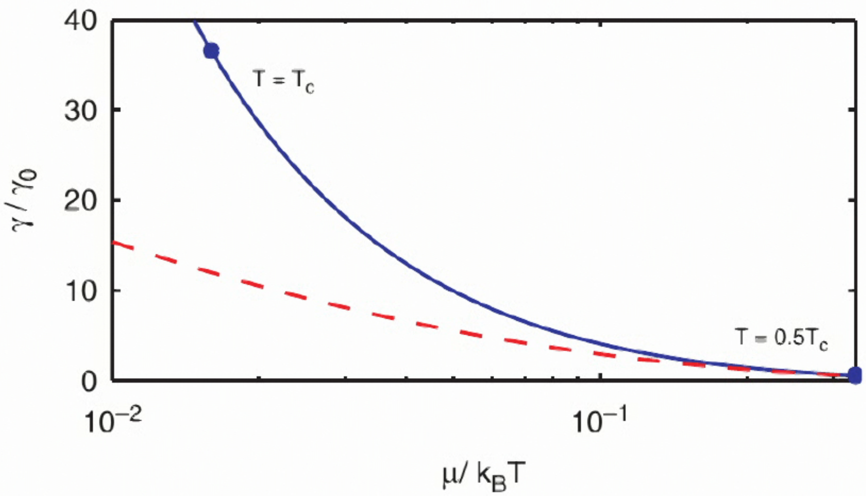


[Liu, Donadello, Lamporesi, Ferrari, Gou, Dalfovo, Proukakis, *Commun. Phys.* **1** 24 (2018)]

[Lamporesi, Donadello, Serafini, Dalfovo, Ferrari, *Nat. Phys.* **9** 656 (2013)]

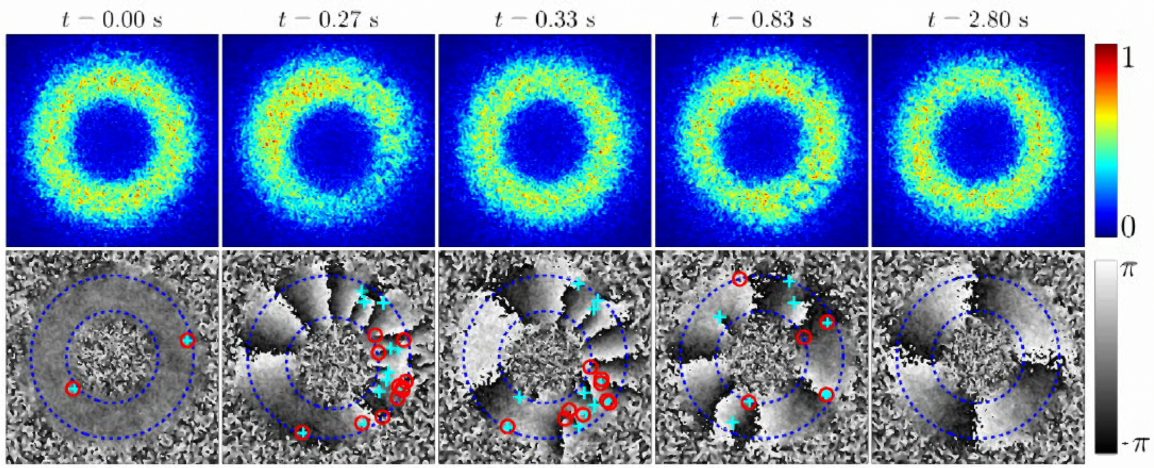
Quantitatively matching experiments: idealism

- In theory, the dimensionless damping rate *γ* can be predicted *a priori*
  - This is a *close-to-equilibrium* prediction
  - Complicated cut-off dependence



Quantitatively matching experiments: realism

- One notable success of a priori treatment
  - Much more common to fit γ to experimental results, $\gamma < \sim 0.02$

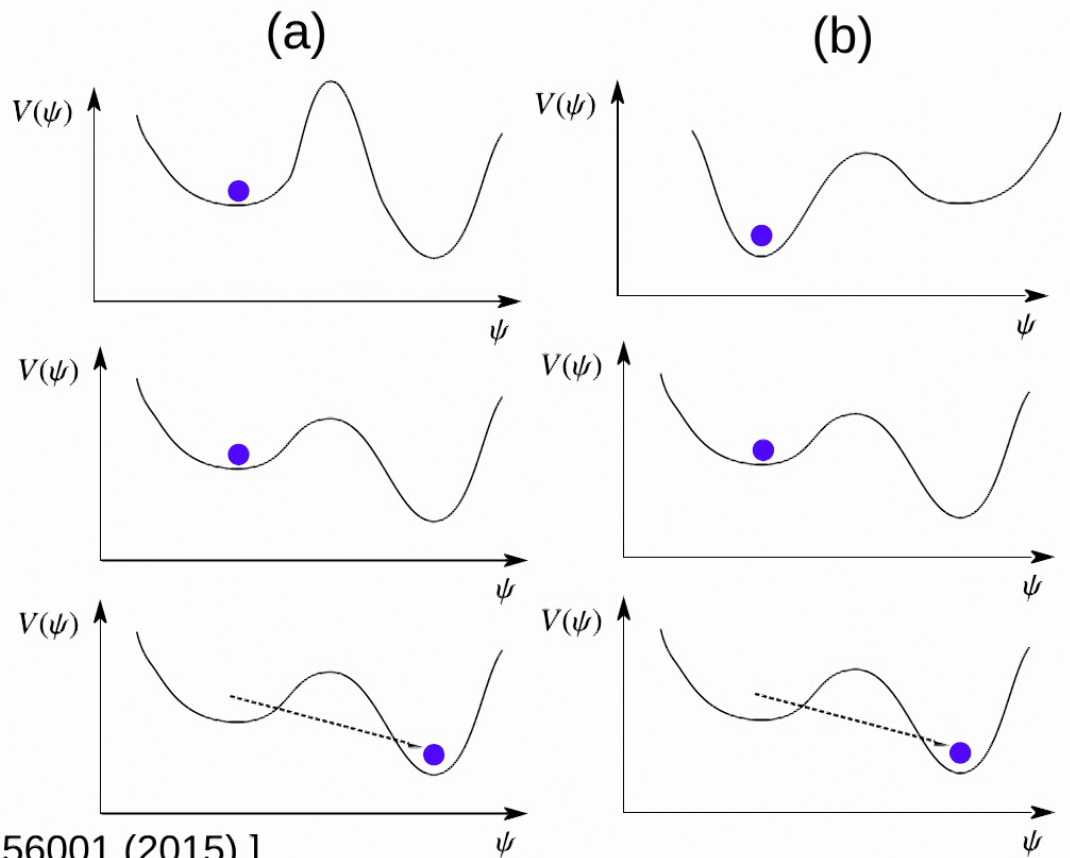


Quantitative match: persistent current formation

[Rooney, Neely, Anderson, Bradley, PRA **88** 063620 (2013)]

Finite-temperature bubbles: Fialko *et al* model

- Simple growth SPGPE
- Thermalize either:
  - (a) in false vacuum with high barrier (time-averaged case)
  - (b) in true vacuum (time-modulated case)
- At time zero either:
  - (a) lower barrier
  - (b) switch the vacua (experimental adjustment of RF phase)
- Observe nucleation and growth of bubbles



[Fialko et al., Europhys. Lett. **110** 56001 (2015).]

Time-averaged Fialko et al. model

- BEC occupying two coupled hyperfine spin states: pseudo-spin-1/2
- Spin states coupled by time-modulated RF field: time-averaged description

Hamiltonian and couplings

$$H = \int dx \left\{ -\frac{\hbar^2}{2m} \psi^\dagger \nabla^2 \psi + V(\psi, \psi^\dagger) \right\}$$

$$V = \frac{g}{2} \sum_i (\psi_i^\dagger \psi_i)^2 - \mu \psi^\dagger \psi - \mu \epsilon^2 \psi^\dagger \sigma_x \psi + \frac{g}{4} \epsilon^2 \lambda^2 (\psi^\dagger \sigma_y \psi)^2,$$

SPGPE

$$i \frac{\partial \psi_j}{\partial t} = \mathcal{P} \left\{ (1 - i\gamma) \left(-\frac{1}{2} \nabla^2 \psi_j + \frac{\partial \hat{V}}{\partial \psi_j^\dagger} \right) + \eta_j \right\}$$

$$\langle \eta_i(x,t) \eta_j(x',t') \rangle = 2\gamma T \delta(x - x') \delta(t - t') \delta_{ij}$$

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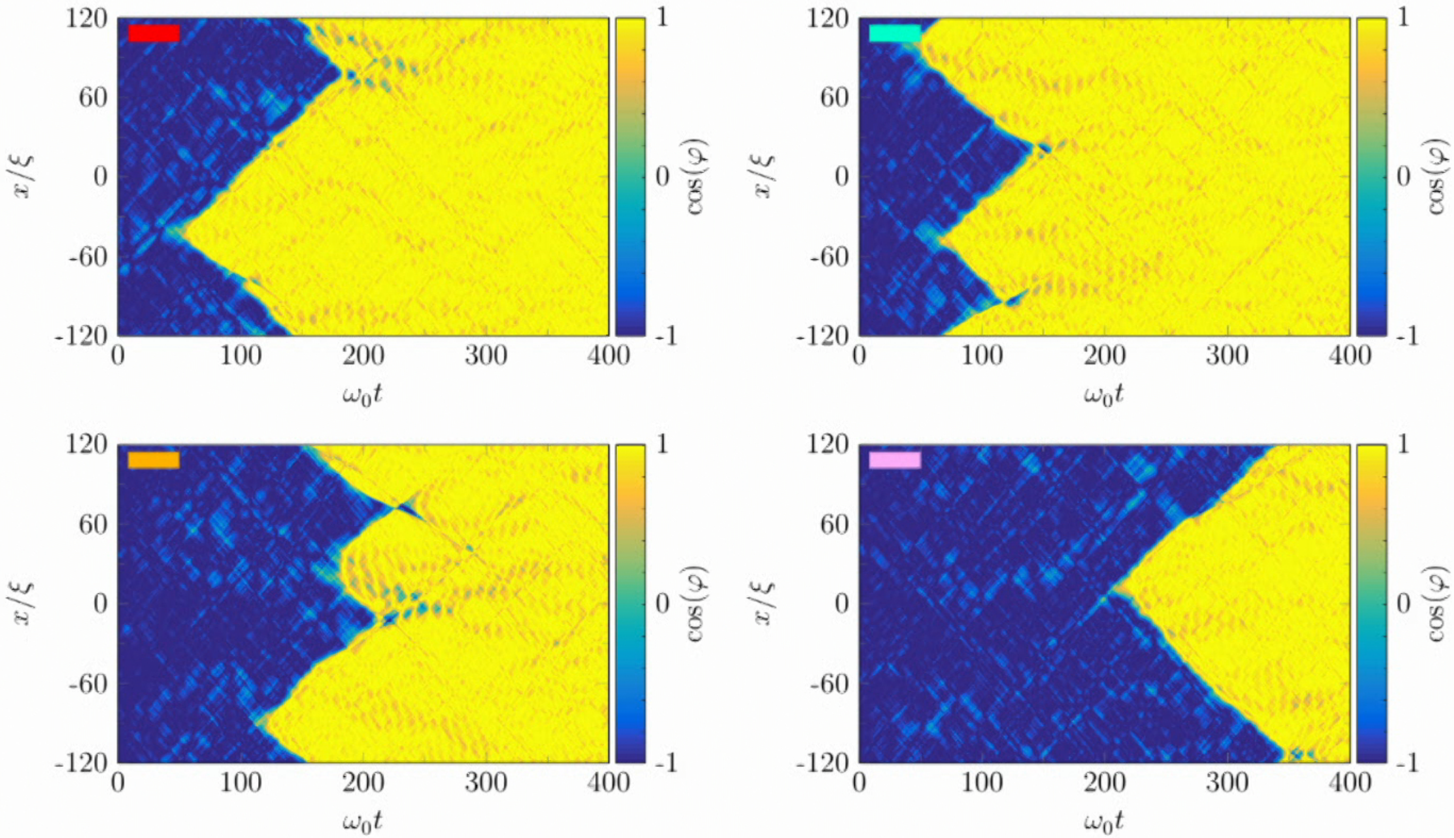
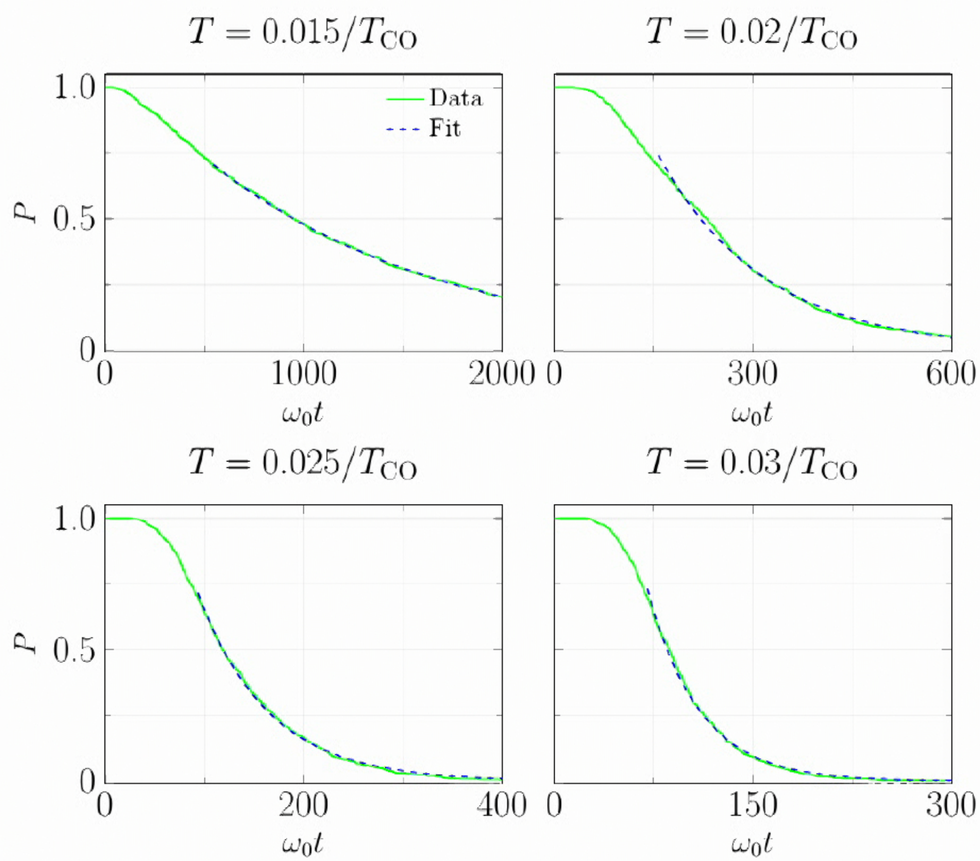
Space-time trajectories



Survival probability

- Nucleation threshold:

$$\langle \cos(\varphi) \rangle > -0.8$$

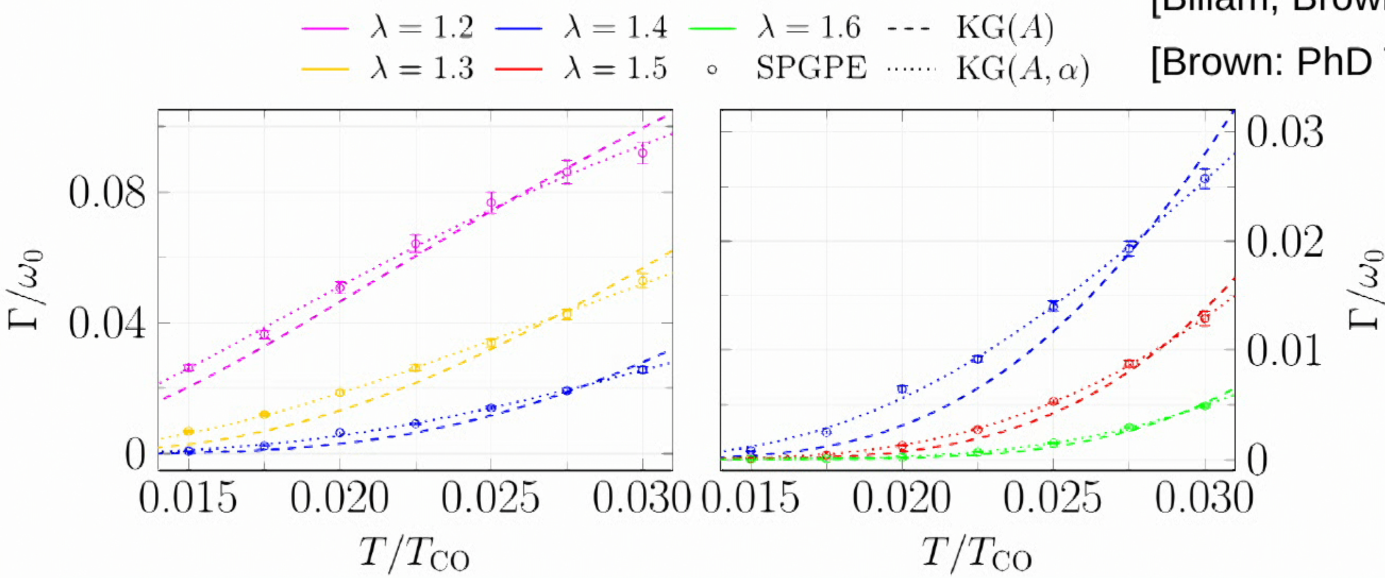


Time averaged model: fit to instantons

- Reasonable agreement fitting prefactor A_0 in $\Gamma \approx \mathcal{V} A_0 B^{1/2} e^{-B}, \quad B = \alpha(\lambda)\epsilon/T$
- Fits extremely good if also fitting exponent α (renormalisation effects)
- Good fits achievable for varying γ

[Billam, Brown, Moss, PRA **102** 043324 (2020)]

[Brown: PhD Thesis (in preparation)]



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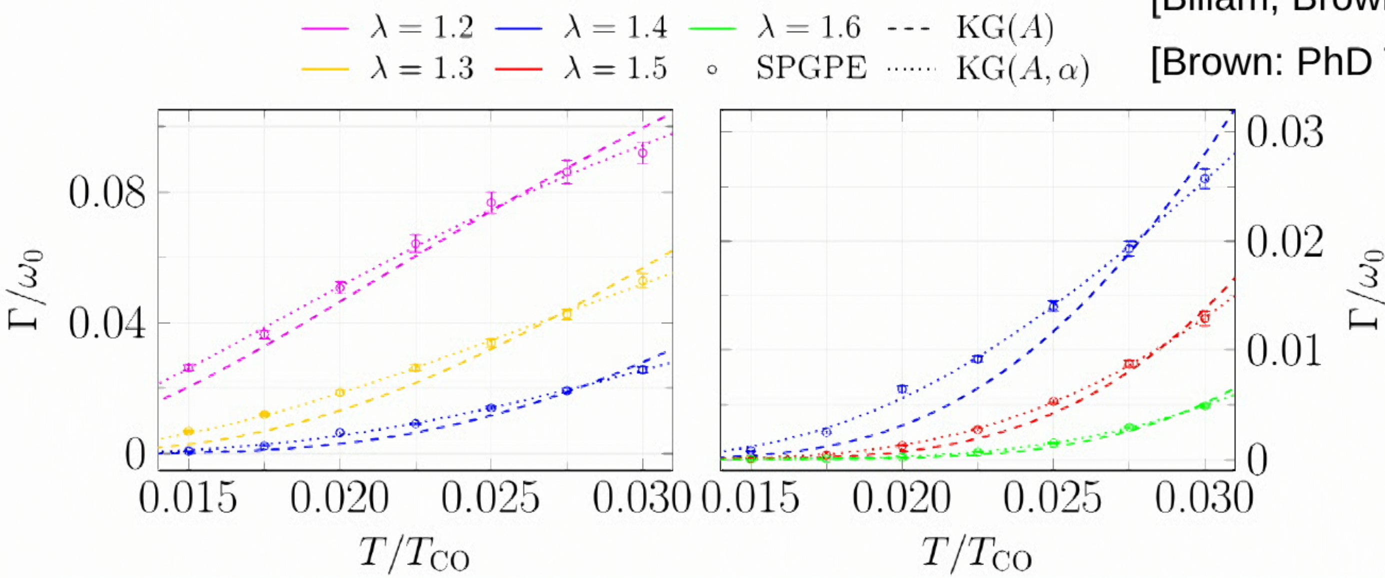
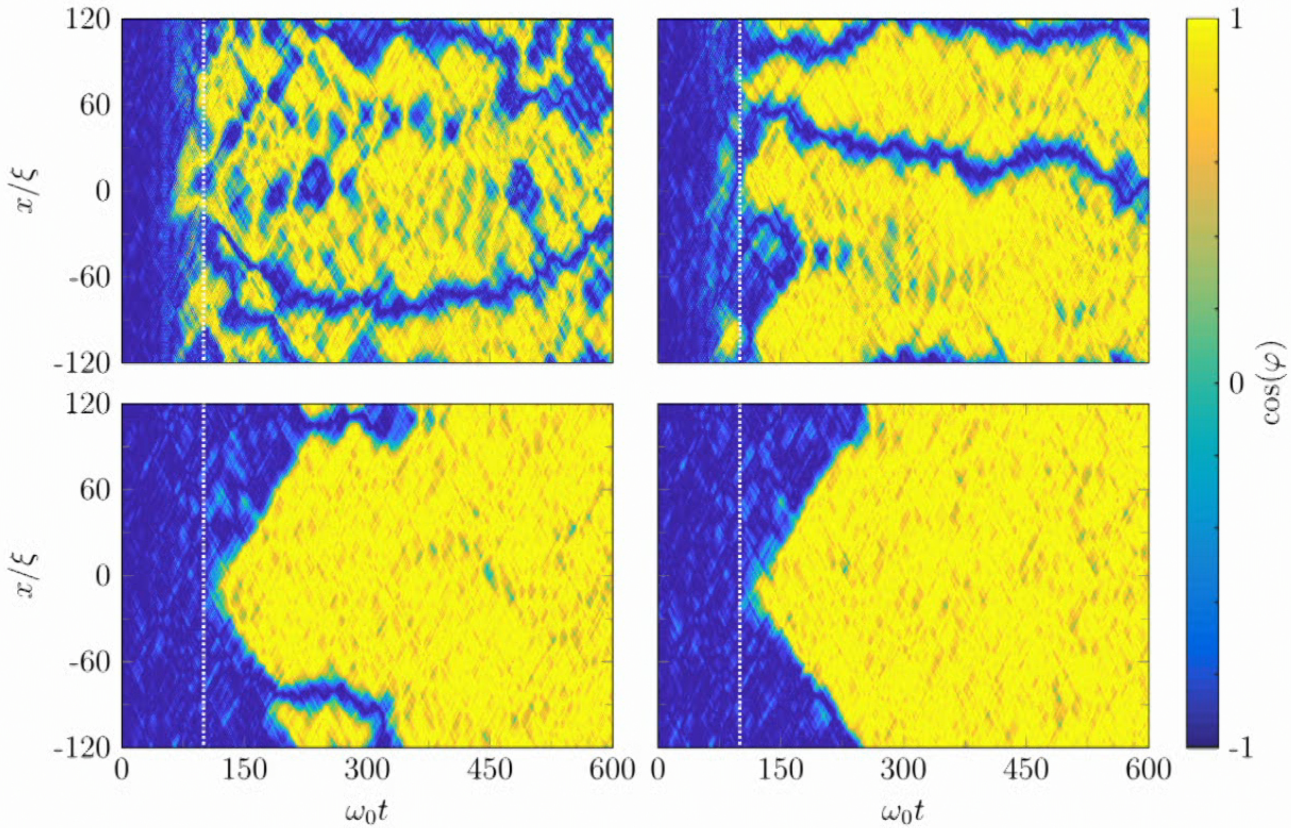


Full modulated model: agreement but γ question

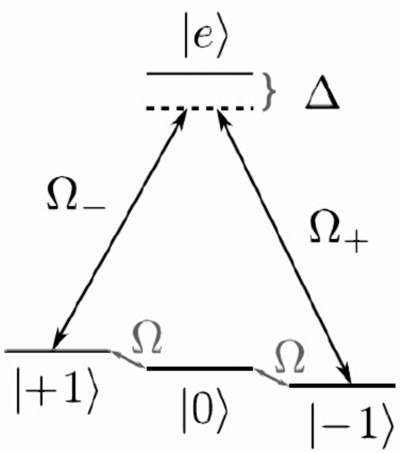
- Full modulated model potentially suffers from parametric instability
- Is this eliminated by damping at finite temperature?
- Yes, but much higher γ than the *a priori* value required

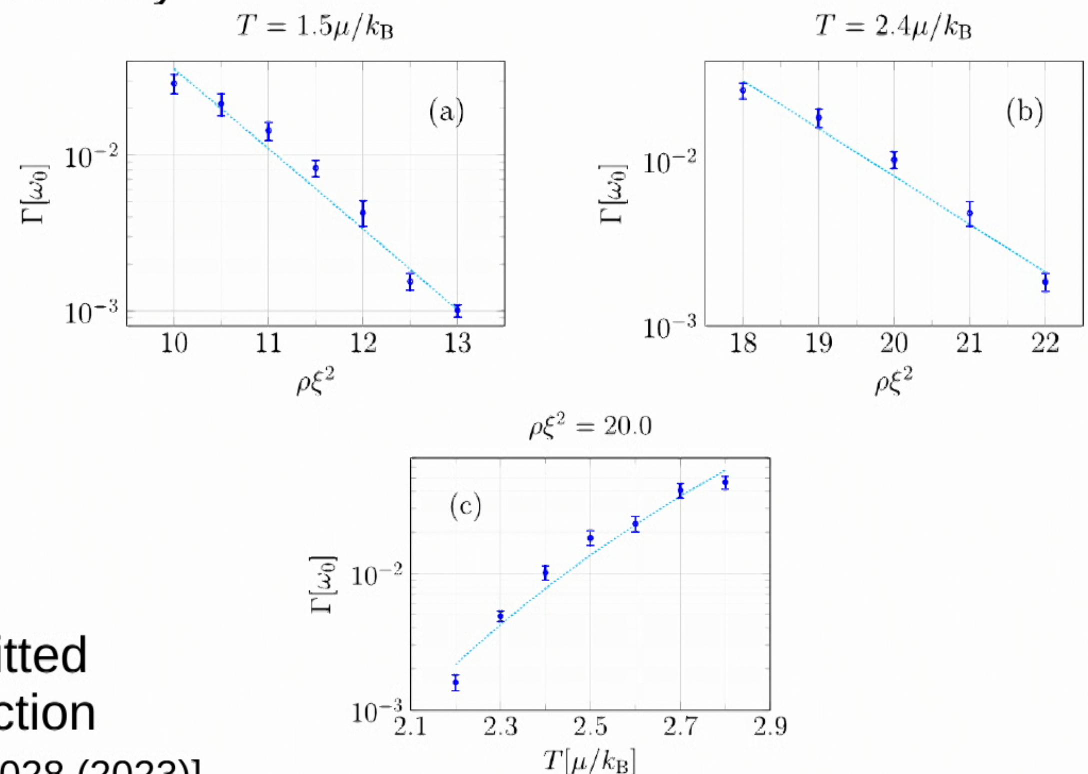


[Billam, Brown, Groszek, Moss, PRA **104** 053309 (2021)]

Avoiding instability: 2D spin-1 system

- Described by Kate in her talk on Monday



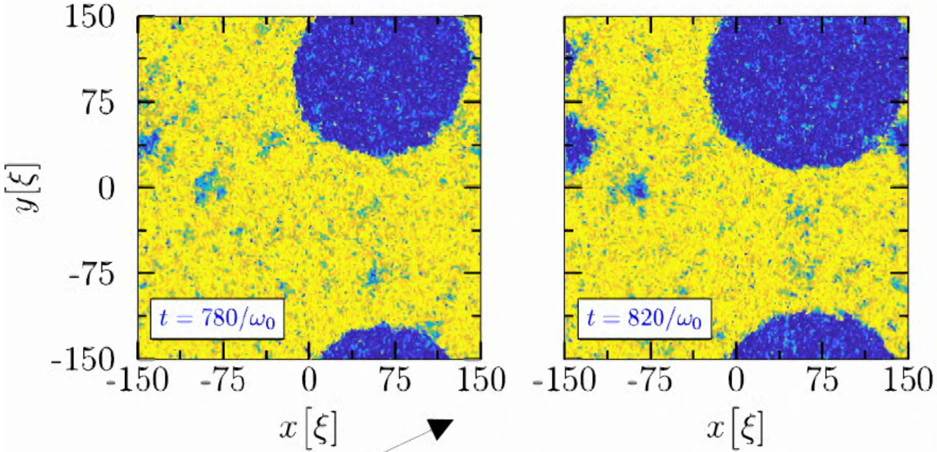


- We fit prefactor and exponent
- Within 95% confidence interval, fitted exponents match instanton prediction

[Billam, Brown, Moss, New J. Phys. **25** 043028 (2023)]

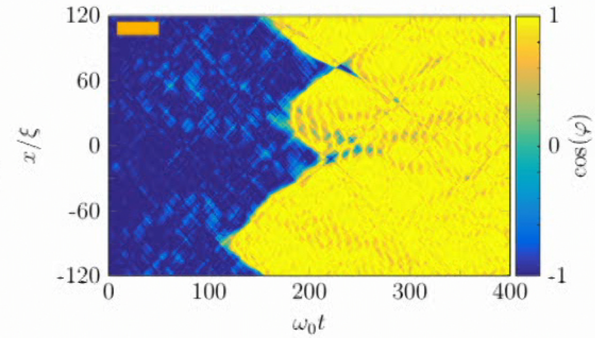
Outlook

- Want to address questions about bubble dynamics and correlations:

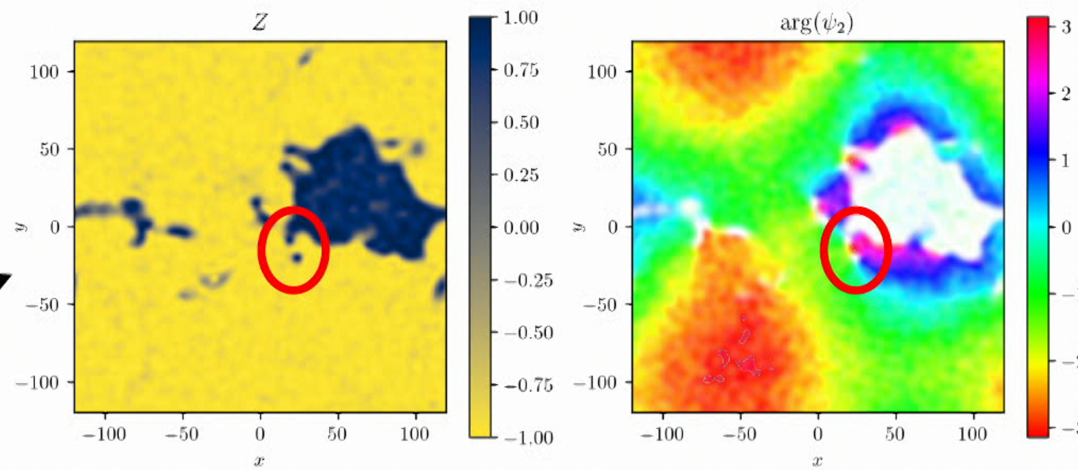


“Barnacles” (?) in spin 1, 2D

1D bubble collisions in Fialko et al. model



Half-quantum vortices in ferromagnetic model (Ian’s talk)



Reasons to explore full SPGPE

- These effects all involve substantially out-of-equilibrium dynamics
- Effects of dissipation, owing to bath of thermal particles, on bubble growth and mergers may be relevant to these effects

$$(S)d\psi|_\varepsilon = \mathcal{P}\{-iV_\varepsilon(\mathbf{r},t)\psi\, dt + i\psi\, dW_\varepsilon(\mathbf{r},t)\},$$

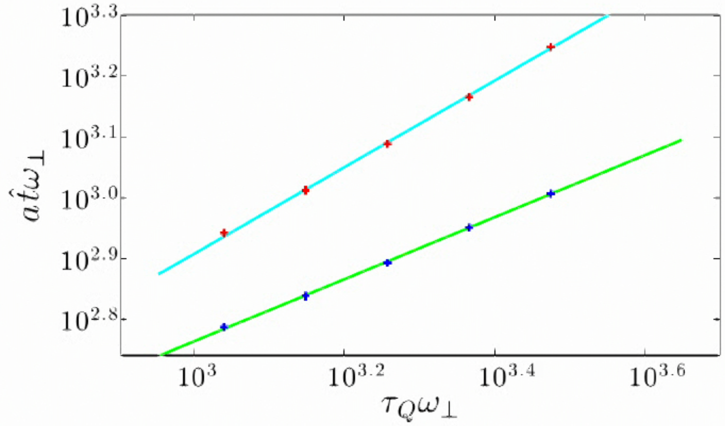
Number-conserving scattering processes

Nonlocal potential that 'resists' c-field currents

Multiplicative noise with unusual correlations

Full SPGPE: effects on KZM

- Implemented for quasi-1D KZ quench
- Results depart significantly from the 'simple growth' SPGPE



Exponent	$\alpha = z\nu/(1+z\nu)$	$\beta = \nu/2(1+z\nu)$
Number-damping SPGPE	0.5119 ± 0.0178	0.1236 ± 0.0098
Full SPGPE	0.7145 ± 0.0358	0.0966 ± 0.0128
Mean field	0.5	0.125

[McDonald, Bradley, PRA **92** 033616 (2015)]

Conclusion

- Introduced the Stochastic Projected Gross-Pitaevskii Equation for finite-temperature ultracold atom modelling
- Investigated finite-temperature vacuum decay in a range of atomic analogue systems, using SPGPE with growth (noise and damping) terms
- Agreement with thermal instanton calculations is good (renormalization effects in the exponent appear small)
- Outlook:
  - Interesting questions about bubble mergers and correlations to address
  - Scattering terms from full SPGPE may be important to explore these