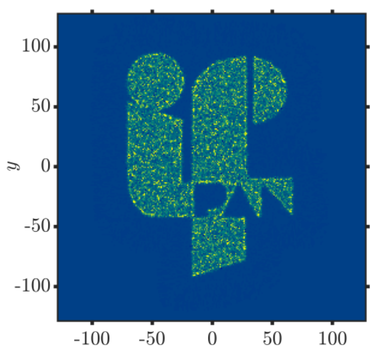
Scalable full quantum dynamics of dissipative Bose-Hubbard systems and multi-time correlations

(if we get to them...)



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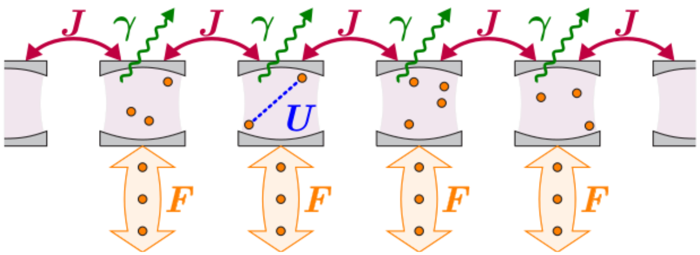
References:

- PD, Ferrier, Matuszewski, Orso, Szymańska, PRX Quantum **2**, 010319 (2021).
- PD, Quantum **5**, 455 (2021).

Driven dissipative Bose-Hubbard model

$$\widehat{H} = \sum_j \widehat{H}_j - \sum_{\text{connections } i,j} \left[J_{ij}\widehat{a}_j^\dagger \widehat{a}_i + J_{ij}^* \widehat{a}_i^\dagger \widehat{a}_j \right]$$



Vincentini, Minganti, Rota, Orso, Ciuti, PRA **97**, 013853 (2018)

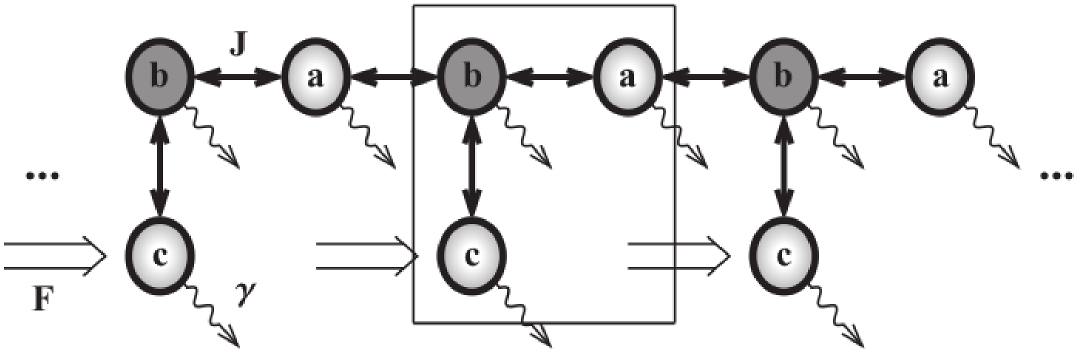
$$\widehat{H}_j = -\Delta_j \widehat{a}_j^\dagger \widehat{a}_j + \frac{U_j}{2} \widehat{a}_j^\dagger \widehat{a}_j^\dagger \widehat{a}_j \widehat{a}_j + F_j \widehat{a}_j^\dagger + F_j^* \widehat{a}_j$$

driving

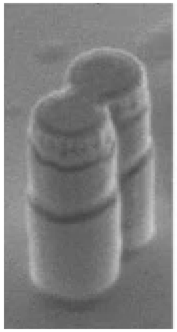
$$\frac{\partial \widehat{\rho}}{\partial t} = -i \left[\widehat{H}, \widehat{\rho} \right] + \sum_j \frac{\gamma_j}{2} \left[2\widehat{a}_j \widehat{\rho} \widehat{a}_j^\dagger - \widehat{a}_j^\dagger \widehat{a}_j \widehat{\rho} - \widehat{\rho} \widehat{a}_j^\dagger \widehat{a}_j \right]$$

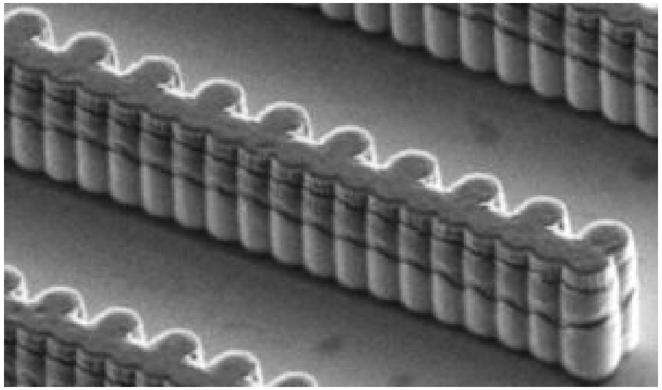
dissipation

Also structured lattices – e.g. Lieb lattice



Casteels, Rota, Storme, Ciuti, PRA **93**, 043833 (2016)





Baboux, Ge, Jacqmin, Biondi, Galopin, Lemaitre, Le Gratiet, Sagnes, Schmidt, Tureci, Amo, Bloch, PRL **116**, 066402 (2016)

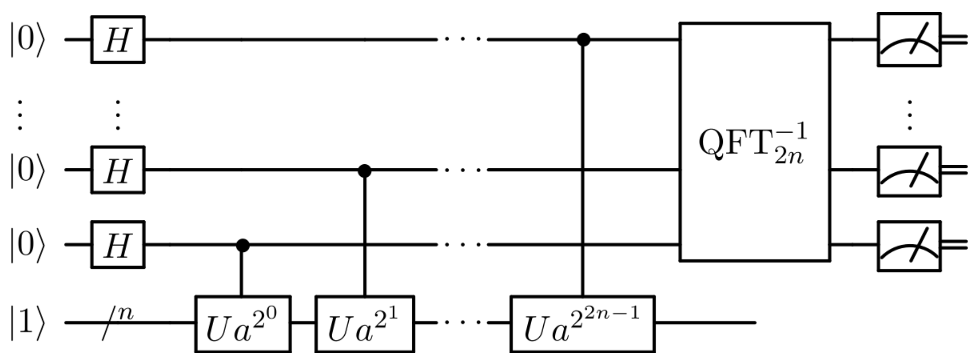
Two different kinds of quantum complexity

Suppose we have M d-level systems

Size of a (mixed) state in Hilbert space: $\sim \frac{1}{2} d^{2M}$

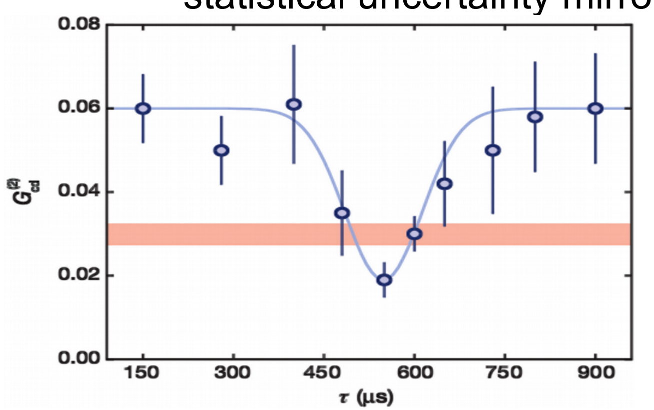
(1) Universal quantum computer, Shor's, Grover's algorithms, etc...

* needs precise knowledge of microscopic subsystem observables



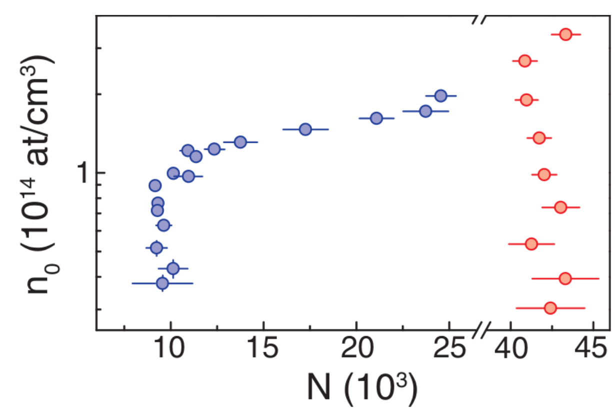
(2) Quantum behaviour of (most?) experimental systems

* knowledge of bulk or locally averaged quantities suffices
* statistical uncertainty mirrors experimental reality



Lopes, Imanaliev, Aspect, Cheneau, Boiron, Westbrook, *Nature* **520**, 66 (2015)

Cabrera, Tanzi, Sanz, Naylor, Thomas, Cheiney, Tarruell, *Science* **359**, 301 (2018)



NARODOWE CENTRUM NAUKI

Positive-P representation

M subsystems (modes, sites, volumes) labeled by j

Coherent state basis, complex, *local* α_j $\quad |\alpha_j\rangle_j = e^{-|\alpha_j|^2/2}\, e^{\alpha_j \widehat{a}_j^\dagger} |\text{vac}\rangle$

Local operator kernel $\quad \widehat{\Lambda}(\boldsymbol{\lambda}) = \bigotimes_j \frac{|\alpha_j\rangle_j \langle \beta_j^*|_j}{\langle \beta_j^*|_j |\alpha_j\rangle_j}$

"ket" amplitude α_j
"bra" amplitude β_j^*

full system configuration $\quad \boldsymbol{\lambda} = \{\alpha_1, \dots, \alpha_M, \beta_1, \dots, \beta_M\}$

Full density matrix $\quad \widehat{\rho} = \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\, \widehat{\Lambda}(\boldsymbol{\lambda})$

Correlations between subsystems are all in the distribution of configurations

$P_+(\boldsymbol{\lambda})$ The distribution is positive, real ⟶ let's SAMPLE IT !

Identities and observables

Crucial element: <u>differential identities</u>

Follow from the operator kernel:

$$\widehat{\Lambda}(\boldsymbol{\lambda}) = \bigotimes_j \frac{|\alpha_j\rangle_j \langle \beta_j^*|_j}{\langle \beta_j^*|_j |\alpha_j\rangle_j}$$

$$\widehat{a}_j \widehat{\Lambda} = \alpha_j \widehat{\Lambda},$$

$$\widehat{a}_j^\dagger \widehat{\Lambda} = \left[\beta_j + \frac{\partial}{\partial \alpha_j}\right] \widehat{\Lambda}$$

$$\widehat{\Lambda} \widehat{a}_j = \left[\alpha_j + \frac{\partial}{\partial \beta_j}\right] \widehat{\Lambda}$$

$$\widehat{\Lambda} \widehat{a}_j^\dagger = \beta_j \widehat{\Lambda}.$$

Observable: occupation

$$\widehat{\rho} = \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\, \widehat{\Lambda}(\boldsymbol{\lambda})$$

$$\begin{aligned}
\widehat{N}_j &= \langle \widehat{a}_j^\dagger \widehat{a}_j \rangle = \mathrm{Tr}\left[\widehat{a}_j^\dagger \widehat{a}_j \widehat{\rho}\right] \\
&= \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\ \mathrm{Tr}\left[\widehat{a}_j^\dagger \widehat{a}_j \widehat{\rho}\right] \\
&= \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\, \alpha_j \left[\beta_j + \frac{\partial}{\partial \alpha_j}\right] \mathrm{Tr}\left[\widehat{\Lambda}\right] \\
&= \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\, \alpha_j \beta_j \\
&= \lim_{\mathcal{S}\to\infty} \langle \alpha_j \beta_j \rangle_{\mathrm{stoch.}}
\end{aligned}$$

$$\mathrm{Tr}\left[\widehat{\Lambda}\right] = 1$$

$$\widehat{\rho} = \int d^{4M}\boldsymbol{\lambda}\, P_+(\boldsymbol{\lambda})\, \widehat{\Lambda}(\boldsymbol{\lambda})$$

we have *S* samples of $\boldsymbol{\lambda}$
the configurations
distributed according to $P_+(\boldsymbol{\lambda})$

Density matrix $\widehat{\rho}$ $\leftrightarrow$ distribution P_+ for the fields $\leftrightarrow$ random samples of the fields α β

Master equation:

$$\hbar = 1$$

$$\frac{\partial\widehat{\rho}}{\partial t} = -i\left[\widehat{H},\widehat{\rho}\right] + \frac{\gamma}{2}\left(2\widehat{a}\widehat{\rho}\widehat{a}^\dagger - \widehat{a}^\dagger\widehat{a}\widehat{\rho} - \widehat{\rho}\widehat{a}^\dagger\widehat{a}\right)$$

$$\widehat{H} = \frac{U}{2}\widehat{a}^\dagger\widehat{a}^\dagger\widehat{a}\widehat{a} - \Delta\widehat{a}^\dagger\widehat{a}$$

apply identities

Fokker Planck equation

$$\frac{\partial P_+}{\partial t} = \left\{-\frac{\partial}{\partial\alpha}\left(-iU\alpha\beta + i\Delta - \frac{\gamma}{2}\right)\alpha - \frac{\partial}{\partial\beta}\left(iU\alpha\beta - i\Delta - \frac{\gamma}{2}\right)\beta + \frac{\partial^2}{\partial\alpha^2}\left(\frac{-iU}{2}\right)\alpha^2 + \frac{\partial^2}{\partial\beta^2}\left(\frac{iU}{2}\right)\beta^2\right\}P_+$$

deterministic (ket) — deterministic (bra) — quantum noise

stochastic correspondence

Stochastic (Langevin) equations:

$$\frac{d\alpha}{dt} = \left(-iU\alpha\beta + i\Delta - \frac{\gamma}{2}\right)\alpha + \sqrt{-iU}\,\alpha\xi(t)$$

$$\frac{d\beta}{dt} = \left(+iU\alpha\beta - i\Delta - \frac{\gamma}{2}\right)\beta + \sqrt{+iU}\,\beta\widetilde{\xi}(t)$$

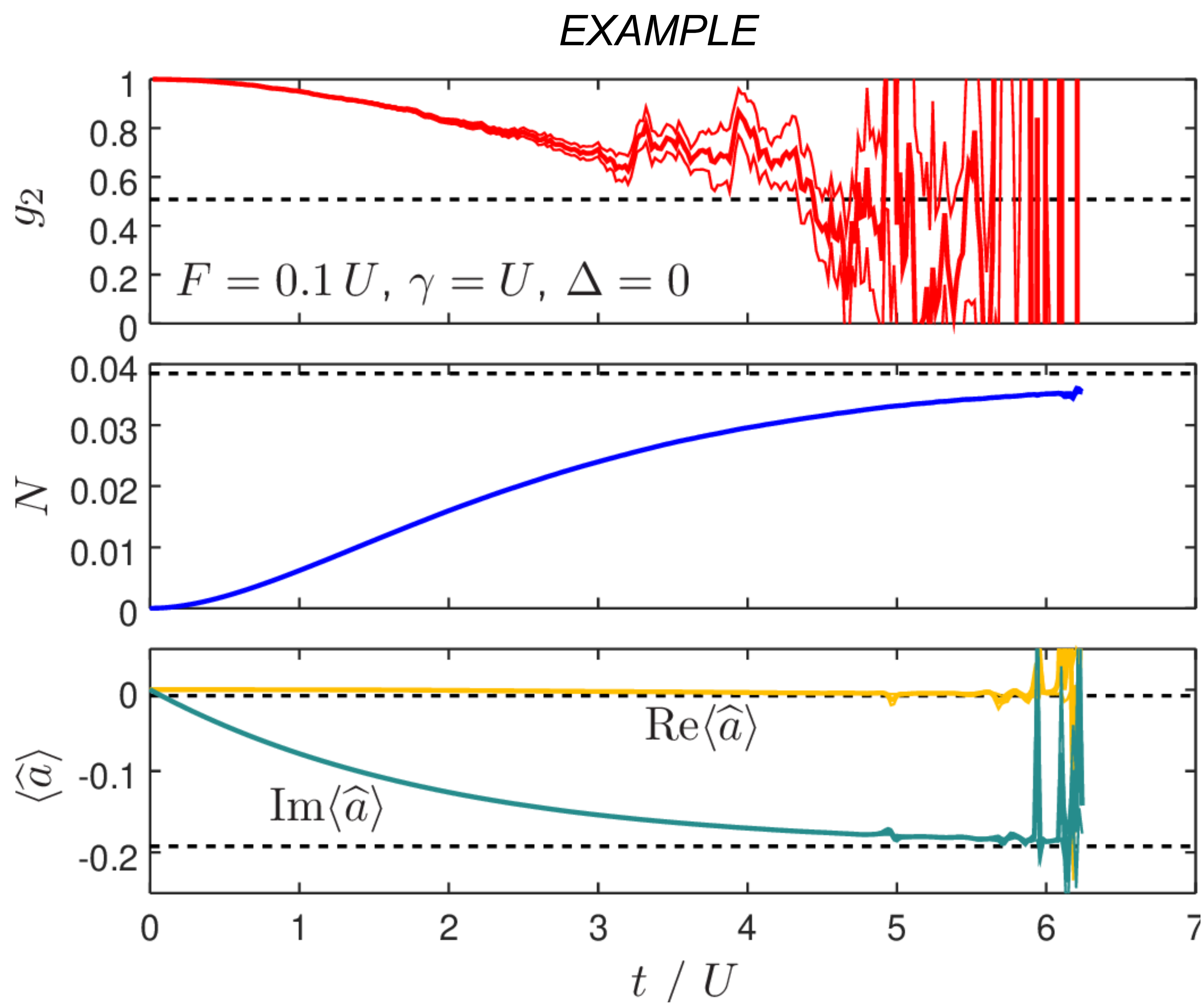
mean field part — quantum noise part

different noises

White noise

$$\langle\xi(t)\xi(t')\rangle_{\text{stoch}} = \delta(t-t')$$

Particularly for closed Hamiltonian systems.



Dealing with noise amplification

- It was found that the simulation time is limited:

$$t_{\rm sim} \approx \begin{cases} \dfrac{2.5}{\max_j [U_j N_j^{2/3}]} & \text{if } \max_j N_j \gg 1, \\ \dfrac{C}{\max_j U_j} & \text{if } \max_j N_j \ll 1, \end{cases}$$

PD, Drummond, *J Phys A* **39**, 1163 (2006)

- Various ways have been developed to improve this performance:
  - * stochastic Gauges — PD, Drummond, *PRA* **66**, 033812 (2002), J Phys A **39**, 2723 (2006); PD *et al*, PRA **79**, 043619 (2009); Wuster, Corney, Rost, PD, PRE **96**, 013309 (2017)
  - * quantum interpolation — PD, *PRL* **103,** 130402 (2009); Ng, Sorensen, PD, PRB **88**, 144304 (2013)
- Or it can be optimal to just use approximate representations:
  - * truncated Wigner — Sinatra, Lobo, Castin, J Phys B 35, 3599 (2002); Norrie, Ballagh, Gardiner, *PRA* **73**, 043617 (2006), PRL **94**, 040401 (2005)
  - * STAB (Stochastic adaptive Bogoliubov) — PD, Chwedeńczuk, Trippenbach, Zin, PRA 83, 063625 (2011); Kheruntsyan *et al*, *PRL* **108**, 260401 (2012)

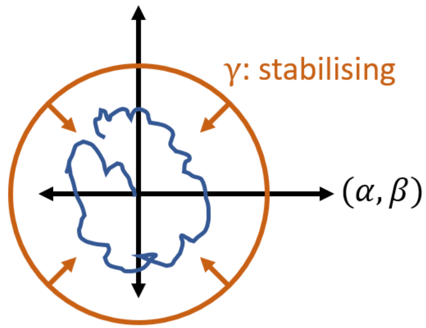
- It was also found that simulation time grows with dissipation to an external bath:

$$t_{\rm sim} \sim \frac{2 - \log N}{U - \gamma}$$

- But not really tested at the time ....

Positive-P simulations stabilised by the dissipation

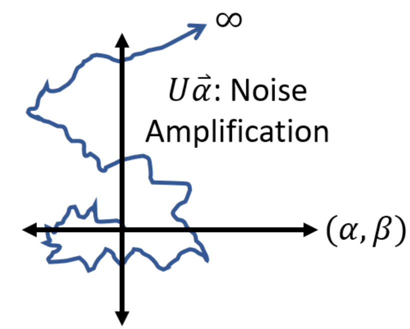
(d) **Open Systems**

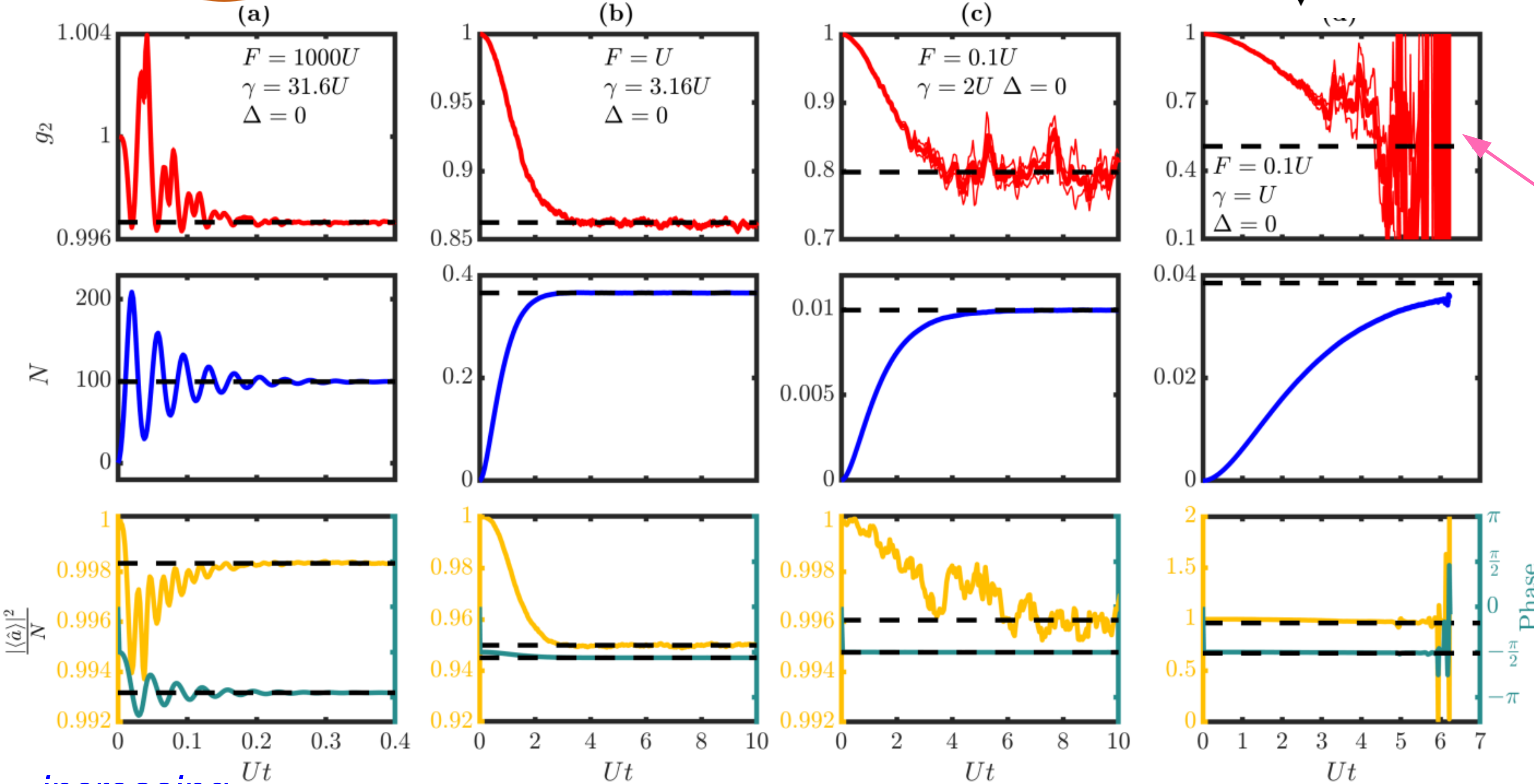


stationary state can be reached
and studied
in a full quantum description

Closed Systems

(c)

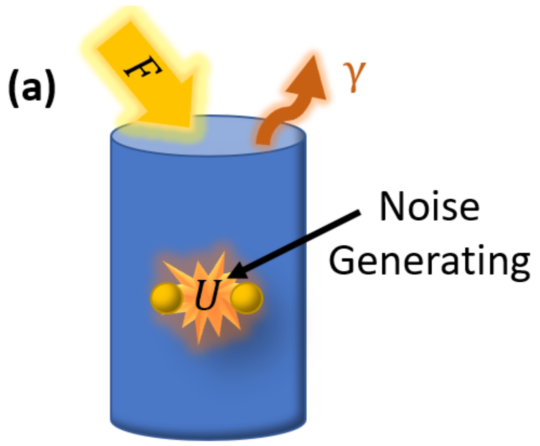




instability
triggered
γ too low

increasing dissipation

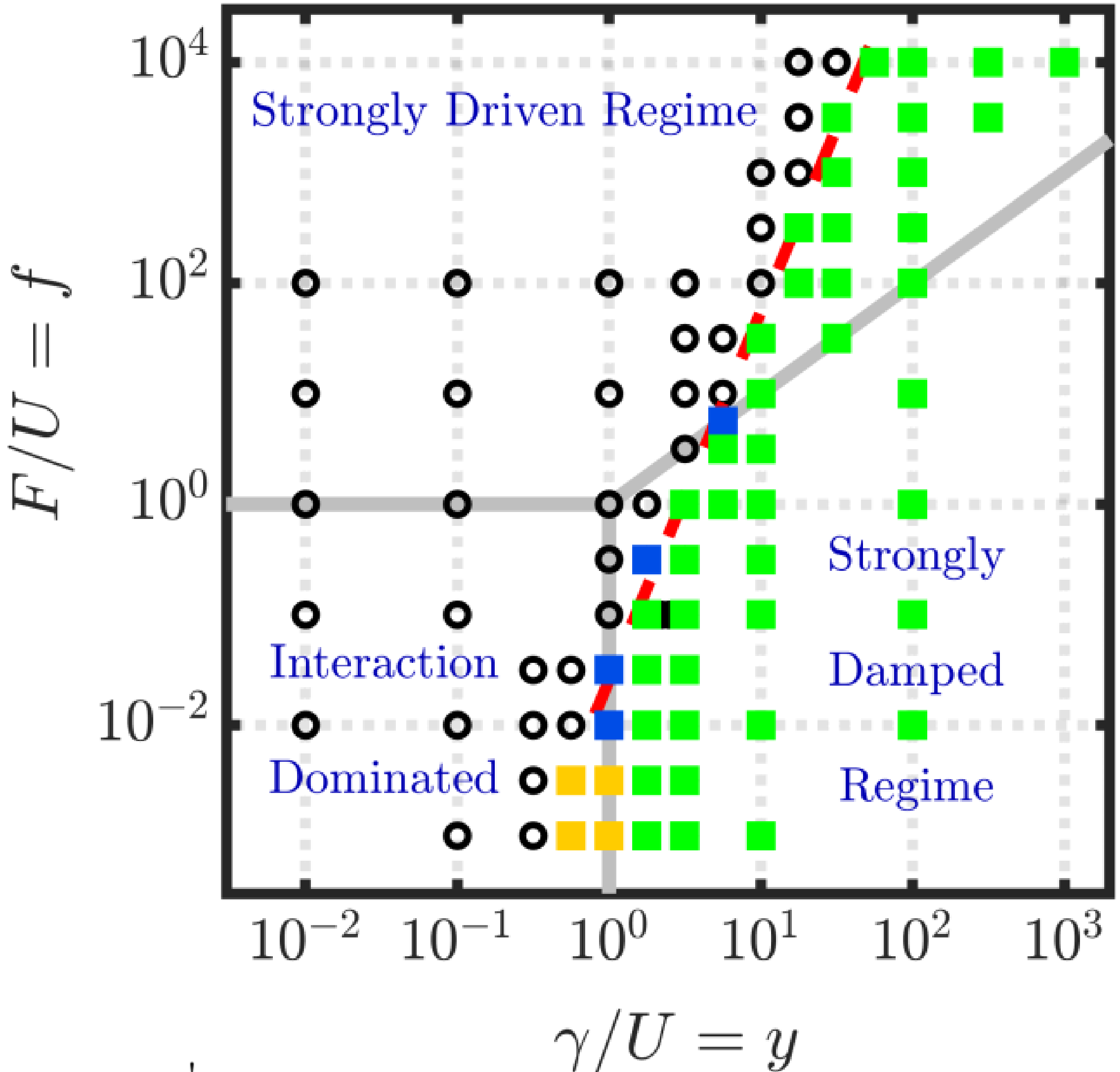
- Remarkably, stability is determined by single-site parameters!



Regime of stability:

$$\gamma \gtrsim 3U\left(\frac{F}{U}\right)^{0.30}$$

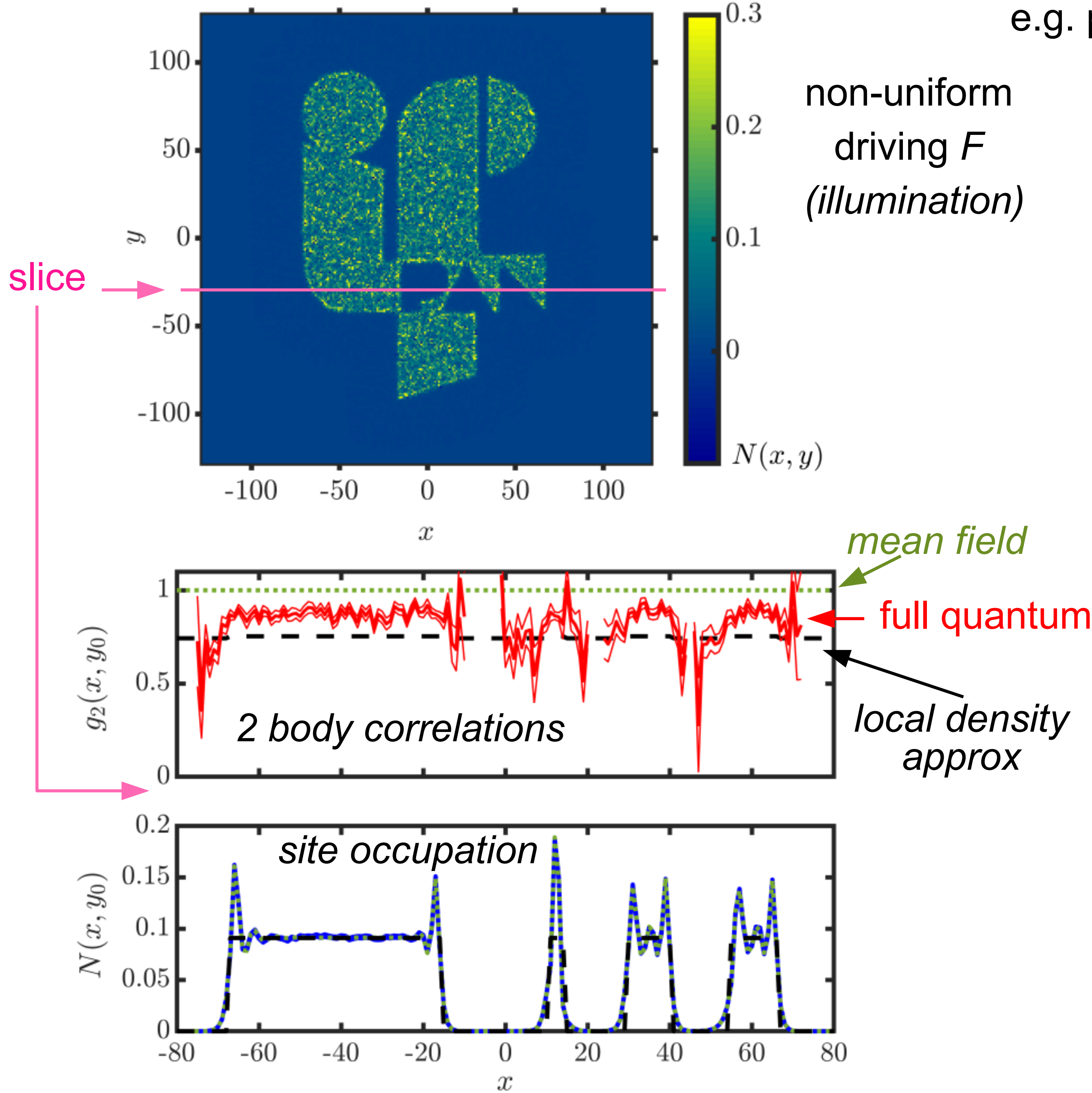
$$\gamma \gtrsim U \quad \text{when} \quad F \lesssim 0.01U$$



$$\hat{H}_j = -\Delta_j \hat{a}_j^\dagger \hat{a}_j + \frac{U_j}{2}\hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j + F_j \hat{a}_j^\dagger + F_j^* \hat{a}_j$$

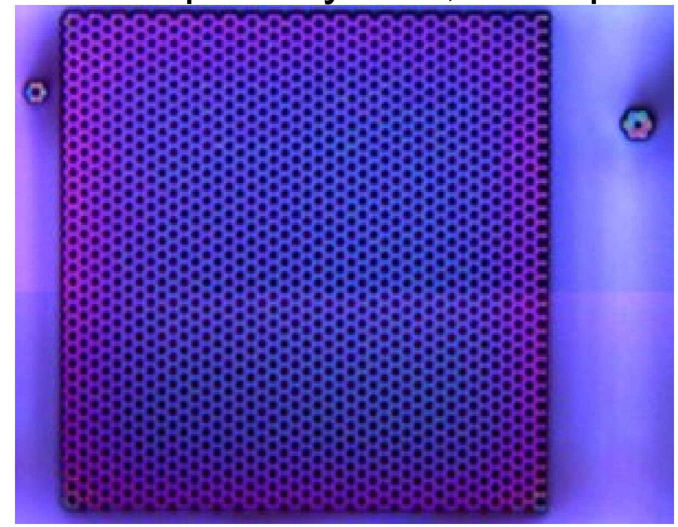
PD, Ferrier, Matuszewski, Orso, Szymańska, PRX Quantum **2**, 010319 (2021).

Large systems – example simulation 256 x 256 lattice

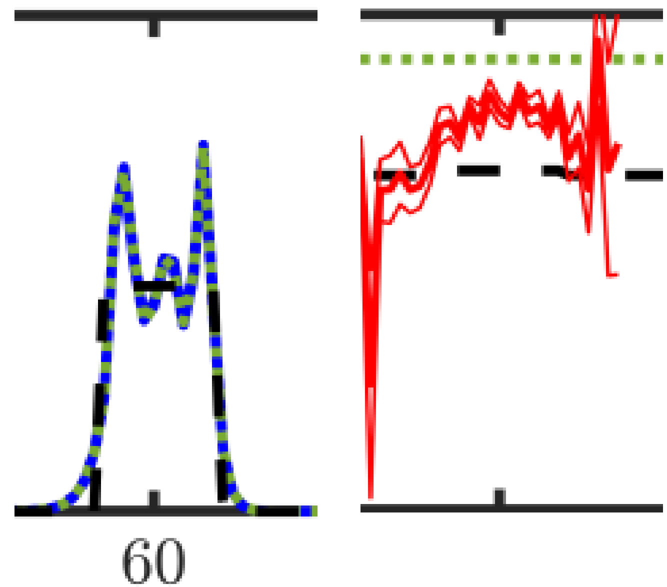


PD, Ferrier, Matuszewski, Orso, Szymańska, PRX Quantum **2**, 010319 (2021).

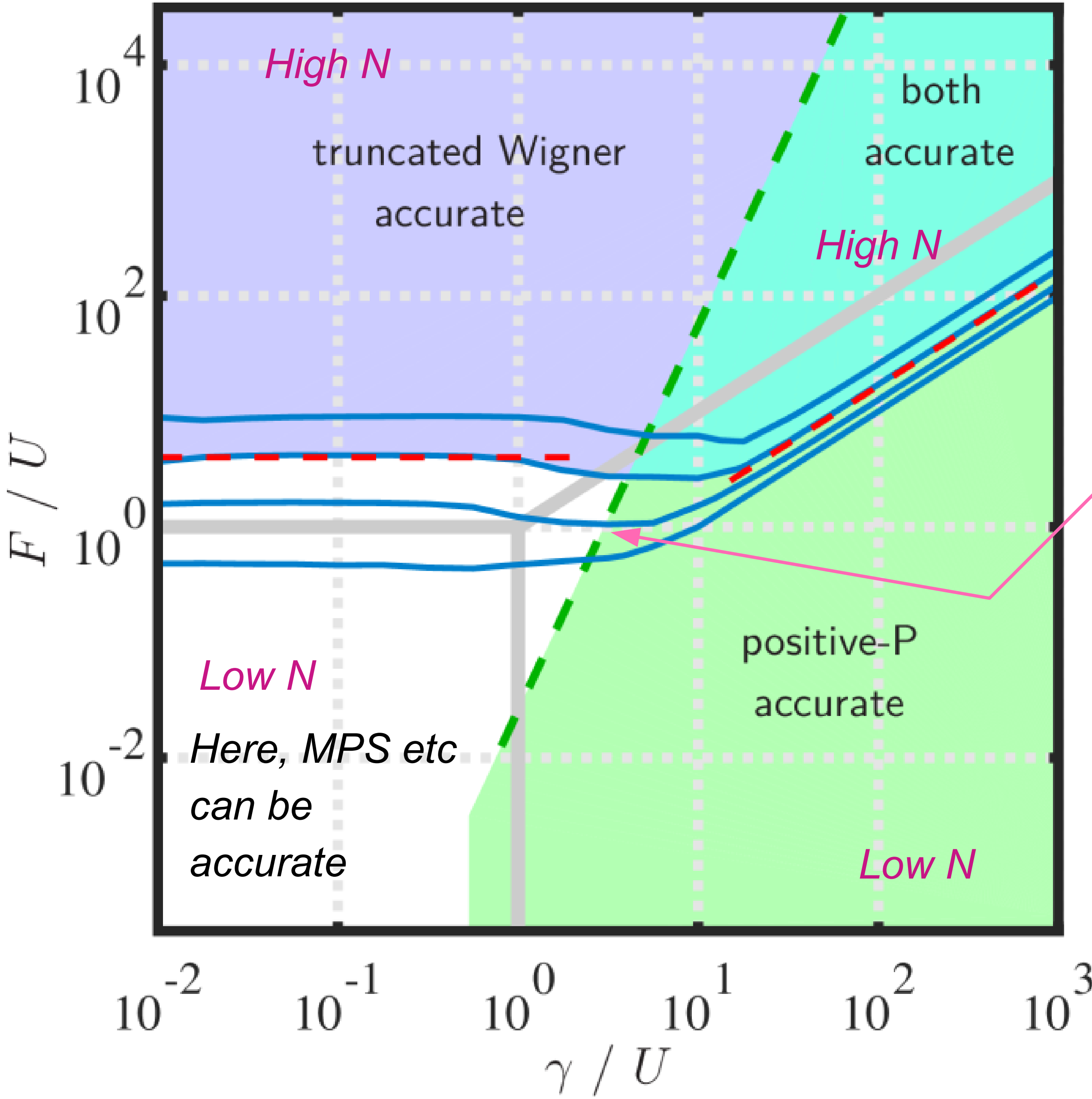
e.g. photonic quasicrystals, micropillars

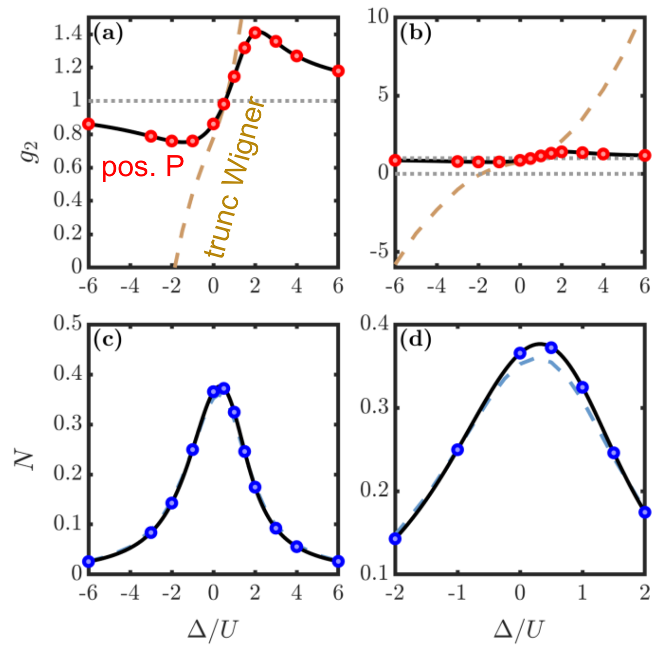


Milicevic, Ozawa, Montambaux, Carusotto, Galopin, Lemaitre, Le Gratiet, Sagnes, Bloch, Amo, PRL **118**, 107403 (2017)



Phase space methods - regimes of applicability





Have a dissipative system you want to simulate?

non-uniform ?
time-dependent ??

Contact us ;-)

PD, Ferrier, Matuszewski, Orso, Szymańska, PRX Quantum **2**, 010319 (2021).

Unequal time correlations

- Expressed in terms of Heisenberg operators

$$\widehat{A}(t) = e^{i(t-t_0)\widehat{H}/\hbar}\ \widehat{A}(t_0)\ e^{-i(t-t_0)\widehat{H}/\hbar}$$

- Time ordered correlation functions.
  Correspond to all sequences of measurements

$$\langle \widehat{A}_1(t_1)\widehat{A}_2(t_2)\cdots\widehat{A}_{\mathcal{N}}(t_{\mathcal{N}})\widehat{B}_1(s_1)\widehat{B}_2(s_2)\cdots\widehat{B}_{\mathcal{M}}(s_{\mathcal{M}})\rangle \qquad t_1 \leqslant t_2 \leqslant \ldots \leqslant t_{\mathcal{N}}, \quad s_1 \geqslant s_2 \geqslant \ldots \geqslant s_{\mathcal{M}}$$

time grows (→) time grows (←)

- e.g.

$$\langle \widehat{a}^\dagger(0)\widehat{a}^\dagger(\tau)\widehat{a}(\tau)\widehat{a}(0)\rangle$$

particle present both at *t=0* and *t=tau*

$$\langle \widehat{a}^\dagger(\tau)\widehat{a}^\dagger(\tau)\widehat{a}(0)\widehat{a}(0)\rangle$$

anomalous pair correlation:
anihilate pair at *t=0* create at *t=tau*

Partial analogy positive-P <-> Heisenberg equations of motion

Correspondence in observable calculations:

$$\widehat{a} \leftrightarrow \alpha \qquad \widehat{a}^\dagger \leftrightarrow \beta$$

Heisenberg equations of motion:

$$\frac{d\,\widehat{a}(t)}{dt} = \left(-iU\widehat{a}^\dagger(t)\widehat{a}(t) + i\Delta - \frac{\gamma}{2}\right)\widehat{a}(t)$$

$$\frac{d\,\widehat{a}^\dagger(t)}{dt} = \widehat{a}^\dagger(t)\left(+iU\widehat{a}^\dagger(t)\widehat{a}(t) - i\Delta - \frac{\gamma}{2}\right)$$

$$\widehat{H} = \frac{U}{2}\widehat{a}^\dagger\widehat{a}^\dagger\widehat{a}\widehat{a} - \Delta\widehat{a}^\dagger\widehat{a}$$

positive-P equations of motion

$$\frac{d\alpha}{dt} = \left(-iU\alpha\beta + i\Delta - \frac{\gamma}{2}\right)\alpha + \sqrt{-iU}\,\alpha\xi(t)$$

$$\frac{d\beta}{dt} = \left(+iU\alpha\beta - i\Delta - \frac{\gamma}{2}\right)\beta + \sqrt{+iU}\,\beta\widetilde{\xi}(t)$$

Indeed, many unequal time correlations have remarkably simple expressions

$$g^{(2)}_{1,1}(\tau) = \frac{\langle \widehat{a}_1^\dagger(t)\,\widehat{a}_1^\dagger(t+\tau)\,\widehat{a}_1(t+\tau)\,\widehat{a}_1(t)\rangle}{\langle \widehat{a}_1^\dagger(t)\,\widehat{a}_1(t)\rangle\langle \widehat{a}_1^\dagger(t+\tau)\,\widehat{a}_1(t+\tau)\rangle} = \frac{\mathrm{Re}\langle \alpha_1(t)\,\alpha_1(t+\tau)\,\widetilde{\alpha}_1^*(t+\tau)\,\widetilde{\alpha}_1^*(t)\rangle_s}{N_1(t)\,N_1(t+\tau)}$$

PD Quantum **5**, 455 (2021).

Evaluation of variously ordered correlations

PD Quantum **5**, 455 (2021).

Normal ordering: positive-P variables

$$\langle \hat{a}^\dagger_{p_1}(t_1)\cdots\hat{a}^\dagger_{p_\mathcal{N}}(t_\mathcal{N})\hat{a}_{q_1}(s_1)\cdots\hat{a}_{q_\mathcal{M}}(s_\mathcal{M})\rangle$$
$$= \langle \beta_{p_1}(t_1)\cdots\beta_{p_\mathcal{N}}(t_\mathcal{N})\alpha_{q_1}(s_1)\cdots\alpha_{q_\mathcal{M}}(s_\mathcal{M})\rangle_{\mathrm{stoch}}$$

Anti-normal ordering: Q distribution variables

$$\langle \hat{a}_{p_1}(t_1)\cdots\hat{a}_{p_\mathcal{N}}(t_\mathcal{N})\hat{a}^\dagger_{q_1}(s_1)\cdots\hat{a}^\dagger_{q_\mathcal{M}}(s_\mathcal{M})\rangle$$
$$= \langle \alpha'_{p_1}(t_1)\cdots\alpha'_{p_\mathcal{N}}(t_\mathcal{N})\beta'_{q_1}(s_1)\cdots\beta'_{q_\mathcal{M}}(s_\mathcal{M})\rangle_{\mathrm{stoch}}$$

conversion P ⟶ Q

$$\alpha'_j = \alpha_j + \zeta_j \quad ; \quad \beta'_j = \beta_j + \zeta^*_j$$

$$\langle\zeta_j\rangle_{\mathrm{stoch}} = 0\ ;\ \langle\zeta_j\zeta_k\rangle_{\mathrm{stoch}} = 0\ ;\ \langle\zeta^*_j\zeta_k\rangle_{\mathrm{stoch}} = 1$$

Mixed ordering:

1) sample what is possible using positive-P variables
2) convert variables to doubled-Q
3) sample what is possible using Q variables

identities:

positive-P

$$\hat{a}_j\hat{\Lambda} = \alpha_j\hat{\Lambda},$$
$$\hat{a}^\dagger_j\hat{\Lambda} = \left[\beta_j + \frac{\partial}{\partial\alpha_j}\right]\hat{\Lambda}$$
$$\hat{\Lambda}\hat{a}_j = \left[\alpha_j + \frac{\partial}{\partial\beta_j}\right]\hat{\Lambda}$$
$$\hat{\Lambda}\hat{a}^\dagger_j = \beta_j\hat{\Lambda}.$$

doubled-Q

$$\hat{a}_j\hat{\Lambda}_Q = \left[\alpha_j - \frac{\partial}{\partial\alpha^*_j}\right]\hat{\Lambda}_Q$$
$$\hat{a}^\dagger_j\hat{\Lambda}_Q = \alpha^*_j\hat{\Lambda}_Q,$$
$$\hat{\Lambda}_Q\hat{a}_j = \alpha_j\hat{\Lambda}_Q,$$
$$\hat{\Lambda}_Q\hat{a}^\dagger_j = \left[\alpha^*_j - \frac{\partial}{\partial\alpha_j}\right]\hat{\Lambda}_Q.$$

Order (number of operators)	2nd order	3rd order	4th order
Total permutations	**12**	**56**	**240**
single time correlations	4	8	16
multi-time accessible with P representation	4	14	36
additional accessible with Q representation	4	14	36
additional accessible with mixed order (Sec. 5.4)	–	12	72
Total doable	**12**	**48**	**160**
time ordered not doable	–	–	–
Not time ordered, not doable	–	8	80

Table 2: A tally of $\hat{a}$, $\hat{a}^\dagger$ products involving up to four operators, evaluated at one of two times. The general form considered is $\langle\hat{A}(t_a)\hat{B}(t_b)\hat{C}(t_c)\hat{D}(t_d)\rangle$, where $\hat{A}, \hat{B}, \hat{C}, \hat{D}$ can be either of $\hat{a}$ or $\hat{a}^\dagger$ (same mode), and the time arguments can take up to two distinct times $t = 0$ and $t = \tau > 0$.

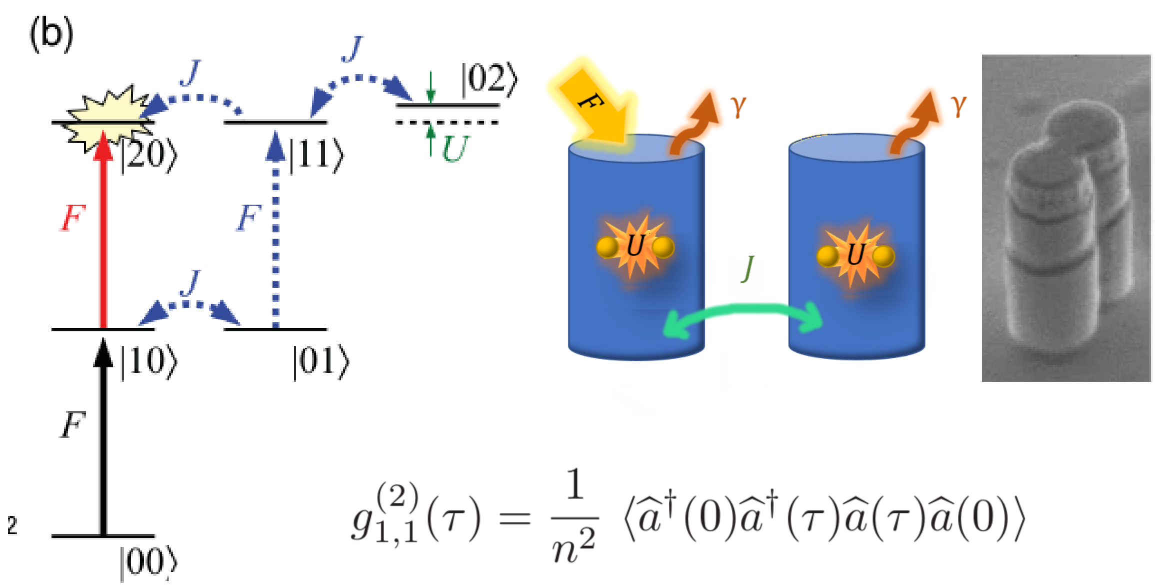
Unconventional photon blockade

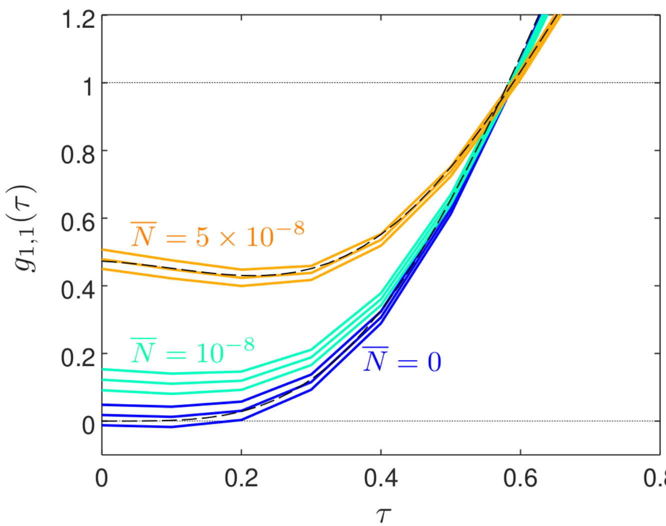
Complete antibunching,
Subtle interference effect $U \ll \gamma$

potential single-photon source

Liew, Savona, PRL **104**, 183601 (2010)
Bamba, Imamoglu, Carusotto, Ciuti, PRA **83**, 021802(R) (2011)

robustness to background photons:

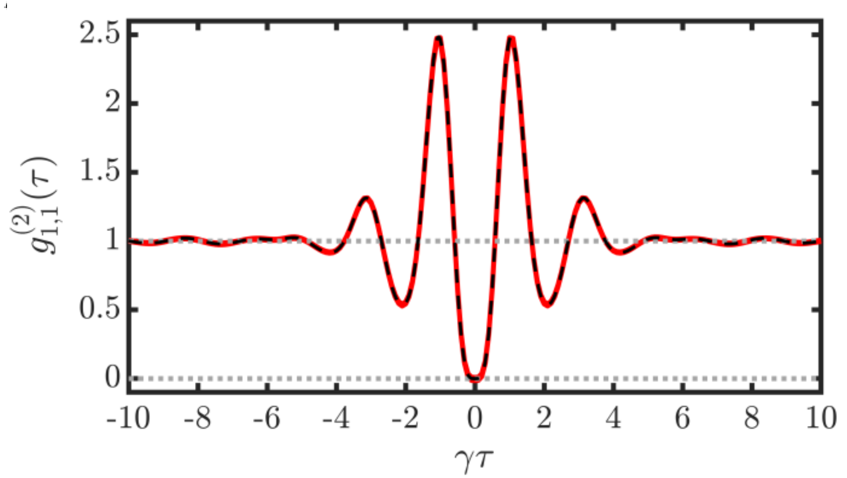




PD Quantum **5**, 455 (2021).

$$g^{(2)}_{1,1}(\tau) = \frac{1}{n^2} \langle \hat{a}^\dagger(0)\hat{a}^\dagger(\tau)\hat{a}(\tau)\hat{a}(0)\rangle$$

$$U = 0.0856,\ J = 3,\ \Delta = -0.275,$$
$$\gamma = 1,\ F = 0.01$$



$$\frac{\partial\hat{\rho}}{\partial t} = -i\left[\hat{H},\hat{\rho}\right] + \frac{\gamma\overline{N}}{2}\sum_j\left[2\hat{a}_j^\dagger\hat{\rho}\hat{a}_j - \hat{a}_j\hat{a}_j^\dagger\hat{\rho} - \hat{\rho}^\dagger\hat{a}_j\hat{a}_j\right]$$
$$+\frac{\gamma(\overline{N}+1)}{2}\sum_j\left[2\hat{a}_j\hat{\rho}\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_j\hat{\rho} - \hat{\rho}\hat{a}_j^\dagger\hat{a}_j\right]. \quad (96)$$

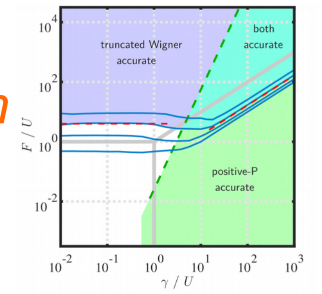
Summary and outlook

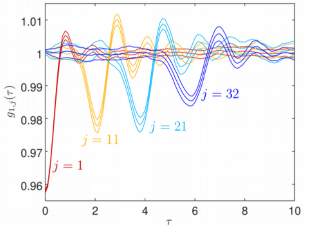
- Full quantum calculations of large Bose-Hubbard models

  positive-P method found to be stable with sufficient dissipation

  scalable. e.g. 10^5 sites is easy

  truncated Wigner accurate in complementary regimes





- Many unequal time correlations accessible

  nontrivial multi-time correlations appear

- Other dissipative models may also be possible.

  e.g. spins, Jaynes-Cummings-Hubbard

  Schwinger bosons — Ng, Sorensen, J Phys A **44**, 065305 (2011); Huber, Kirton, Rabl, SciPost Phys **10**, 045 (2021) (truncated Wigner)

  SU(n) positive-P-like representations — Ng, Sorensen, PD, PRB **88**, 144304 (2013); Begg, Green, Bhaseen arXiv:2011.07924 (stochastic gauges)

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- PD, Ferrier, Matuszewski, Orso, Szymańska, *Fully Quantum Scalable Description of Driven-Dissipative Lattice Models*, PRX Quantum **2**, 010319 (2021).
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