WEAK ADDITIVITY PRINCIPLE FOR CURRENT STATISTICS IN D-DIMENSIONS

Carlos Pérez-Espigares

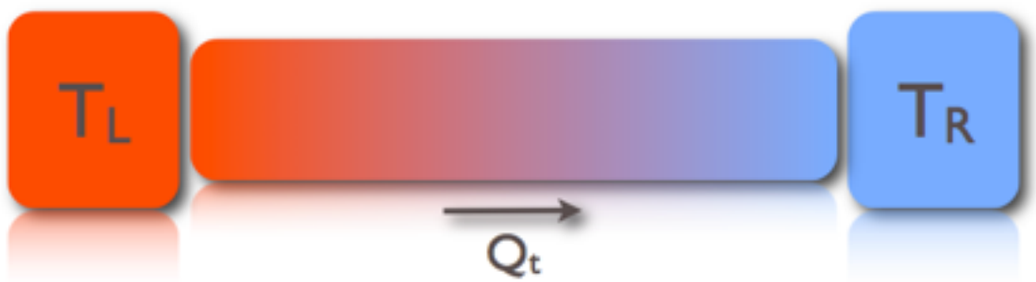
University of Modena and Reggio Emilia (Italy)

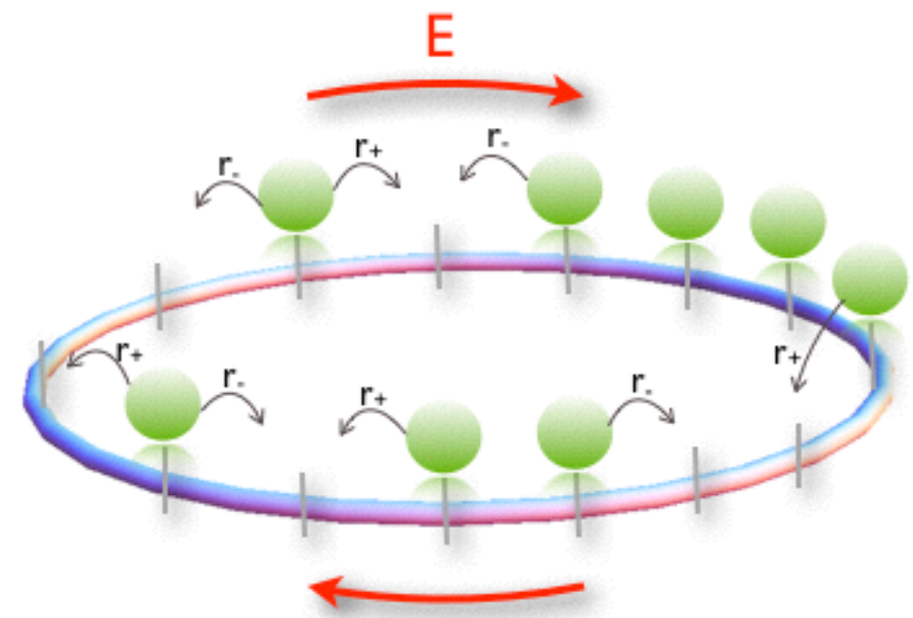
Collaborators
P.L. Garrido
P.I. Hurtado

Large Deviations for Interacting Particle Systems and
Partial Differential Equations, YEP XIII, March 9, 2016

CURRENTS OUT OF EQUILIBRIUM

- **Currents**: hallmarks of nonequilibrium behavior





- **Current statistics**: main objective of nonequilibrium statistical physics

Fundamental observable:
Current Large Deviation Function (LDF)

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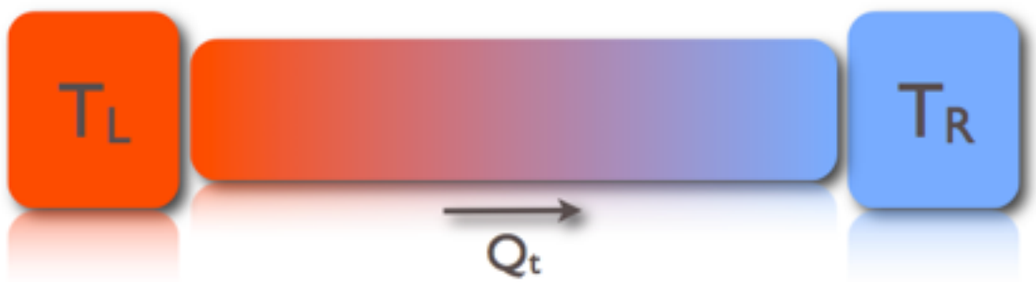

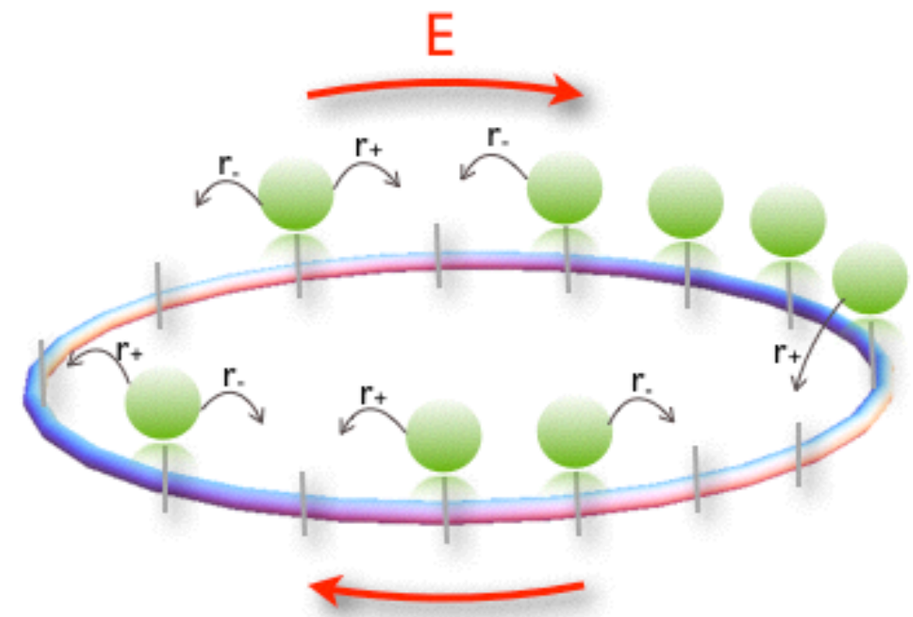

- **Current statistics**: main objective of nonequilibrium statistical physics

Fundamental observable:
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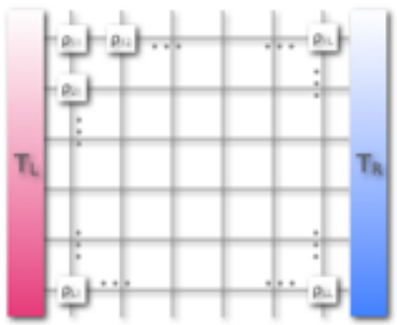
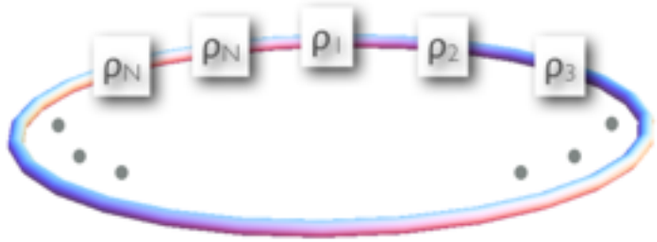
- Despite some exact results (e.g. **fluctuation theorems**), the overall picture remains puzzling

- **Two new powerfull tools:**
  - ☑ Macroscopic Fluctuation Theory (**MFT**)
  - ☑ Advanced simulations of rare events

... and an ideal laboratory:
  - ☑ Stochastic lattice gases

STOCHASTIC LATTICE GASES





$$D(\rho) = 1/2 \quad ; \quad \sigma(\rho) = \rho^2$$

$$(\rho_i, \rho_{i+1}) \to (\rho'_i, \rho'_{i+1})$$

$$\rho'_i = p(\rho_i + \rho_{i+1}) \qquad \rho'_{i+1} = (1-p)(\rho_i + \rho_{i+1})$$

- **KMP**: Diffusive energy transport model
- Local energies $\rho_i \geq 0$
- $p \in [0,1]$ random. Energy is locally conserved!

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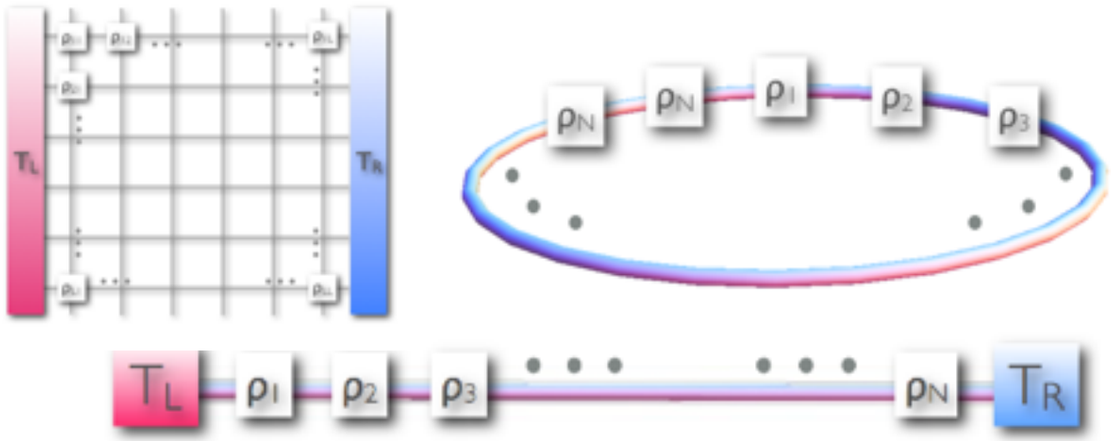

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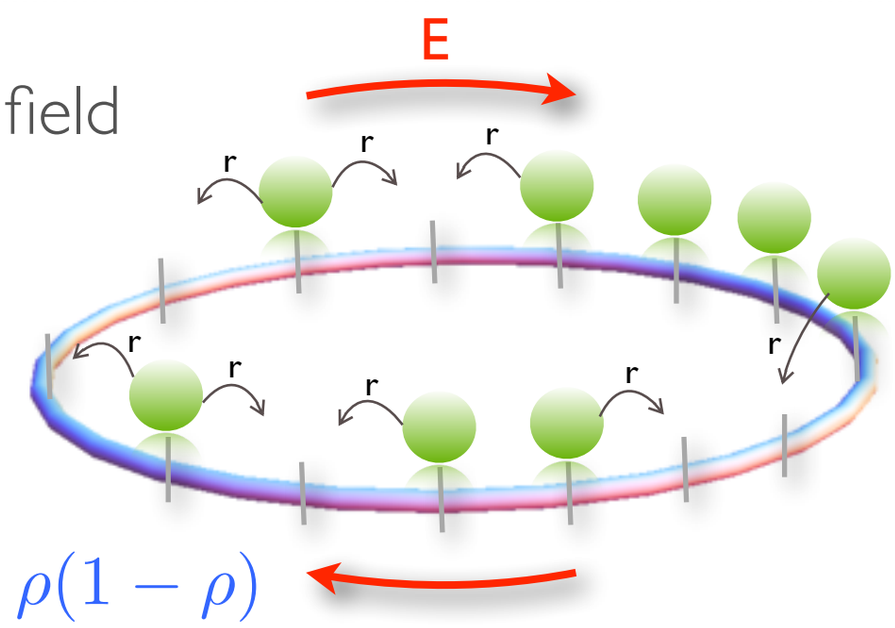
- **WASEP**: Diffusive particle transport under external field
- Occupation numbers $n_i = 0,1$ + jumps with rates

$$r_\pm = \frac{1}{2}\exp(\pm E/N)$$

- 1D, 2D, reservoirs, periodic boundaries, ...



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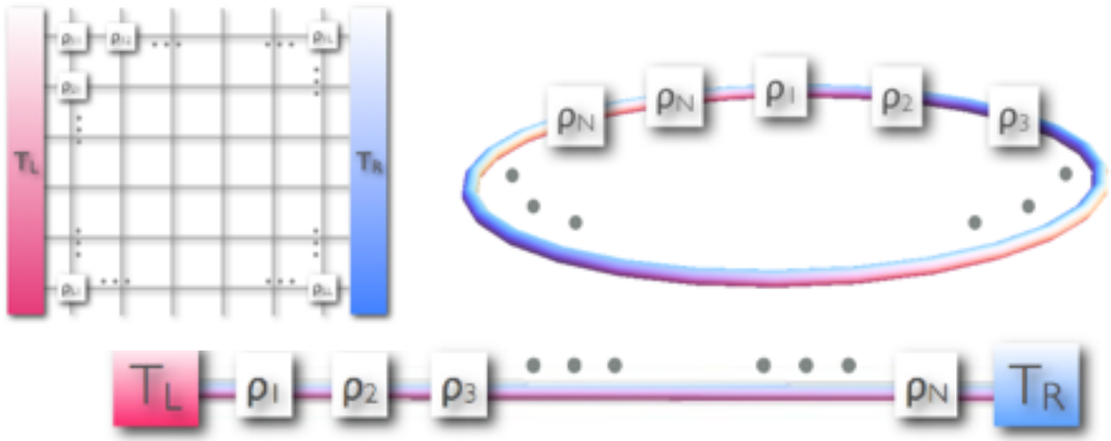

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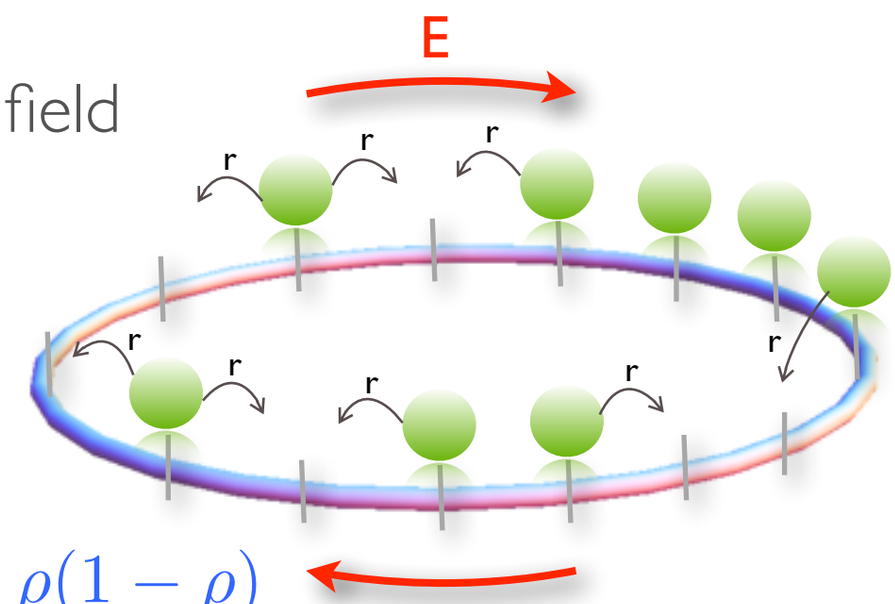

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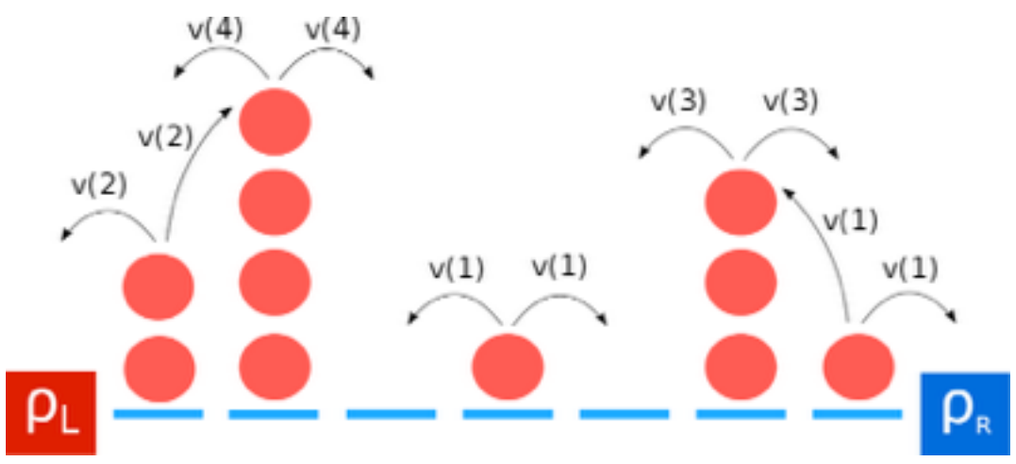

- **ZRP**: Interacting particles diffusing in a lattice
- Jump rates depend on local occupation, $\mathbf{v(n_i)}$
- Product invariant measure!

$$D(\rho) = \gamma'(\rho)/2 \quad ; \quad \sigma(\rho) = \gamma(\rho)$$

SIMULATING RARE EVENTS

Giardinà, Kurchan & Peliti, PRL **96**, 120603 (2006)
Lecomte & Tailleur, JSTAT P03004 (2007)
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- **LDFs are very hard to compute**: exponentially-unlikely rare events

- Way around: **modify dynamics** so rare events are no longer rare.

$$\mathrm{P}(\mathbf{Q}_t, t; C_0) = \sum_{C_t..C_1} U_{C_t C_{t-1}}..U_{C_1 C_0}\, \delta(\mathbf{Q}_t - \sum_{k=0}^{t-1} \mathbf{q}_{C_{k+1} C_k})$$

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- For long times,

$$\mathrm{P}(\mathbf{Q}_t, t) \asymp \mathrm{e}^{+t\mathcal{F}(\mathbf{Q}_t/t)} \Rightarrow \Pi(\boldsymbol{\lambda}, t) \asymp \mathrm{e}^{+t\theta(\boldsymbol{\lambda})}, \;\text{ with }\; \theta(\boldsymbol{\lambda}) = \max_{\mathbf{q}}[\mathcal{F}(\mathbf{q}) + \boldsymbol{\lambda}\cdot\mathbf{q}]$$

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- Modified dynamics $\tilde{U}_{C'C}$ **unnormalized**. Exit rate $Y_C \equiv \sum_{C'} \tilde{U}_{C'C}$

$$U'_{C'C} \equiv Y_C^{-1} \tilde{U}_{C'C} \Rightarrow \Pi(\boldsymbol{\lambda}, t) = \sum_{C_t \ldots C_1} Y_{C_{t-1}} U'_{C_t C_{t-1}} \ldots Y_{C_0} U'_{C_1 C_0}$$

- **Monte Carlo scheme**: Evolve **many copies** of the system with dynamics $U'_{C'C}$ and **clone/kill them with rates** Y_C.

MACROSCOPIC FLUCTUATION THEORY (MFT)

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Rev. Mod. Phys. **87**, 593 (2015)

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- Evolution equation for wide class of systems:

$\mathbf{j}(\mathbf{r},t)$ fluctuating

$$\partial_t \rho(\mathbf{r},t) + \boldsymbol{\nabla}\cdot\boxed{\left(-\hat{D}(\rho)\boldsymbol{\nabla}\rho(\mathbf{r},t) + \hat{\sigma}(\rho)\mathbf{E} + \boldsymbol{\xi}(\mathbf{r},t)\right)} = 0$$

$\mathbf{r} \in \Lambda \equiv [0,1]^d$

- Gaussian white noise: Accounts for **microscopic fluctuations at the macroscale**

$$\langle \boldsymbol{\xi}(\mathbf{r},t)\rangle = 0 \qquad \langle \xi_\alpha(\mathbf{r},t)\xi_\beta(\mathbf{r}',t')\rangle = L^{-d}\sigma_\alpha(\rho)\delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$

$\alpha,\beta \in [1,d]$

- Diffusivity and mobility matrices linked by **local Einstein relation**: $\hat{D}(\rho) = f_0''(\rho)\hat{\sigma}(\rho)$

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- Probability of a **history** $\{\rho(\mathbf{r},t),\mathbf{j}(\mathbf{r},t)\}_0^\tau \longrightarrow \mathrm{P}\left(\{\rho,\mathbf{j}\}_0^\tau\right) \sim \mathrm{e}^{+L^d I_\tau[\rho,\mathbf{j}]}$

$$I_\tau[\rho,\mathbf{j}] = -\frac{1}{2}\int_0^\tau dt\int_\Lambda d\mathbf{r}\,\left(\mathbf{j}-\mathbf{j}_{\boldsymbol{h}}(\rho)\right)\cdot\hat{\Sigma}(\rho)\left(\mathbf{j}-\mathbf{j}_{\boldsymbol{h}}(\rho)\right)$$

$$\mathbf{j}_{\boldsymbol{h}}(\rho) \equiv -\hat{D}(\rho)\boldsymbol{\nabla}\rho + \hat{\sigma}(\rho)\mathbf{E} \qquad \Sigma_\alpha(\rho) \equiv \sigma_\alpha^{-1}(\rho)$$

- Density and current fields coupled via **continuity equation**: $\partial_t\rho(\mathbf{r},t) + \boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r},t) = 0$

CURRENT STATISTICS IN MFT

- Space- and time-averaged **empirical current J**

$$\mathbf{J} = \frac{1}{\tau}\int_0^\tau dt \int_\Lambda d\mathbf{r}\ \mathbf{j}(\mathbf{r},t)$$

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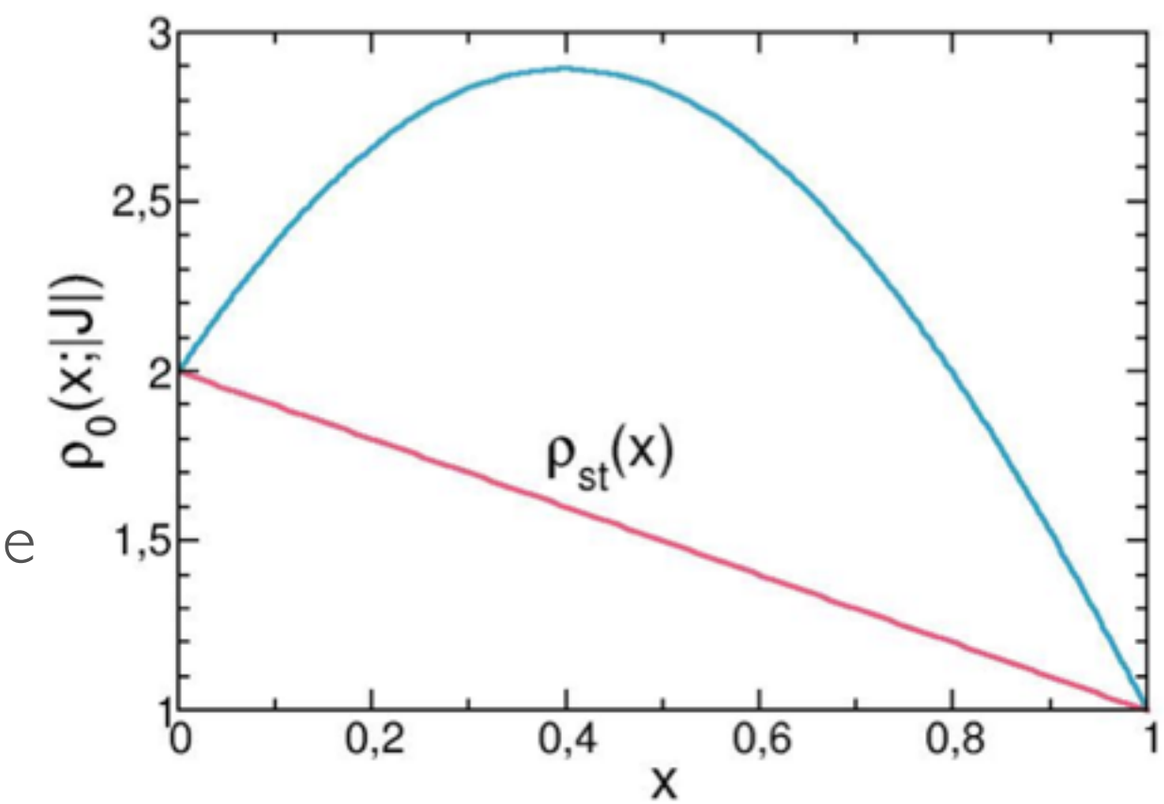
- **Optimal path≠steady profile**: Typical path to sustain a given current fluctuation **J**

$$\rho_{\mathbf{J}}(\mathbf{r},t) \qquad \mathbf{j}_{\mathbf{J}}(\mathbf{r},t)$$

- Complex spatiotemporal variational proble

challenging solution



ONE DIMENSION (1D)

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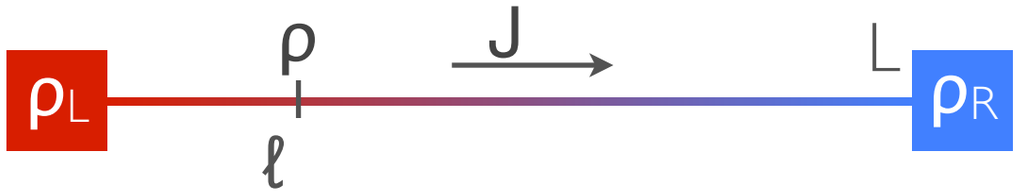
T. Bodineau & B. Derrida, PRL **92**, 180601 (2004)



- The additivity principle (AP) allows to compute explicitly the current distribution in many **1D nonequilibrium systems**

- Original formulation of AP by **iteratively slicing a 1D system**

$$\mathrm{P}_{\tau}^{(L)}(J;\rho_L,\rho_R) = \max_{\rho}[\mathrm{P}_{\tau}^{(L-\ell)}(J;\rho_L,\rho) \times \mathrm{P}_{\tau}^{(\ell)}(J;\rho,\rho_R)]$$

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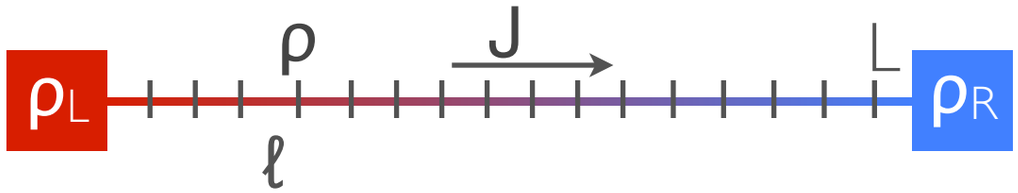

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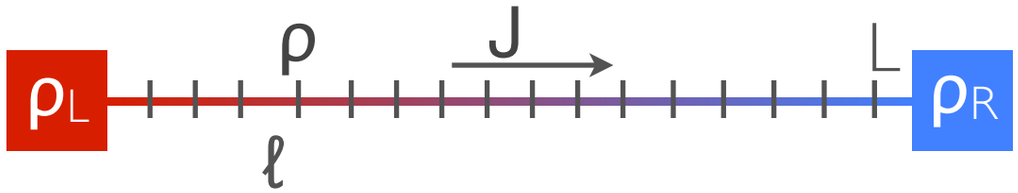

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$$\left.\begin{matrix}\rho_J(x)\\ j_J(x)\end{matrix}\right\}\xrightarrow{\partial_t\rho_J+\partial_x j_J=0} j_J(x)=J \qquad \Rightarrow G(J) = -\min_{\rho(x)}\int_0^1 dx\,\frac{[J+D(\rho)\rho'(x)]^2}{2\sigma(\rho)}$$

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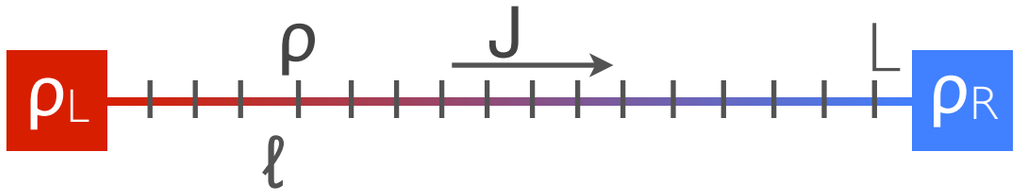

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- **Physical picture**: after a short (microscopic) transient, the system settles into a time-independent state with structured density field (typically different from the stationary one) such that the empirical, space- and time-averaged current equals **J**

TESTING THE ADDITIVITY PRINCIPLE IN 1D

P.I. Hurtado & P.L. Garrido, PRL **102**, 250601 (2009)

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$$\rho'_i = p(\rho_i + \rho_{i+1}) \qquad \rho'_{i+1} = (1-p)(\rho_i + \rho_{i+1})$$

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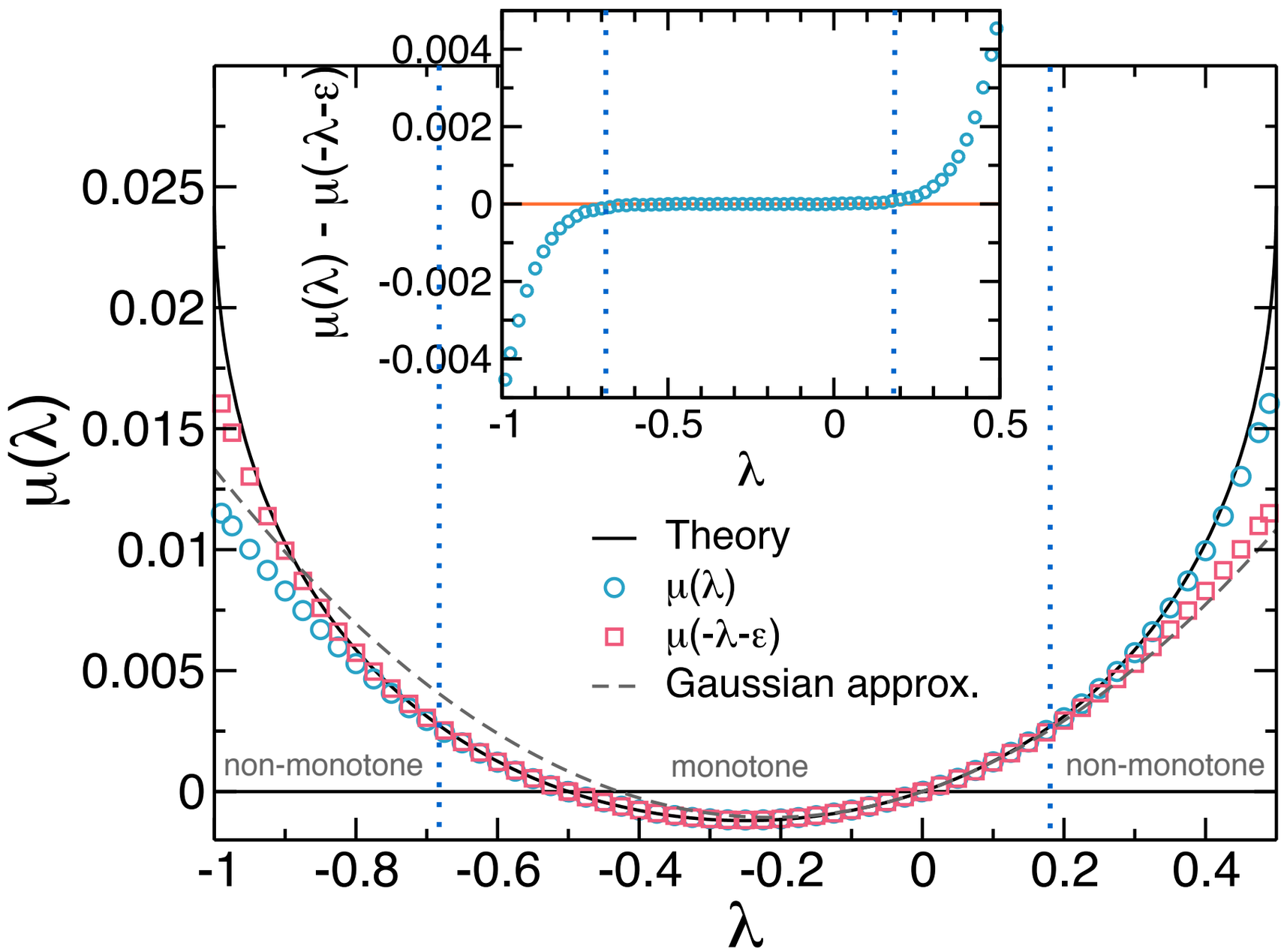

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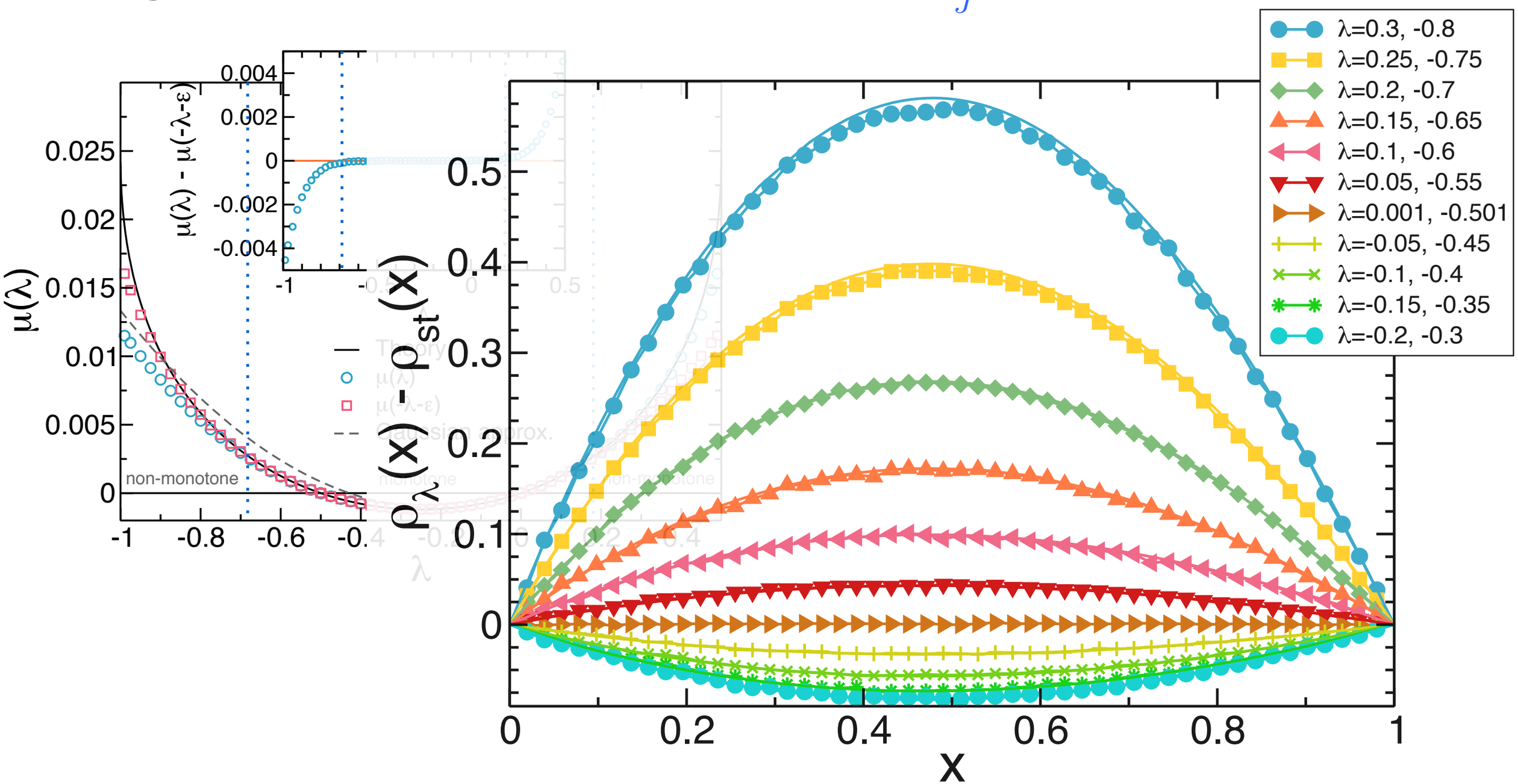

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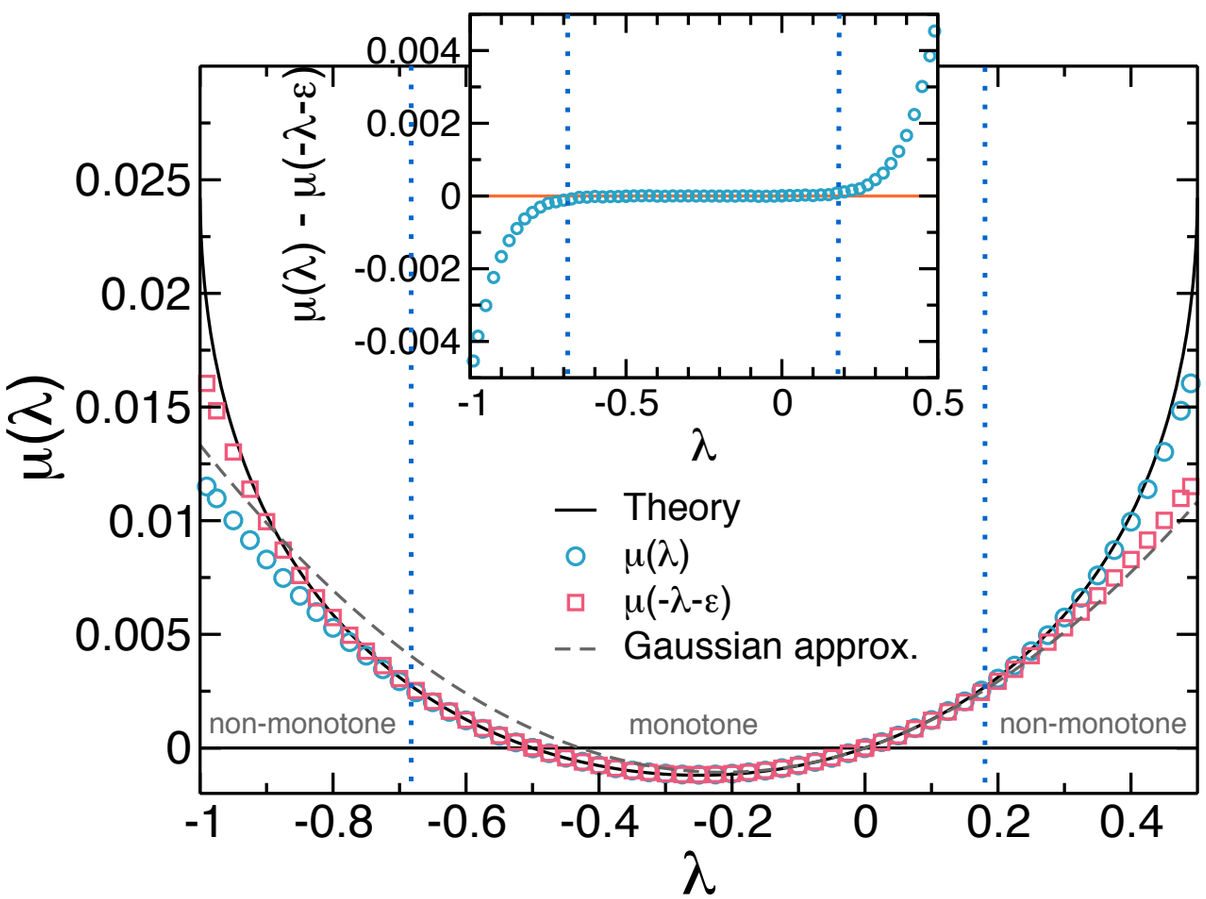

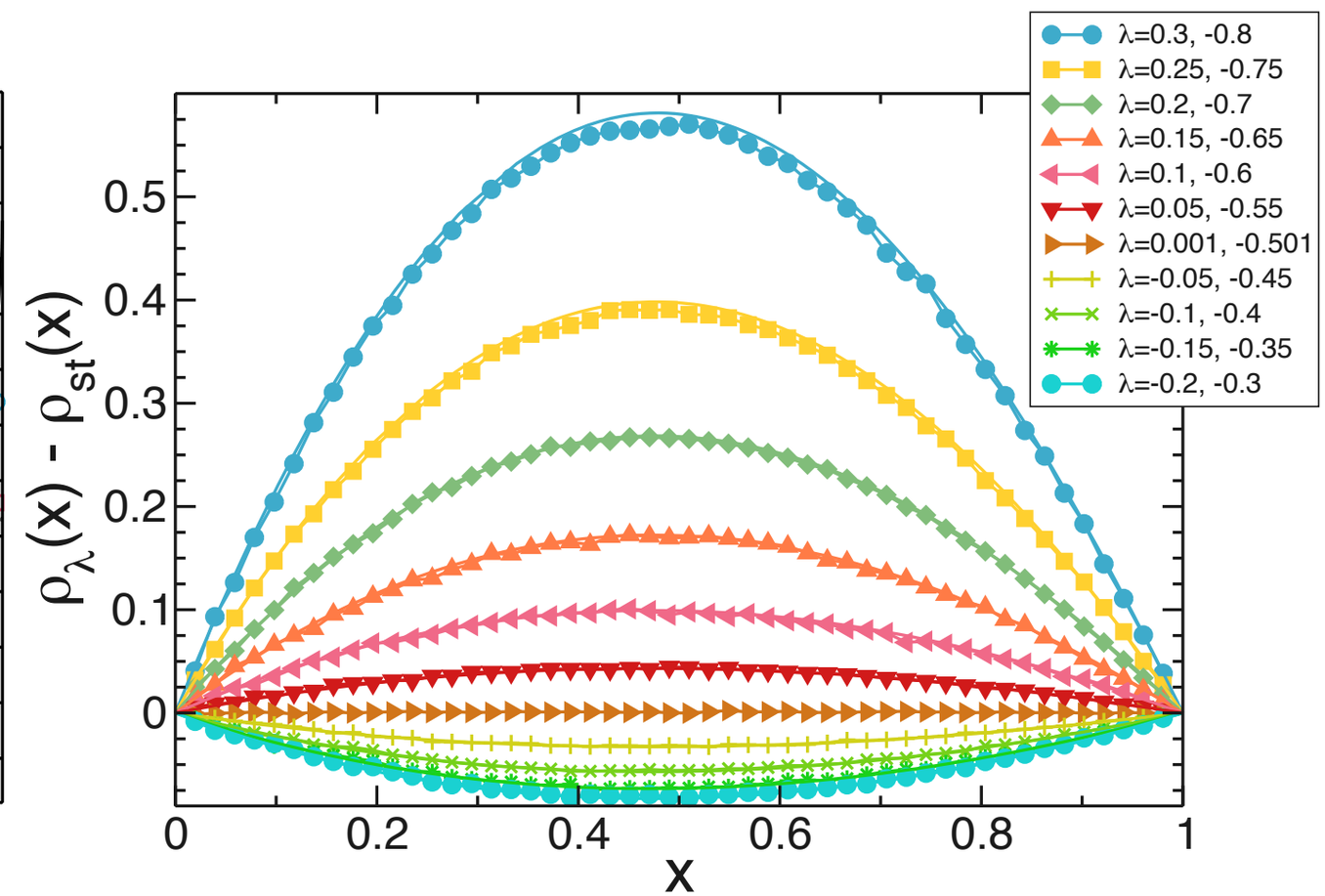

- No violation of additivity principle has been reported to date in open 1D nonequilibrium diffusive systems.

DYNAMIC PHASE TRANSITIONS IN FLUCTUATIONS

- **MFT + Additivity Principle** = powerful tool to compute 1D current LDFs

- However, **MFT allows for dynamic solutions in general**:
  - What is their meaning? $G(J) = -\lim_{\tau\to\infty}\frac{1}{\tau}\min_{\{\rho,\mathbf{j}\}_0^\tau}\left\{\int_0^\tau dt\int_0^1 dx\,\frac{[j(x,t)+D(\rho)\partial_x\rho(x,t)-\sigma(\rho)E]^2}{2\sigma(\rho)}\right\}$
  - Do they appear? Can we observe them?

$$\boxed{\rho_J(x,t) \quad ; \quad j_J(x,t)}$$

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  - Do they appear? Can we observe them? $\boxed{\rho_J(x,t)\quad;\quad j_J(x,t)}$

- **YES!!** Additivity scenario eventually breaks down for large fluctuations via a **dynamic phase transition at the fluctuating level involving a symmetry breaking**

- Optimal path is a **localized traveling wave**. **Observed only for periodic systems!**

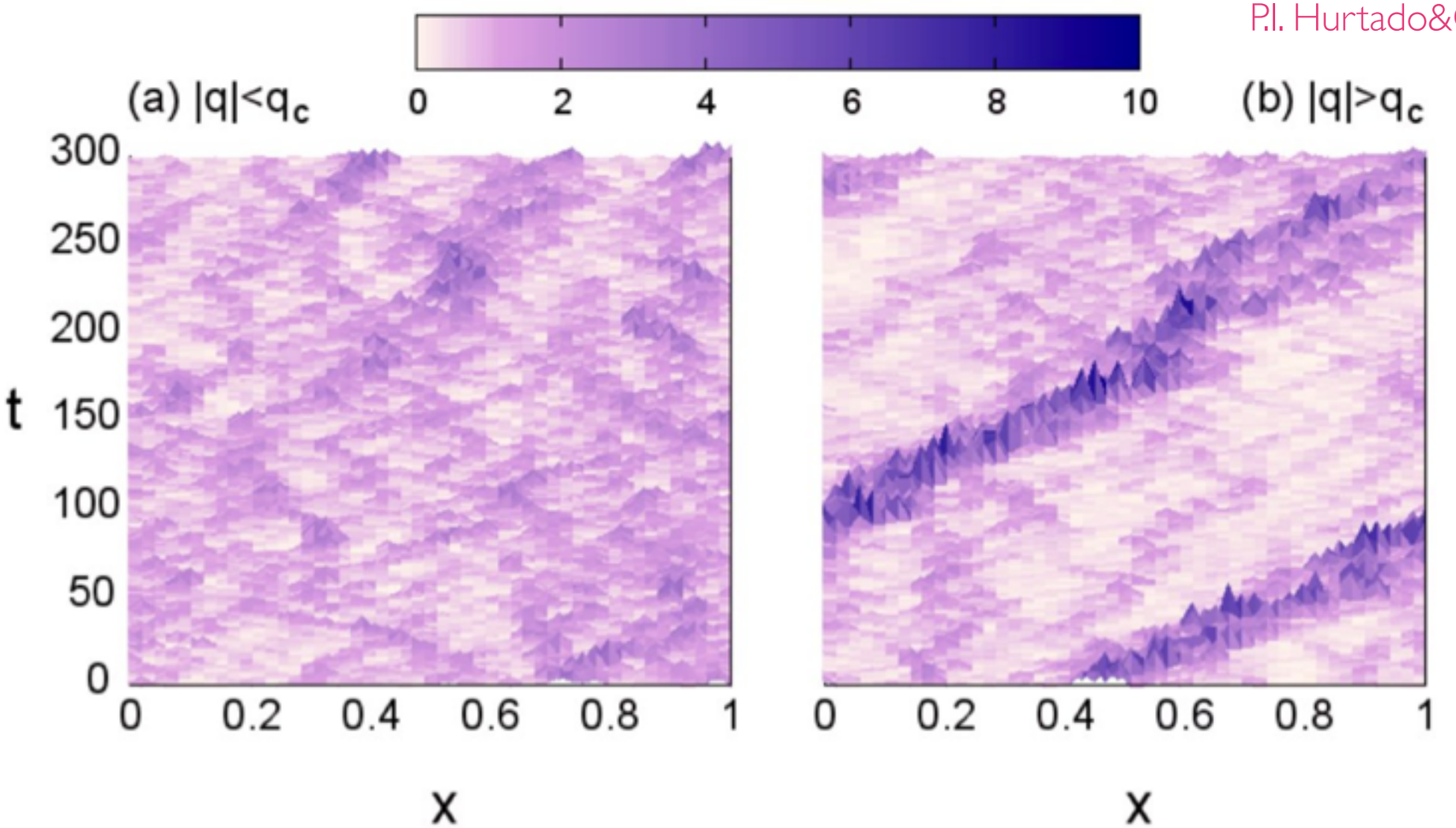
$$\rho_J(x,t)=\omega_J(x-vt)\quad\xrightarrow[\int_0^1\rho_J(x)dx=\rho_0]{\partial_t\rho_J+\partial_x j_J=0}\quad j_J(x,t)=J-v\rho_0+v\omega_J(x-vt)$$

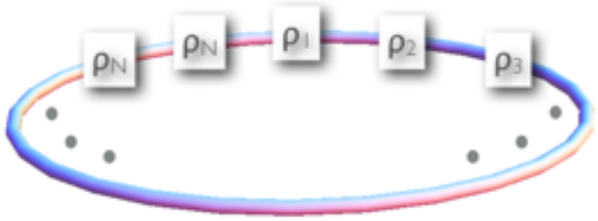
- **Lesson:** rare events are generically associated with **coherent, self-organized patterns** which enhance their probability

Bodineau & Derrida, PRE **72**, 066110 (2005)

SPONTANEOUS SYMMETRY BREAKING IN FLUCTUATIONS

P.I. Hurtado&Garrido, PRL **107**, 180601 (2011)





$$(\rho_i, \rho_{i+1}) \to (\rho'_i, \rho'_{i+1})$$

$$\rho'_i = p(\rho_i + \rho_{i+1})$$

$$\rho'_{i+1} = (1-p)(\rho_i + \rho_{i+1})$$

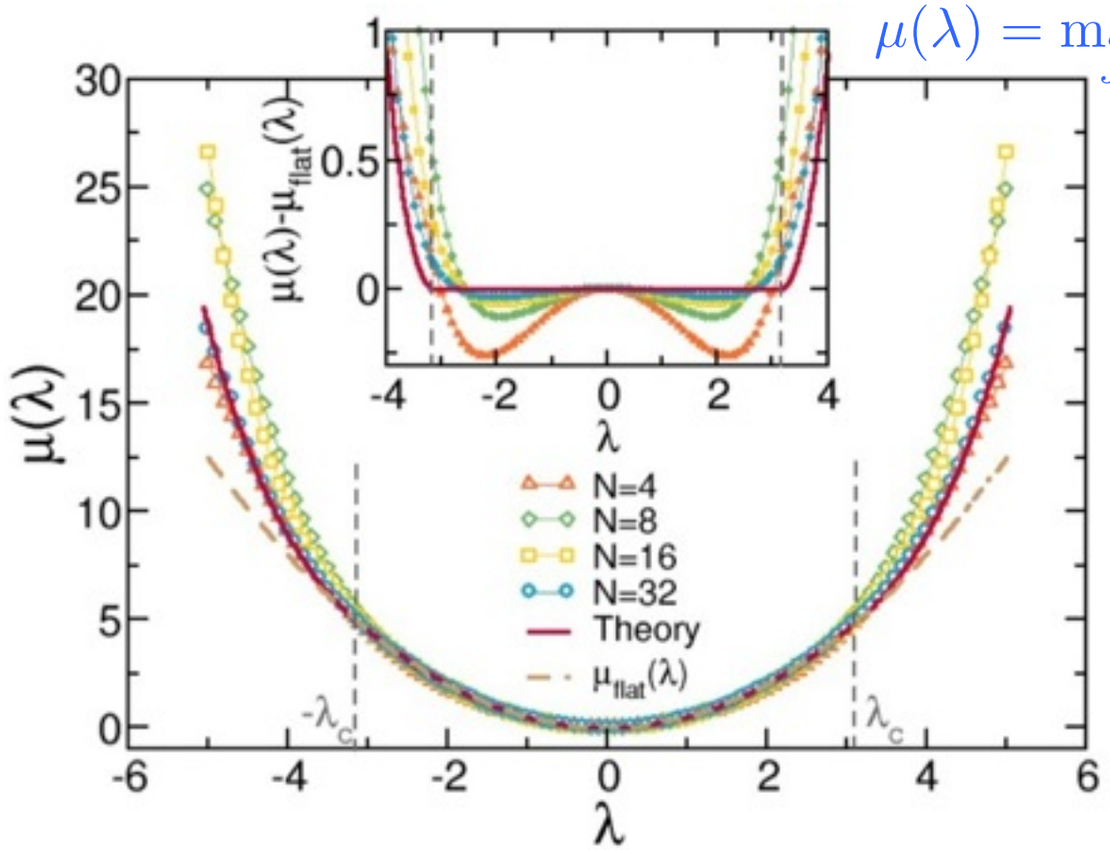
$$|J_c| = 2\pi D(\rho_0)\sqrt{\frac{2\sigma(\rho_0)}{\sigma''(\rho_0)}}$$

- $|J| < J_c$: sum of weakly-correlated events ⟶ Gaussian statistics
- $|J| > J_c$: **coherent traveling wave** + energy localization ⟶ **non-Gaussian statistics**
- Striking phenomenon: **Isolated equilibrium system with no external fields**
- **Spontaneous symmetry breaking in 1d:** translation invariance
- Symmetry-breaking instabilities forbidden in equilibrium may happen in fluctuations

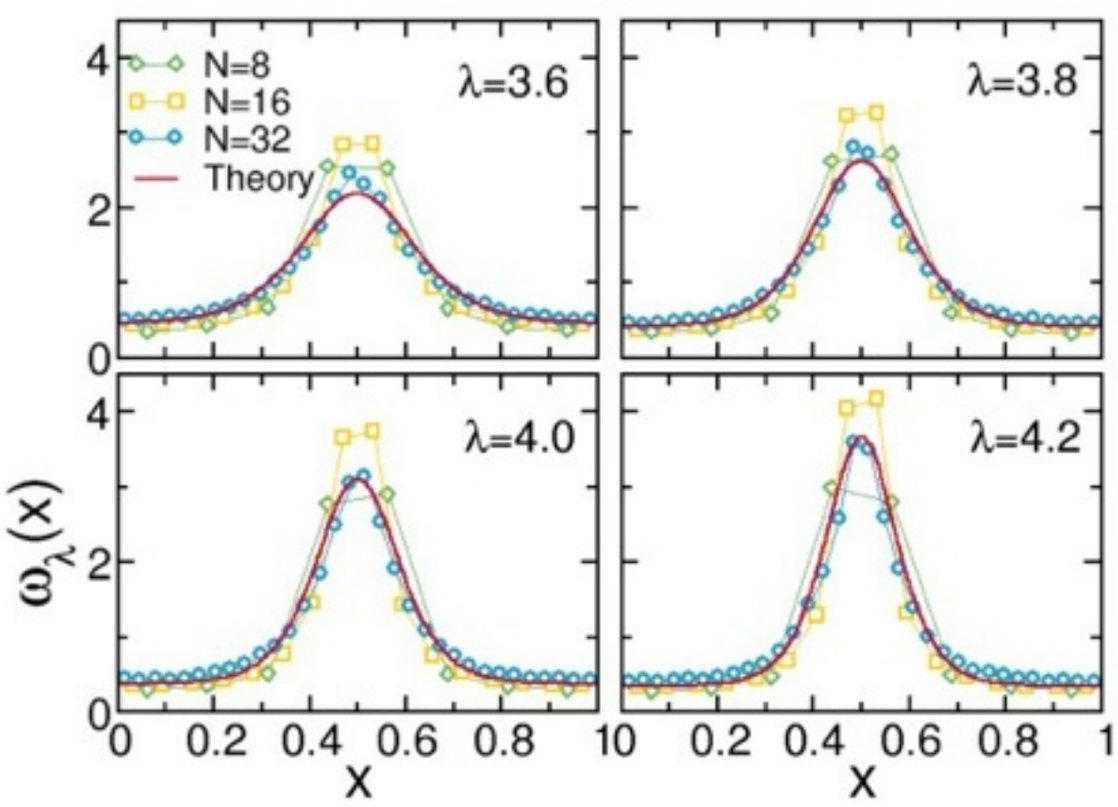
SPONTANEOUS SYMMETRY BREAKING IN FLUCTUATIONS

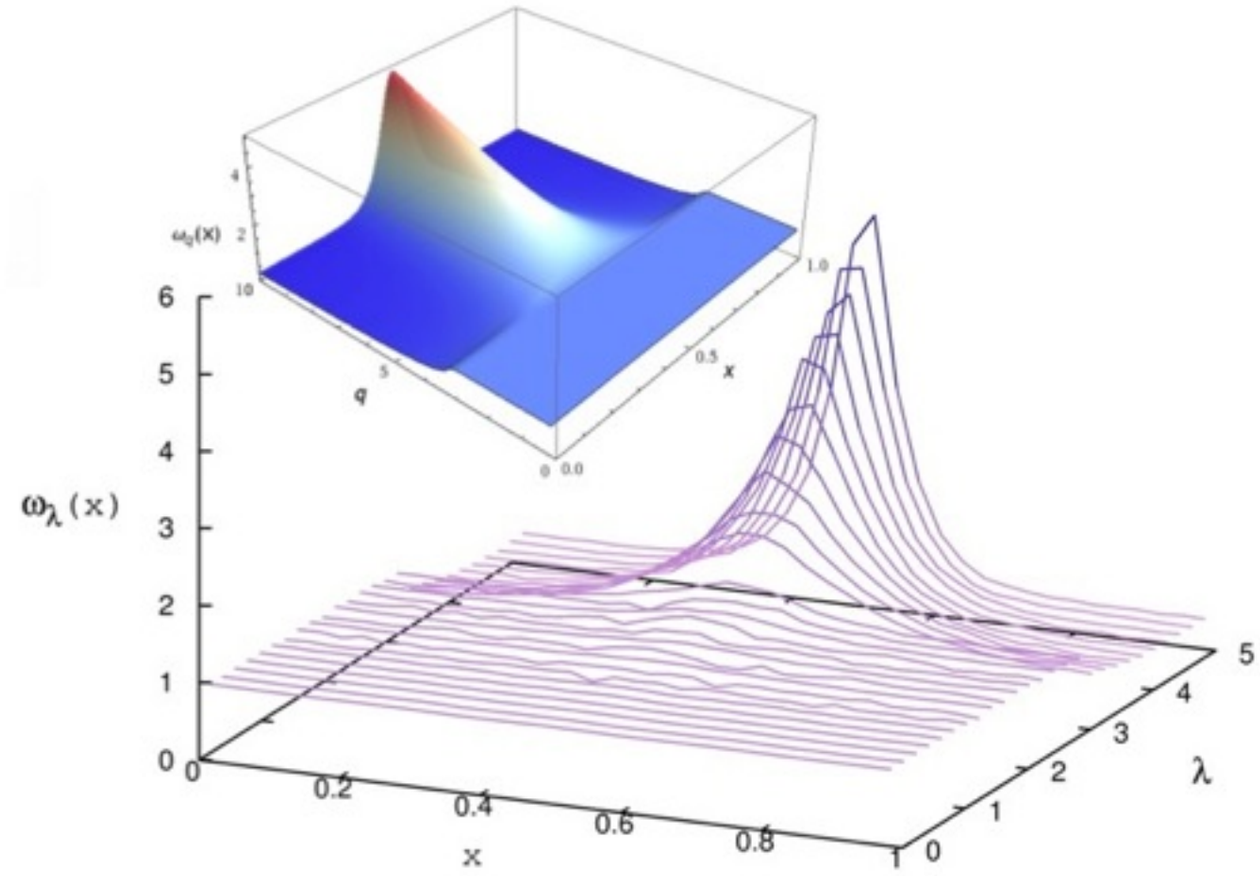
P.I. Hurtado&Garrido, PRL **107**, 180601 (2011)

$$\mu(\lambda) = \max_J [G(J) + \lambda J]$$



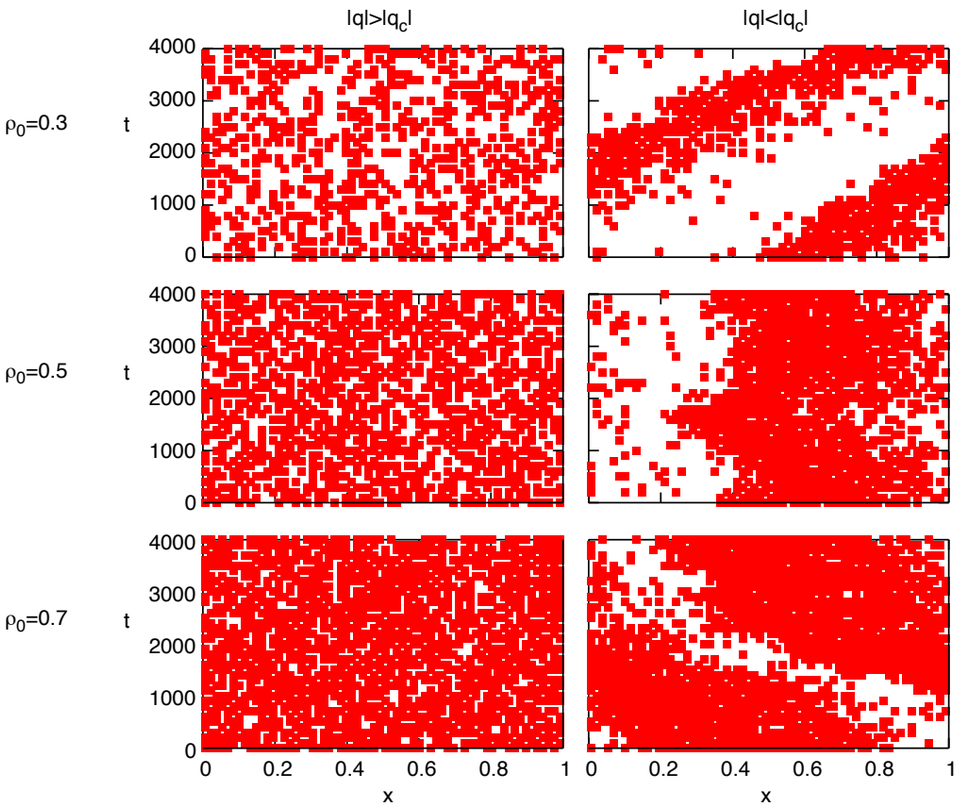
- **Excellent comparison of data with MFT predictions as N↑**
- **|J| > J_c = π**: non-quadratic G(q) and **μ(λ)** → Non-Gaussian statistics
- Clear signature of phase transition in configurations (**λ>$λ_c$= π**): **energy localization + traveling wave**

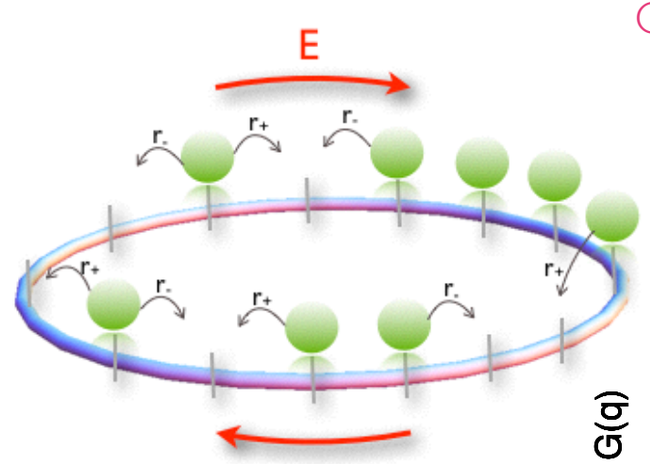


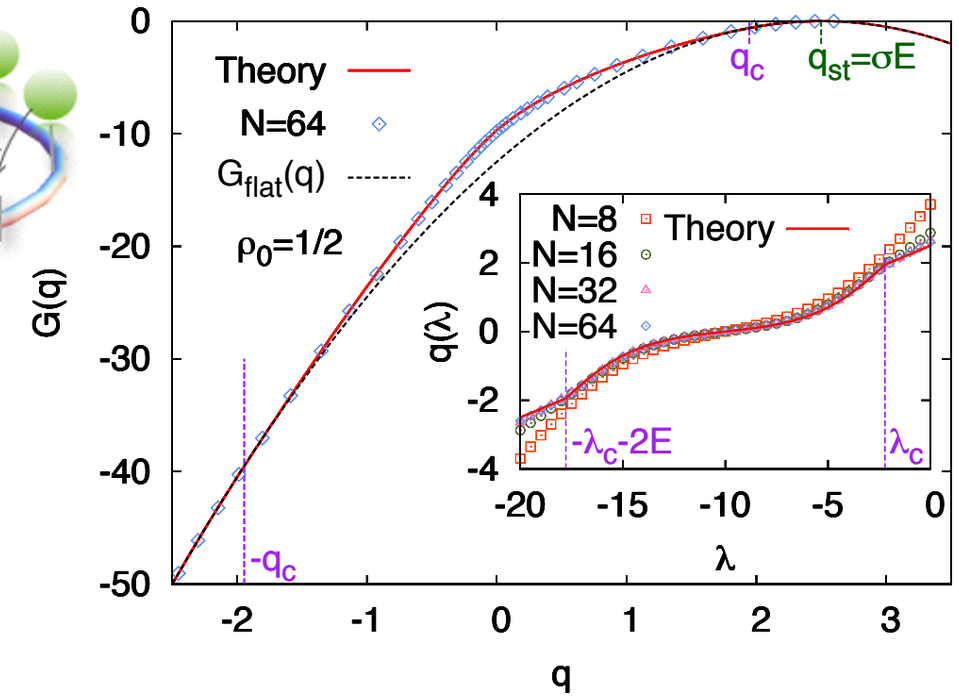


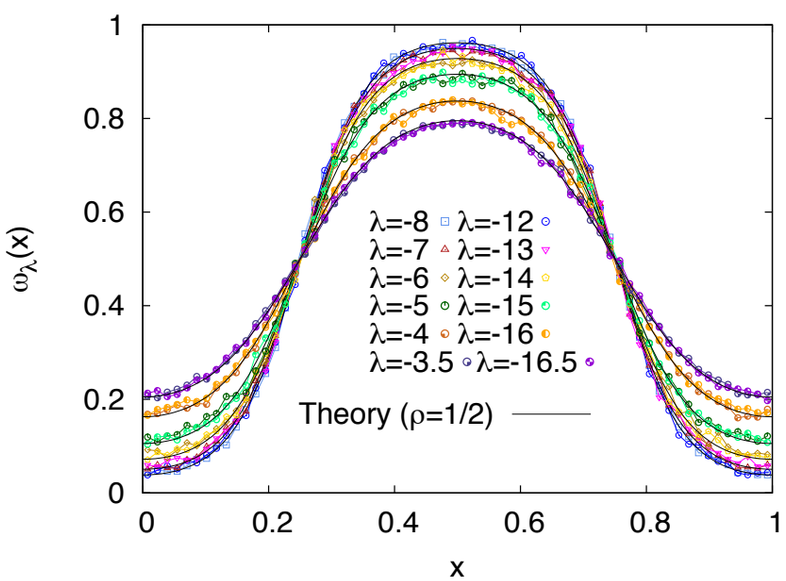
WASEP: SSB IN FLUCTUATIONS, BUT DIFFERENT…

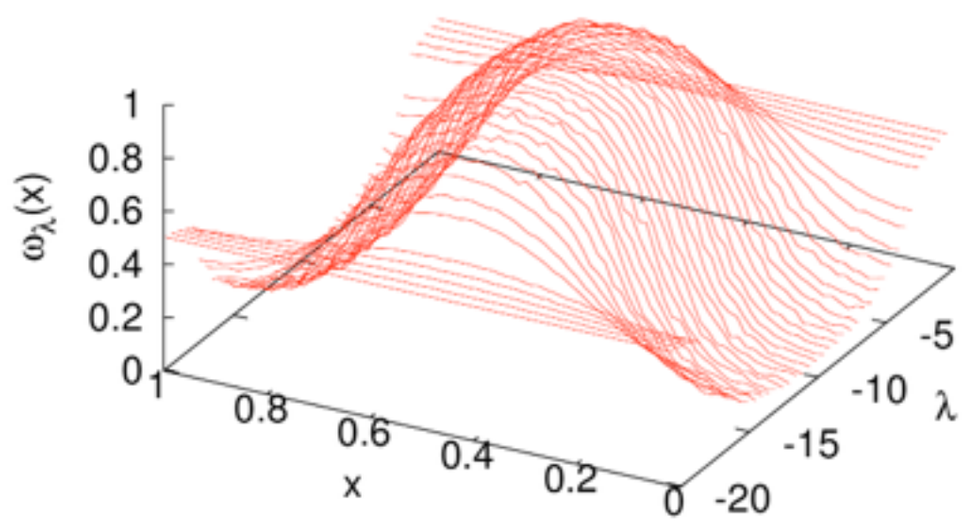
C.P. E., Garrido & Hurtado, PRE **87**, 032115 (2013)

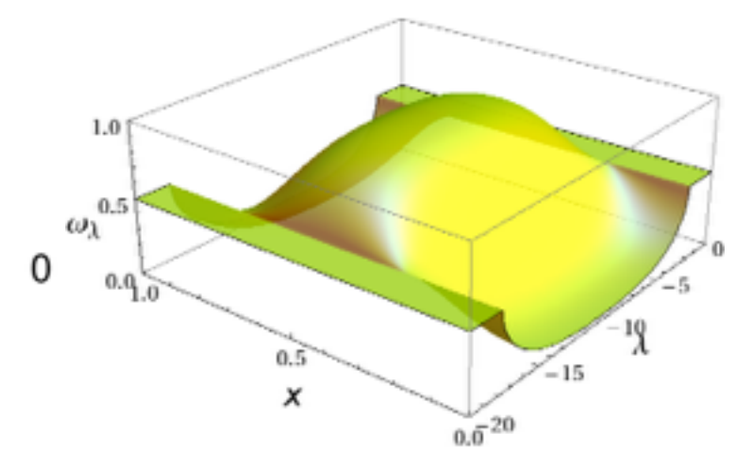






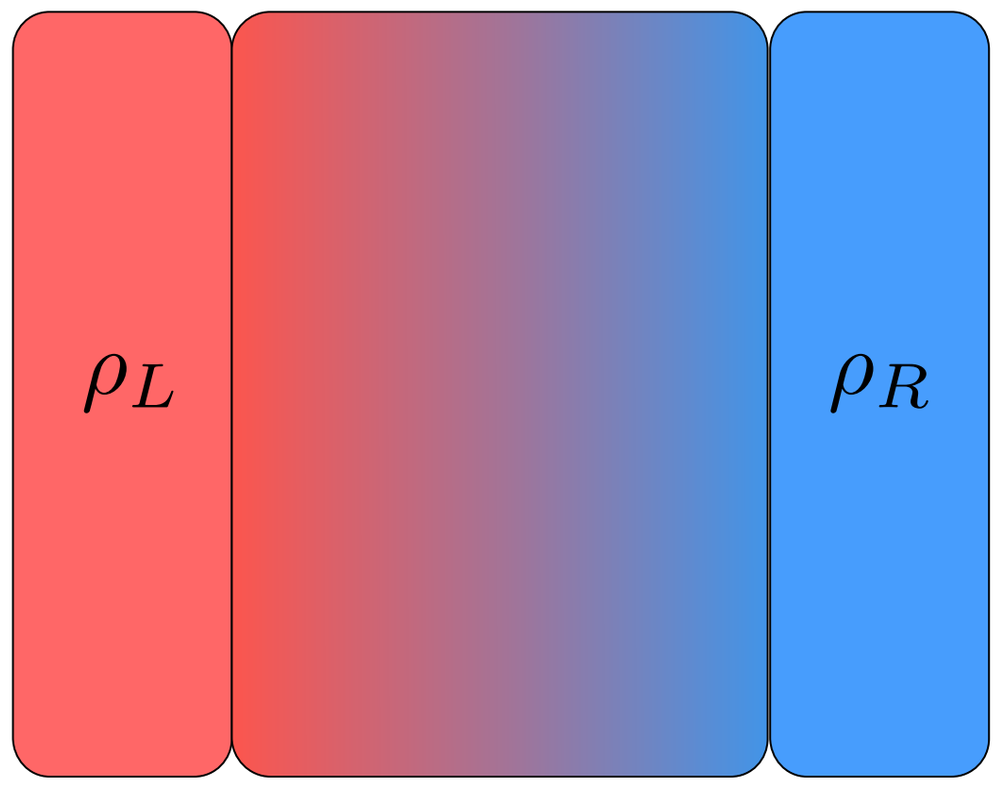




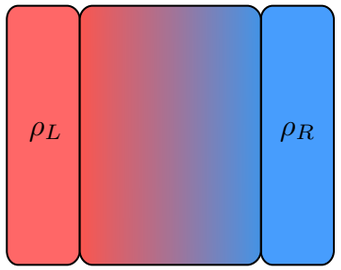


- Main differences with KMP: **critical field |E$_c$|** $\sigma''_{WASEP} < 0 \rightarrow |E_c| = \dfrac{\pi}{\sqrt{\rho_0(1-\rho_0)}}$
- Emergence of a **macroscopic jammed state which hinders transport** of particles to facilitate current fluctuations well below the average

D-DIMENSIONS (D>1)



A WEAK ADDITIVITY PRINCIPLE (WAP) IN D>1



- **Empirical current:**

$$\mathbf{J} = \frac{1}{\tau}\int_0^\tau dt \int_\Lambda d\mathbf{r}\ \mathbf{j}(\mathbf{r},t) \equiv (J_\parallel, \mathbf{J}_\perp)$$

- Probability of a current fluctuation: $\mathrm{P}_\tau(\mathbf{J}) \sim \mathrm{e}^{+\tau L^d G(\mathbf{J})}$

Geometry:

- ☑ **Gradient** along x-direction
- ☑ **Periodic** along all other, (d-1) directions

(no external field **E** for simplicity)

$$G(\mathbf{J}) = -\lim_{\tau\to\infty}\frac{1}{2\tau}\min_{\{\rho,\mathbf{j}\}_0^\tau}\left\{\int_0^\tau dt\int_\Lambda d\mathbf{r}\ \left(\mathbf{j}+\hat{D}(\rho)\boldsymbol{\nabla}\rho\right)\cdot\hat{\Sigma}(\rho)\left(\mathbf{j}+\hat{D}(\rho)\boldsymbol{\nabla}\rho\right)\right\}$$

C.P. E., Garrido & Hurtado, preprint (2015)

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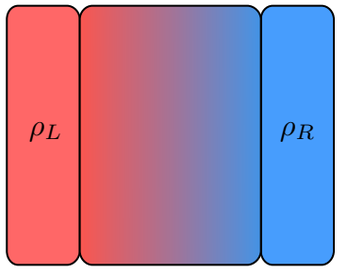

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- **Additivity**: assume dominant paths to be time-independent

$$\left.\begin{matrix}\rho(\mathbf{r})\\ \mathbf{j}(\mathbf{r})\end{matrix}\right\}\xrightarrow{\partial_t\rho+\boldsymbol{\nabla}\cdot\mathbf{j}=0}\boxed{\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r})=0}$$

- **The relevant current fields are divergence-free but possibly structured**

C.P. E., Garrido & Hurtado, preprint (2015)

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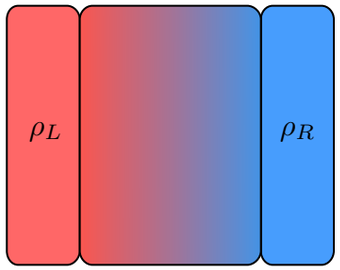

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- **The relevant current fields are divergence-free but possibly structured**

- **Periodicity** suggests relevant fields exhibit **structure only along gradient, x-direction**

$$\left.\begin{matrix}\rho(x)\\ \mathbf{j}(x)\end{matrix}\right\}\xrightarrow[\mathbf{J}\equiv(J_\parallel,\mathbf{J}_\perp)]{\boldsymbol{\nabla}\cdot\mathbf{j}(x)=0}\mathbf{j}(x)=\left(J_\parallel,\mathbf{j}_\perp(x)\right)\qquad\text{with}\quad\mathbf{J}_\perp=\int_0^1 dx\,\mathbf{j}_\perp(x)$$

C.P. E., Garrido & Hurtado, preprint (2015)

A WEAK ADDITIVITY PRINCIPLE (WAP) IN D>1

- **Current LDF under wAP**: $G_{\mathrm{w}}(\mathbf{J}) = -\min_{\substack{\rho(x)\\ \mathbf{j}_\perp(\mathbf{x})}} \int_0^1 dx\, \mathcal{L}_{\mathrm{w}}(\rho, \mathbf{j}_\perp; \mathbf{J})$

$$\mathcal{L}_{\mathrm{w}}(\rho, \mathbf{j}_\perp; \mathbf{J}) = \frac{[J_{\|} + D_1(\rho)\rho'(x)]^2}{2\sigma_1(\rho)} + \sum_{\alpha=2}^{d} \frac{j_\perp^{(\alpha)}(x)^2}{2\sigma_\alpha(\rho)}$$

... + **constraints**:

- ☑ Boundary conditions
- ☑ **Empirical ⊥ current**:

$$\mathbf{J}_\perp = \int_0^1 dx\, \mathbf{j}_\perp(\mathbf{x})$$

C.P. E., Garrido & Hurtado, preprint (2015)

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... + constraints:

- ☑ Boundary conditions
- ☑ Empirical ⊥ current:

$$\mathbf{J}_\perp = \int_0^1 dx\, \mathbf{j}_\perp(\mathbf{x})$$

- Introduce (d-1) Lagrange multipliers

$$\mathcal{L}_{\rm w}^{(\boldsymbol{\lambda}_\perp)}(\rho, \mathbf{j}_\perp; \mathbf{J}) \equiv \mathcal{L}_{\rm w}(\rho, \mathbf{j}_\perp; \mathbf{J}) - \boldsymbol{\lambda}_\perp \cdot \mathbf{j}_\perp(\mathbf{x})$$

- Differential equation for the optimal density profile $\rho_{\mathbf{J}}(x)$

$$D_1(\rho)^2 \rho'(x)^2 = {J_\parallel}^2 + \sigma_1(\rho)\left[2K - \sum_{\alpha=2}^{d} {\lambda_\perp^{(\alpha)}}^2 \sigma_\alpha(\rho)\right]$$

- Optimal current field and Lagrange multipliers: $\mathbf{j}_{\mathbf{J}}(x) = \left(J_\parallel, \mathbf{j}_{\perp,\mathbf{J}}(x)\right)$

$$\boxed{j_{\perp,\mathbf{J}}^{(\alpha)}(x) = \lambda_\perp^{(\alpha)} \sigma_\alpha(\rho_{\mathbf{J}})} \xrightarrow[\alpha \in [2,d]]{} \lambda_\perp^{(\alpha)} = J_\perp^{(\alpha)} \Big/ \int_0^1 dx\, \sigma_\alpha(\rho_{\mathbf{J}})$$

- $j_J(x)$ structured along gradient direction in all orthogonal components, and locally coupled to $\rho_J(x)$ via the mobility $\sigma(\rho)$

Villavicencio-Sánchez & Harris, arXiv:1508.07945 (2015)

C.P. E., Garrido & Hurtado, preprint (2015)

WEAK VS STRONG ADDITIVITY

- **Strong Additivity Principle (sAP)**: straightforward extension of the 1d-AP to high-d

$$G_{\rm s}(\mathbf{J}) = -\min_{\rho(x)} \int_0^1 dx\, \mathcal{L}_{\rm s}(\rho;\mathbf{J}) = -\int_0^1 dx\, \mathcal{L}_{\rm s}(\rho_{\mathbf{J}}^{(\rm s)};\mathbf{J})$$

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- Which conjecture (**weak AP vs strong AP**) yields a **better maximizer of the current MFT action?**

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In general
$\rho_{\mathbf{J}}^{(\rm s)}(x) \neq \rho_{\mathbf{J}}^{(\rm w)}(x)$

C.P. E., Garrido & Hurtado, preprint (2015)

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In general
$\rho_{\mathbf{J}}^{(\rm s)}(x) \neq \rho_{\mathbf{J}}^{(\rm w)}(x)$

- **Intuition** suggests that the wAP should offer a better solution as it includes **additional degrees of freedom** that the system at hand can *put at work* to improve its large deviation function

C.P. E., Garrido & Hurtado, preprint (2015)

WEAK VS STRONG ADDITIVITY

- Define **functional** $\mathcal{F}_\ell(\psi;\mathbf{J}) \equiv -\int_0^1 dx \mathcal{L}_\ell(\psi;\mathbf{J})$, with $\ell = \mathrm{s}, \mathrm{w}$ such that

$$G_\mathrm{s}(\mathbf{J}) = \mathcal{F}_\mathrm{s}(\rho_\mathbf{J}^{(\mathrm{s})}) \qquad G_\mathrm{w}(\mathbf{J}) = \mathcal{F}_\mathrm{w}(\rho_\mathbf{J}^{(\mathrm{w})})$$

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$$\mathcal{F}_\mathrm{w}(\rho_\mathbf{J}^{(\mathrm{w})}) \geq \mathcal{F}_\mathrm{w}(\psi;\mathbf{J}) \qquad \forall \psi(x) \neq \rho_\mathbf{J}^{(\mathrm{w})}(x)$$

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- Compare both functionals for same profile, $\Delta_\mathrm{ws} \equiv \mathcal{F}_\mathrm{w}(\rho_\mathbf{J}^{(\mathrm{s})}) - \mathcal{F}_\mathrm{s}(\rho_\mathbf{J}^{(\mathrm{s})})$

$$\Delta_\mathrm{ws} = \sum_{\alpha=2}^{d} \frac{{J_\perp^{(\alpha)}}^2}{2} \left[\int_0^1 dx \, \frac{1}{\sigma_\alpha(\rho_\mathbf{J}^{(\mathrm{s})})} - \frac{1}{\int_0^1 dx \, \sigma_\alpha(\rho_\mathbf{J}^{(\mathrm{s})})} \right] \geq 0$$

C.P. E., Garrido & Hurtado, preprint (2015)

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- Last inequality is a particular instance of reverse Hölder inequality

$$\int_0^1 dx \sigma_\alpha^{-1}(\rho) \geq \left[\int_0^1 dx \sigma_\alpha(\rho) \right]^{-1}$$

- Therefore $\mathcal{F}_\mathrm{w}(\rho_\mathbf{J}^{(\mathrm{w})}) \geq \mathcal{F}_\mathrm{w}(\rho_\mathbf{J}^{(\mathrm{s})}) \geq \mathcal{F}_\mathrm{s}(\rho_\mathbf{J}^{(\mathrm{s})}) \;\Rightarrow\; \boxed{G_\mathrm{w}(\mathbf{J}) \geq G_\mathrm{s}(\mathbf{J})}$

C.P. E., Garrido & Hurtado, preprint (2015)

WEAK VS STRONG ADDITIVITY

- When compared to the strong AP, **the weak AP always yields a better maximizer of the macroscopic fluctuation theory action for currents**

$$G_{\mathrm{w}}(\mathbf{J}) \geq G_{\mathrm{s}}(\mathbf{J})$$

- This result **singles out the weak Additivity Principle as the relevant simplifying hypothesis to study current statistics** in general d-dimensional driven diffusive systems

- Interestingly, both the **sAP and wAP yield the same result only for constant mobility, or for current fluctuations parallel to the gradient direction**:

$$\sigma_\alpha(\rho) = \sigma_\alpha \quad \forall \alpha \qquad\qquad \mathbf{J} = (J_{\|}, \mathbf{J}_\perp = 0)$$

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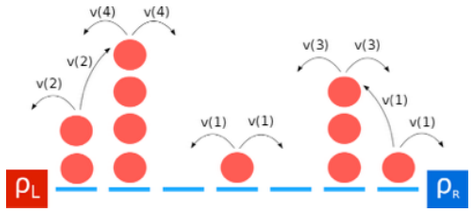
ZRP: WEAK ADDITIVITY VS EXACT RESULTS



C.P. E., Garrido & Hurtado, preprint (2015)

- 2d ZRP with constant jump rates h_α: $D_\alpha(\rho) = \dfrac{h_\alpha}{(1+\rho)^2}$ $\quad \sigma_\alpha(\rho) = 2h_\alpha \dfrac{\rho}{1+\rho}$

Villavicencio-Sánchez & Harris, arXiv:1508.07945 (2015)

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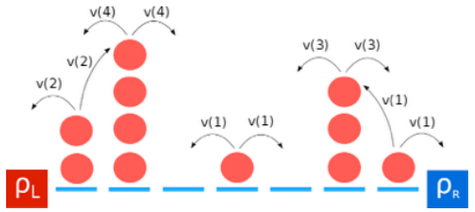

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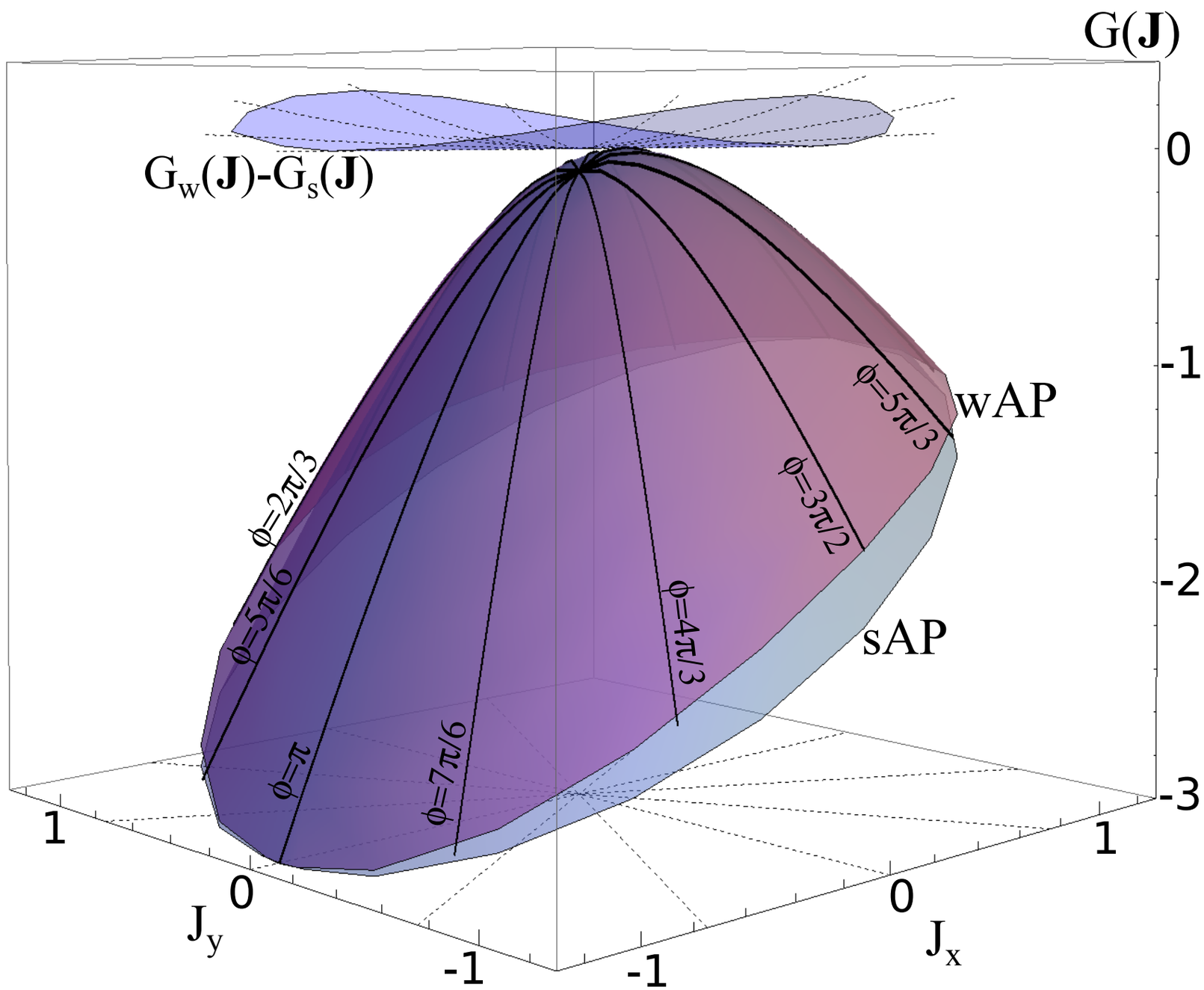

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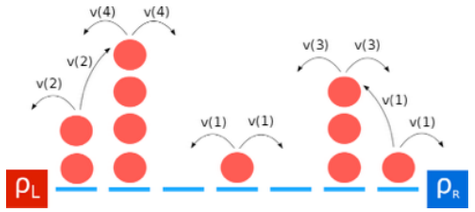

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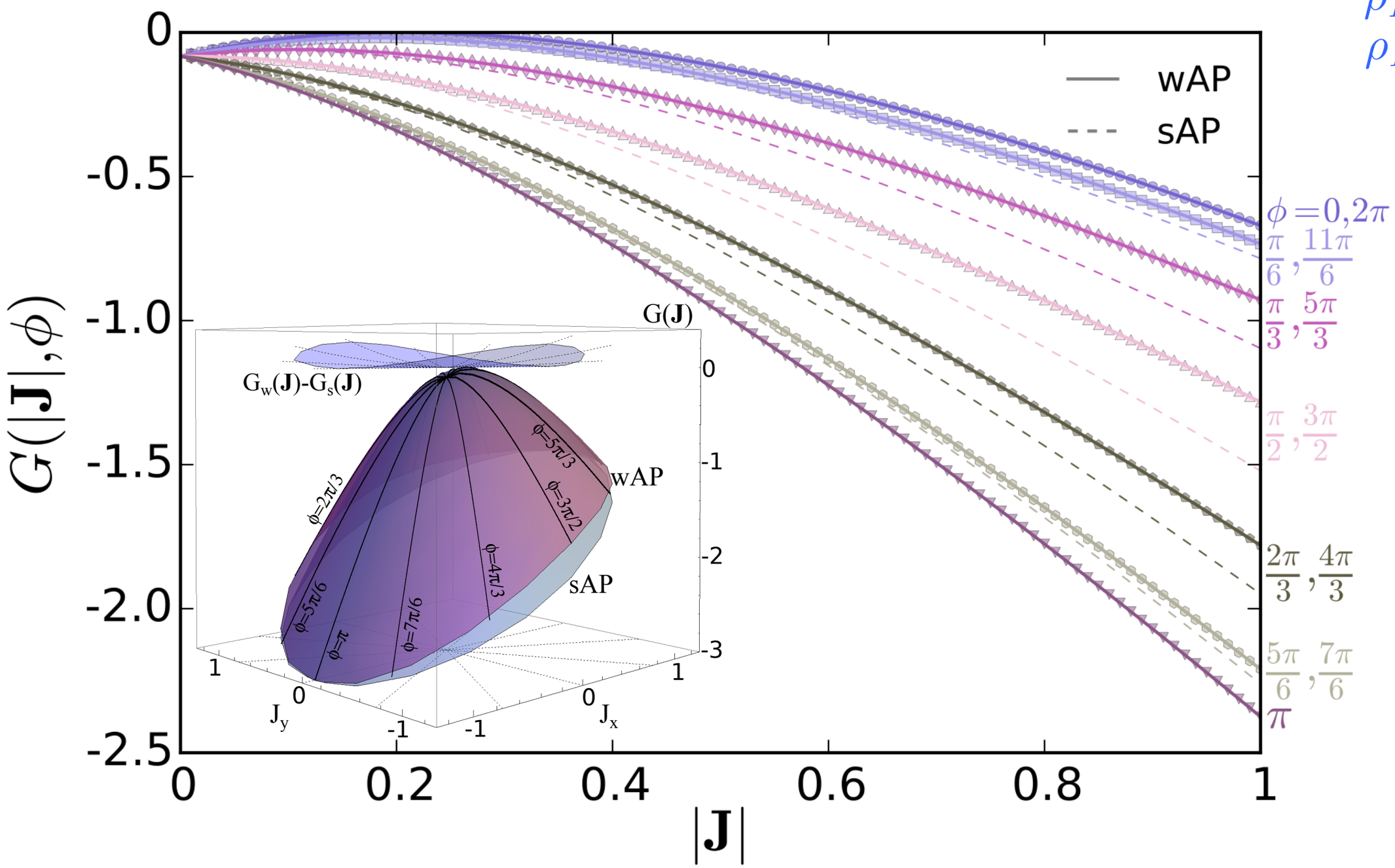

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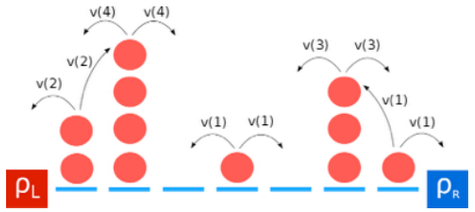

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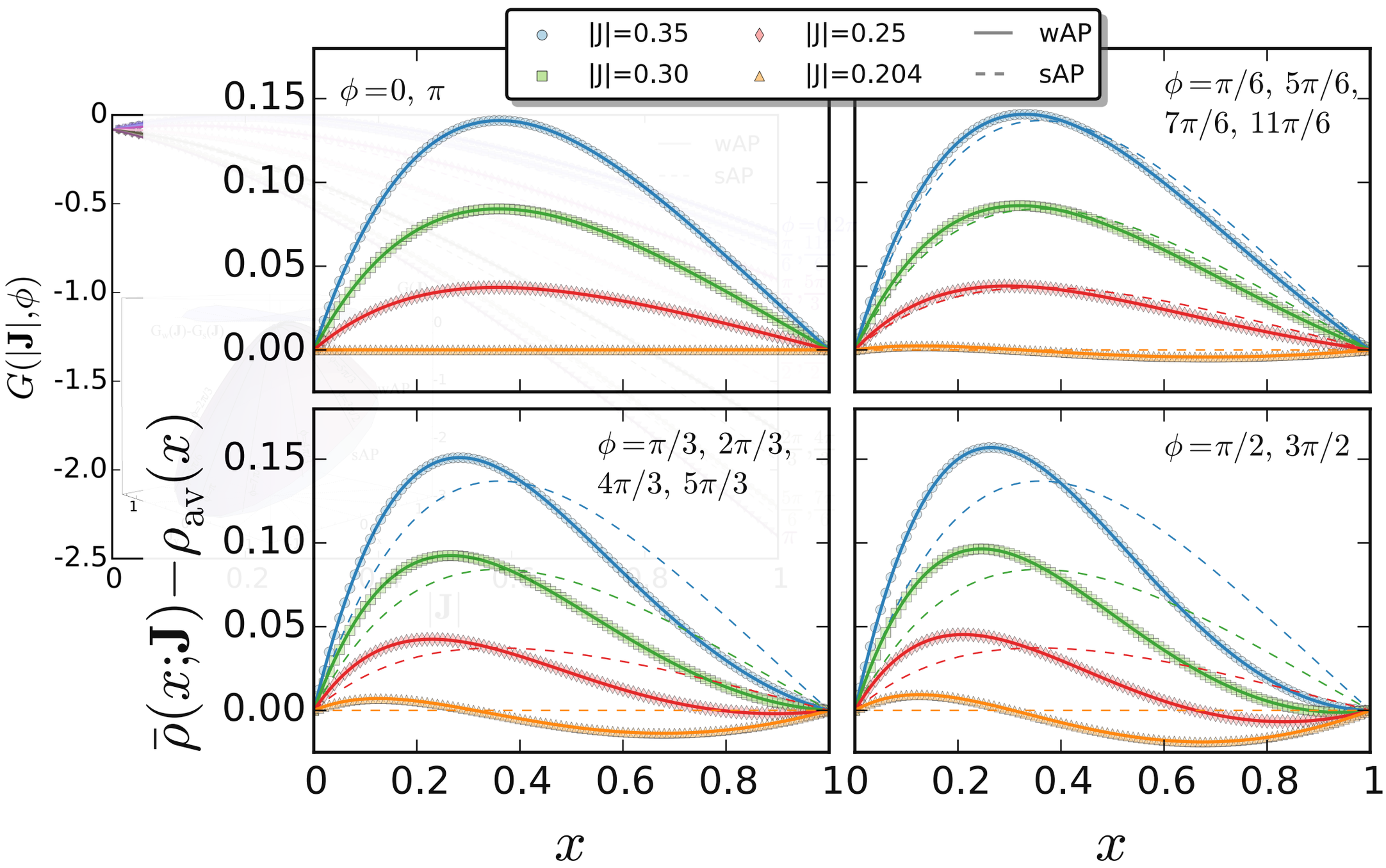

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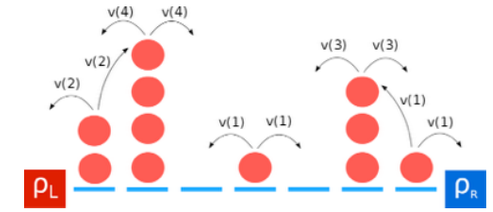

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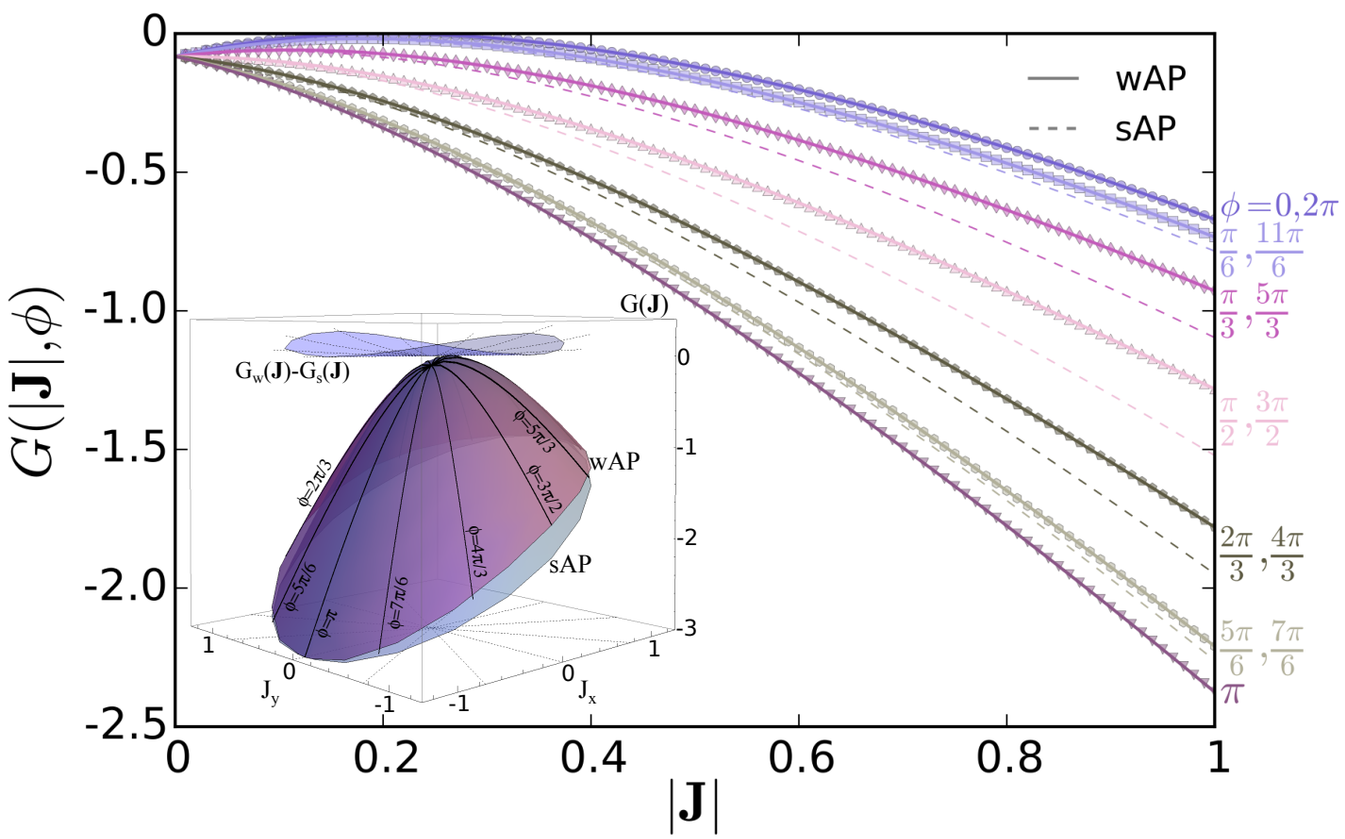
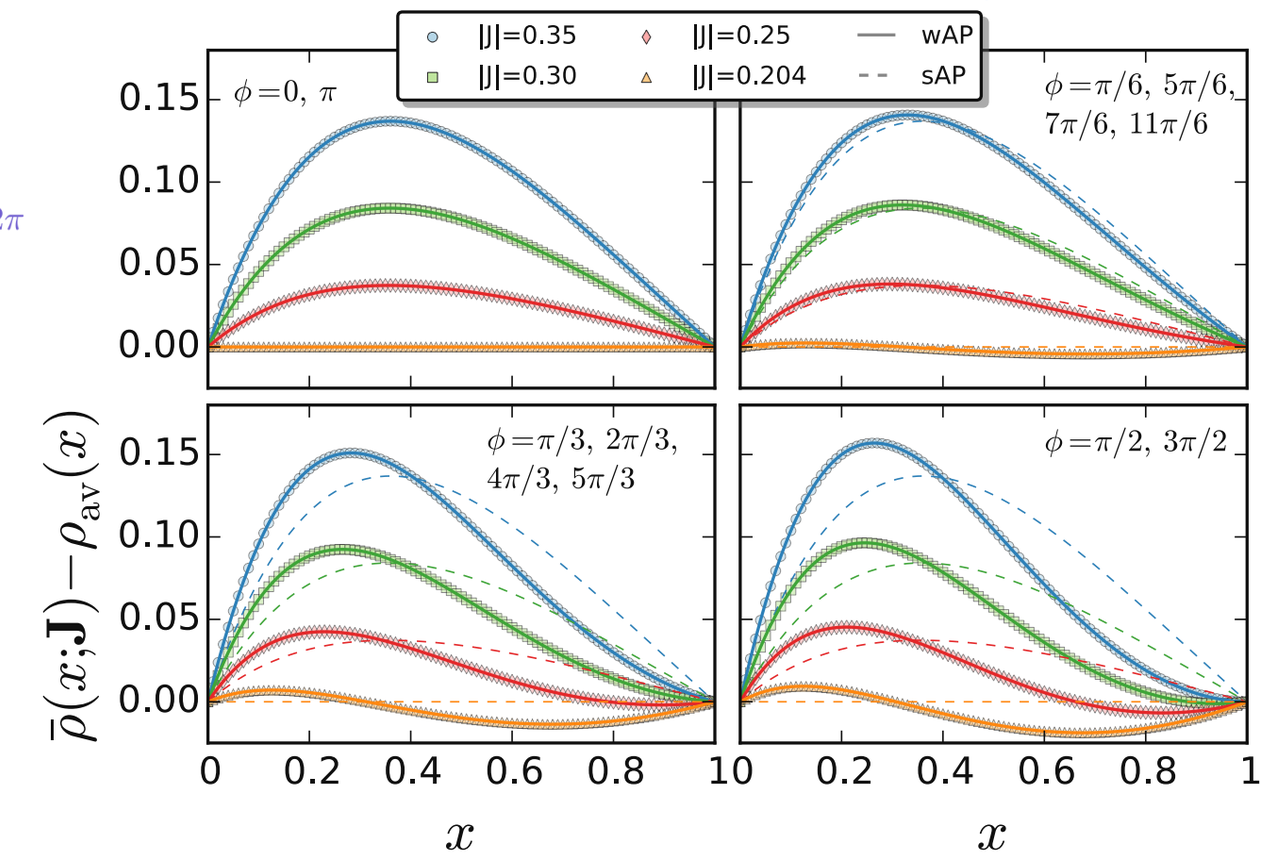
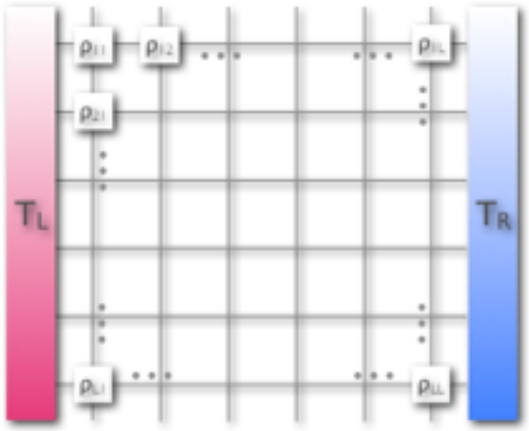




- The **agreement between wAP predictions and exact matrix computations for L=10^5 is excellent**, while **sAP predictions fail outside the gradient direction**, the discrepancy being maximal for orthogonal fluctuations and increasing with **J**

KMP: WEAK ADDITIVITY VS SIMULATIONS

C.P. E., Garrido & Hurtado, preprint (2015)



- More complex 2d-KMP model of heat transport

$$T_L = 2$$
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$$D(\rho) = 1/2 \quad ; \quad \sigma(\rho) = \rho^2$$

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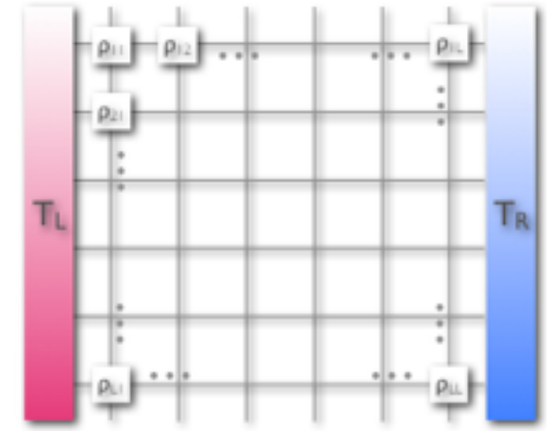

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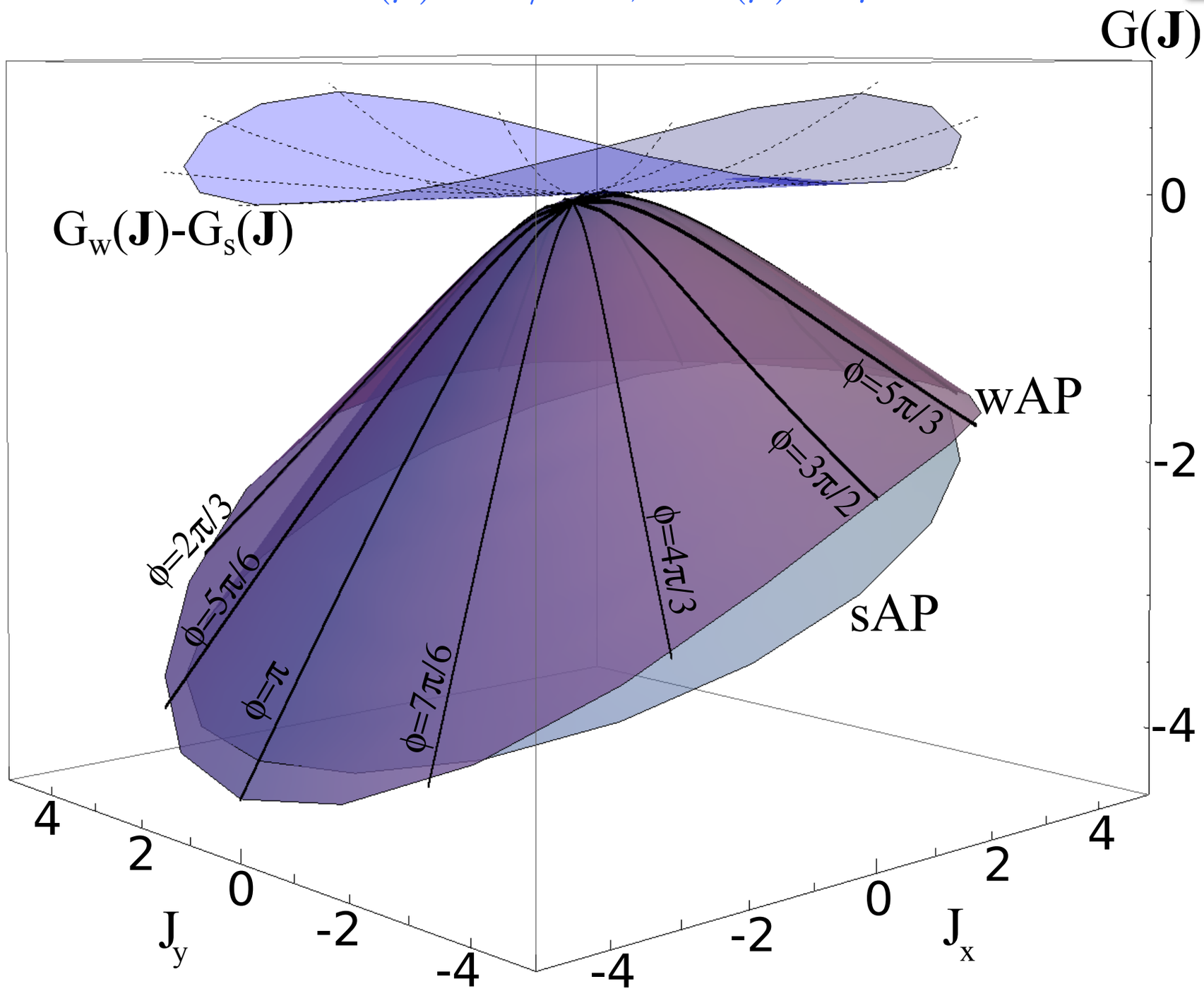

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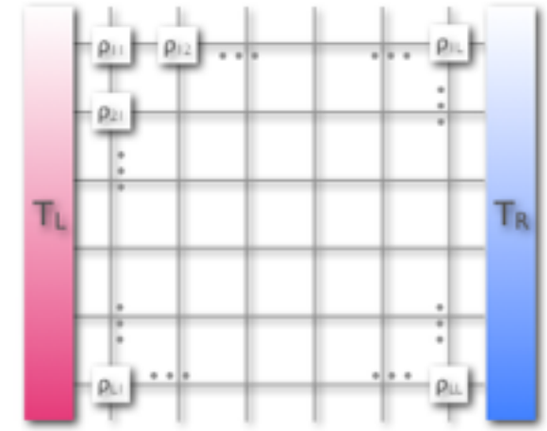

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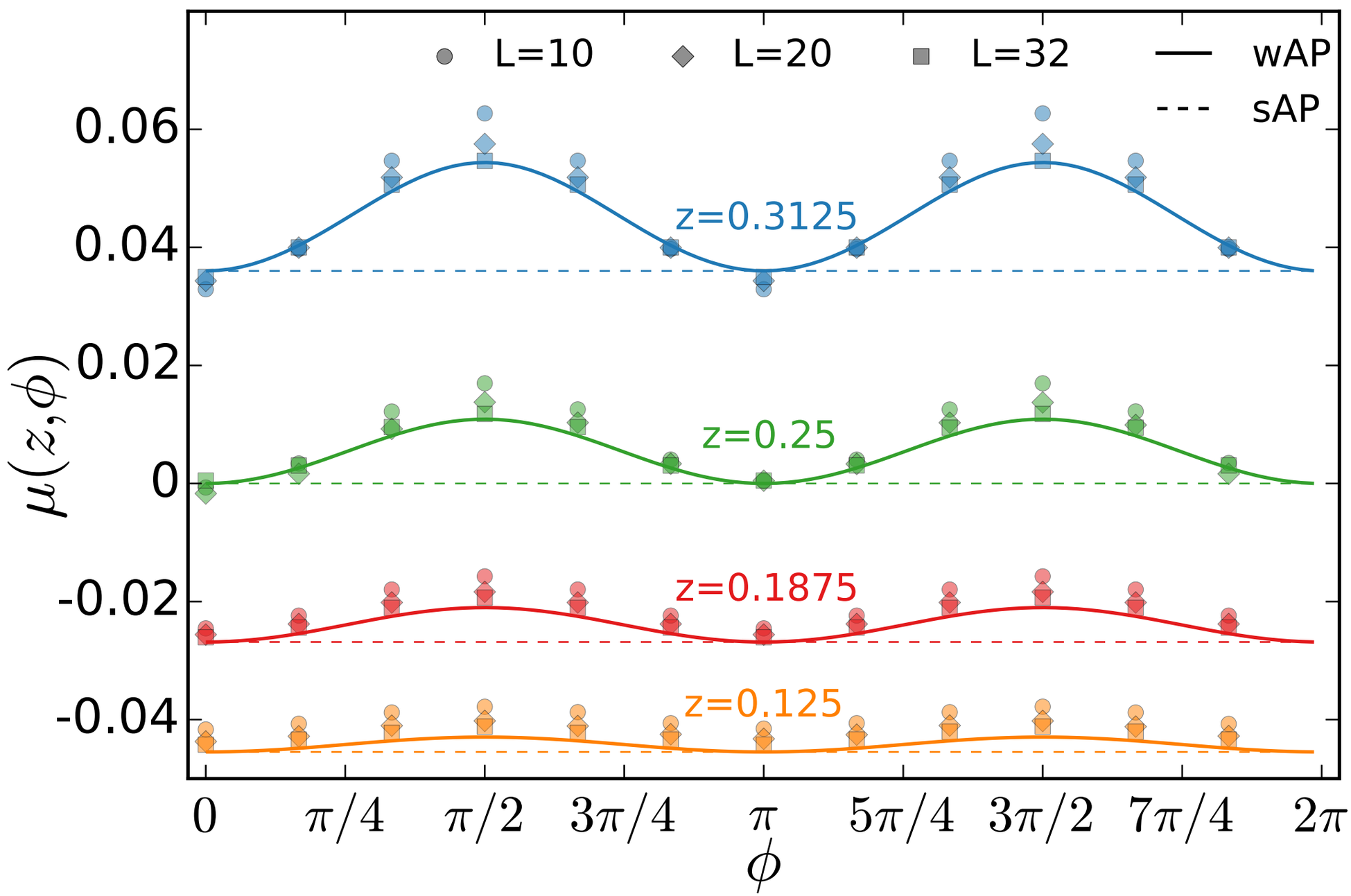

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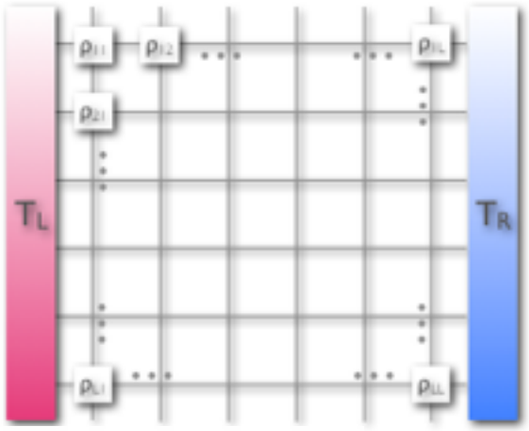

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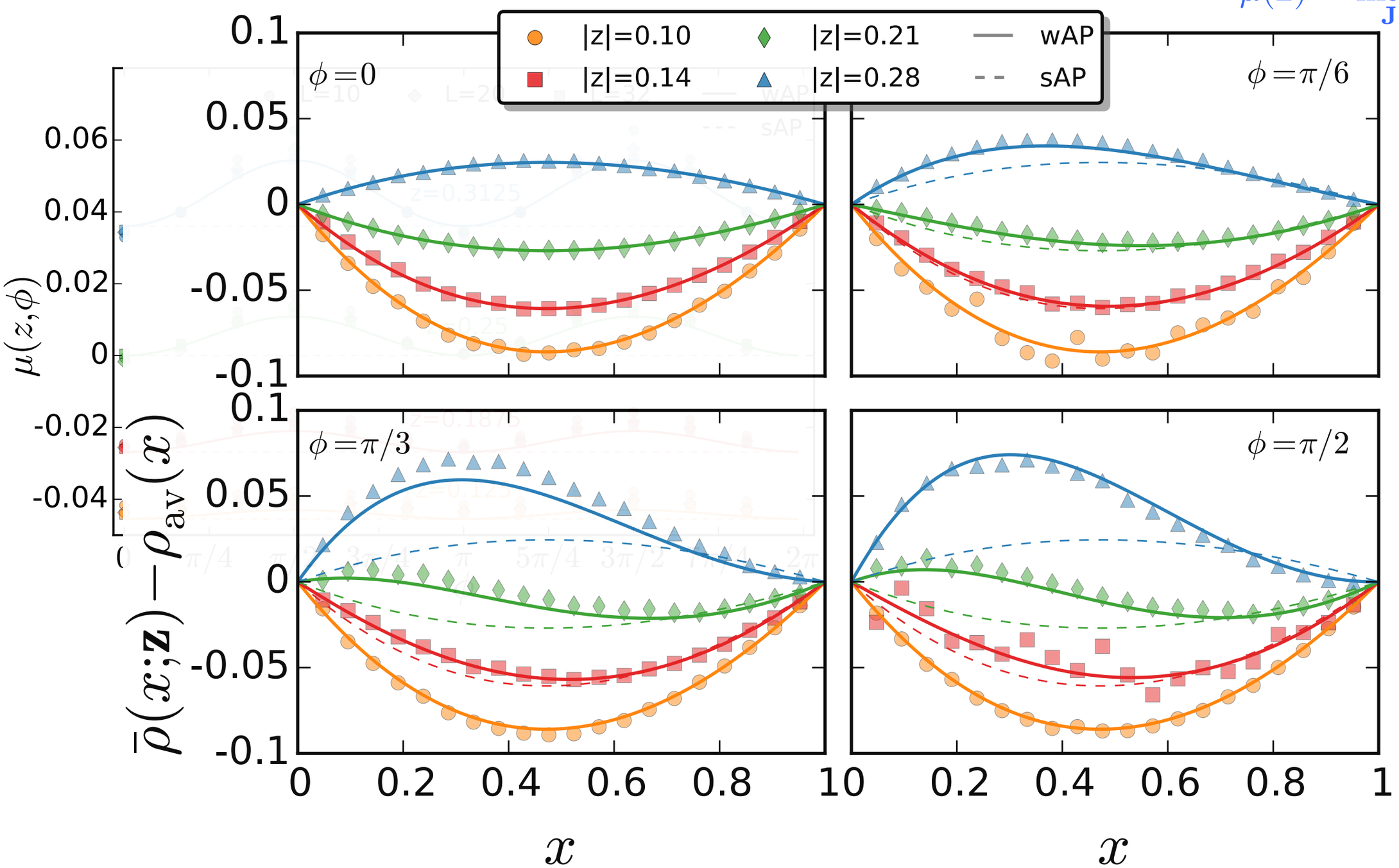

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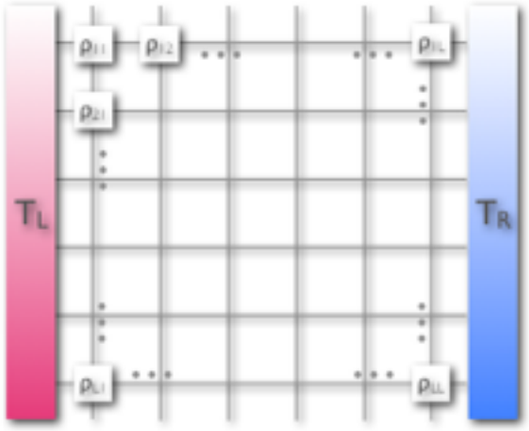

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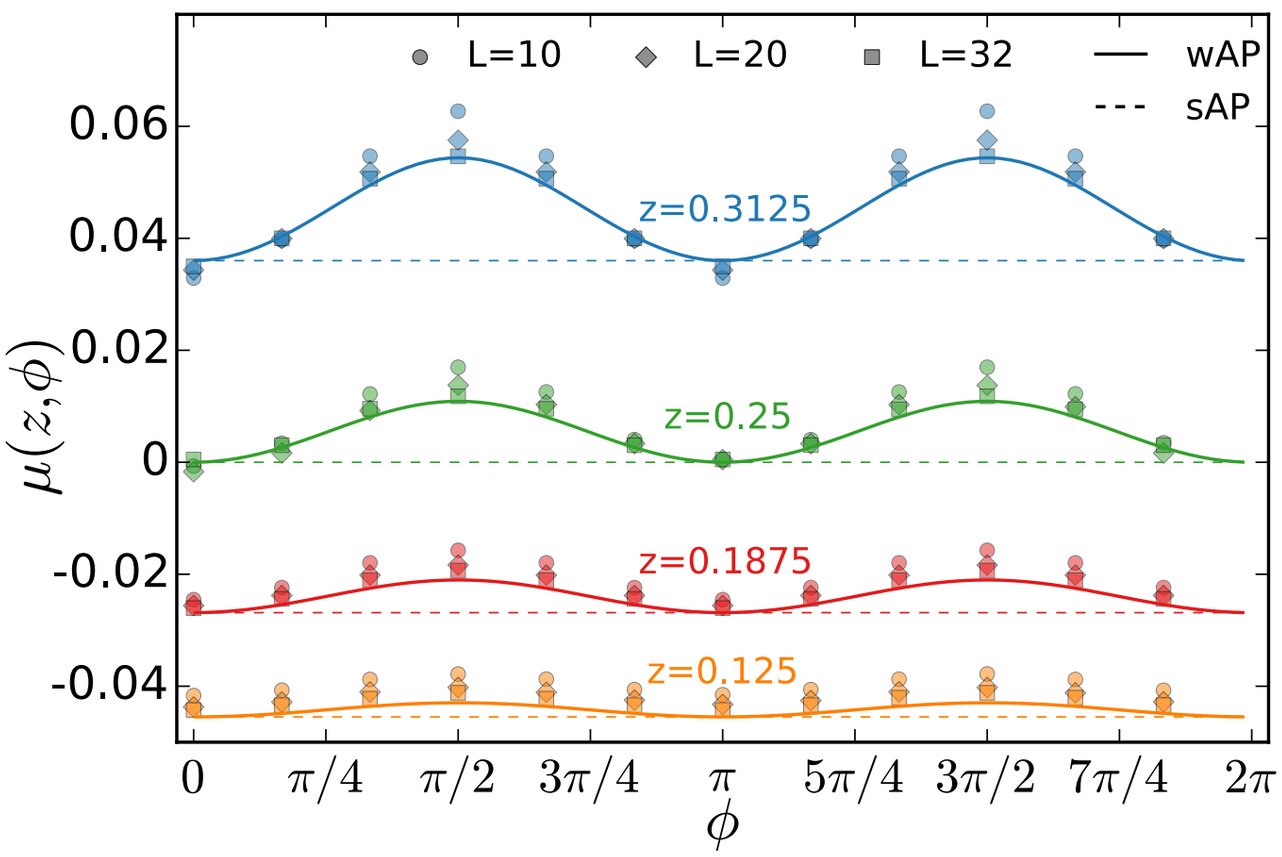
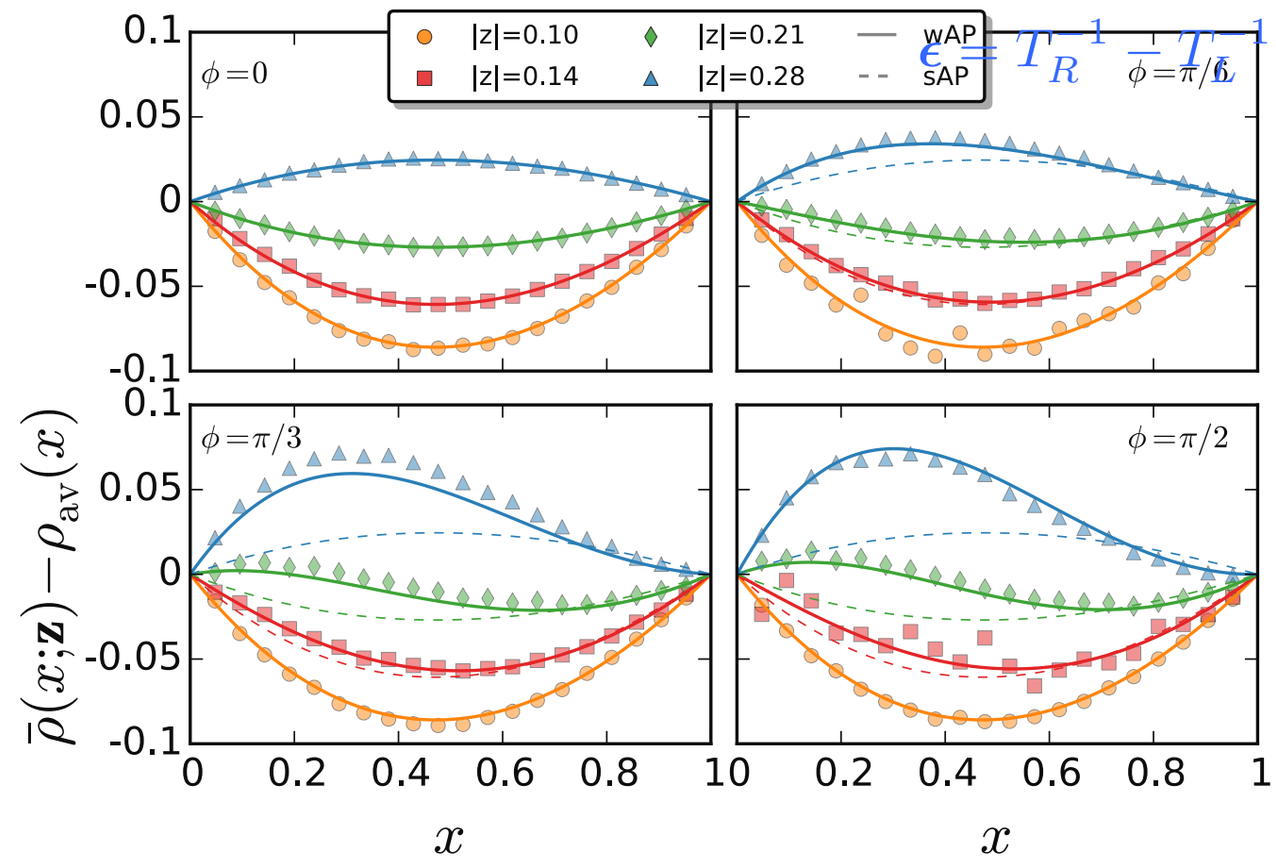




- **Double-bump structure in μ(z) vs ϕ as predicted by wAP**. Moreover, finite-size data clearly converge to the wAP prediction as L increases

OTHER MODELS

- Excellent comparison of wAP predictions against numerical data in other cases:
  - Isotropic 2d Random Walkers (RW) under density gradient
  - Anisotropic 2d Zero Range Process
  - Etc.

C.P. E., Garrido & Hurtado, preprint (2015)

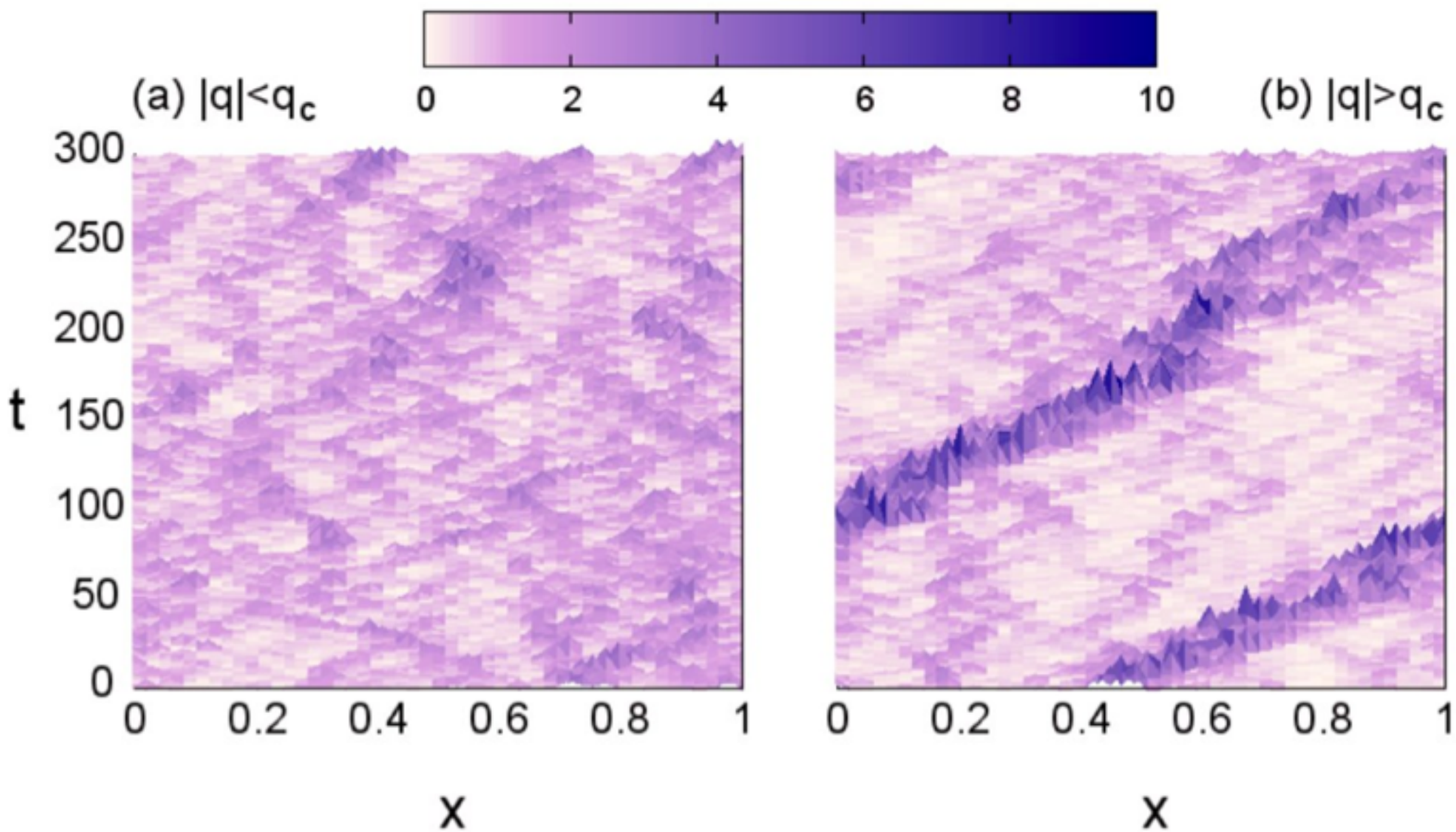
SUMMARY

- The Additivity Principle (AP) of Bodineau & Derrida is a **powerful tool** to compute current LDFs within Macroscopic Fluctuation Theory (MFT)
- **We have extended the Additivity Principle to general, d-dimensional nonequilibrium driven diffusive systems**
- Crucially, the **existence of a divergence-free, structured current vector field at the fluctuating level**, coupled to the local mobility, turns out to be essential to understand current statistics in d>1
- **wAP predictions have been tested** against both exact matrix results and simulations of rare events in different paradigmatic models of transport in d=2, and a **remarkable agreement is found in all cases**.
- We prove that, when compared to the straightforward extension of the AP to high-d (sAP), **the so-called weak AP (wAP) always yields a better maximizer of the macroscopic fluctuation theory action for current statistic**

Thank you

Backup slides

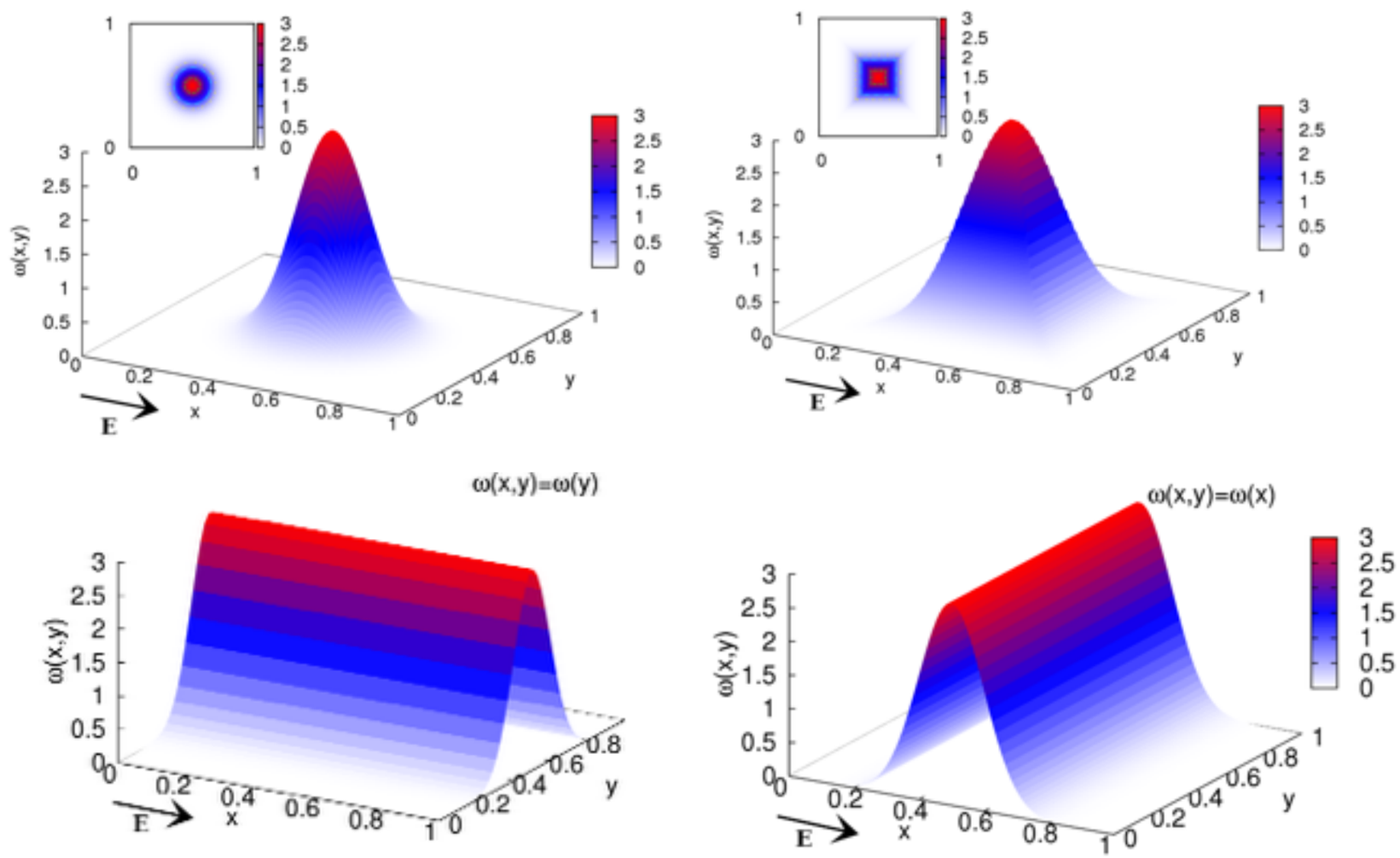
DYNAMIC PHASE TRANSITION IN D-DIMENSIONS ?



DYNAMIC PHASE TRANSITION IN 2D

- **Questions:** Dynamic phase transitions in high-d? Traveling wave structure? Other symmetry-breaking solutions? ...

- **DPT in 2d:** way more complex!! PDE, multiple solutions, ...



Tizón, Espigares, Garrido & Hurtado, preprint (2015)

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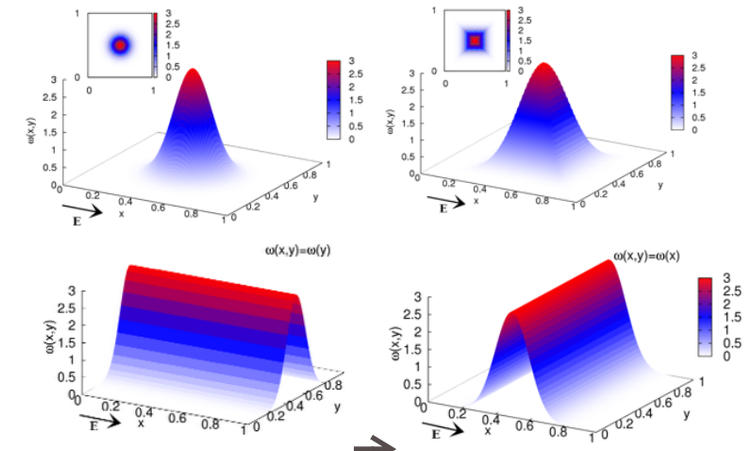
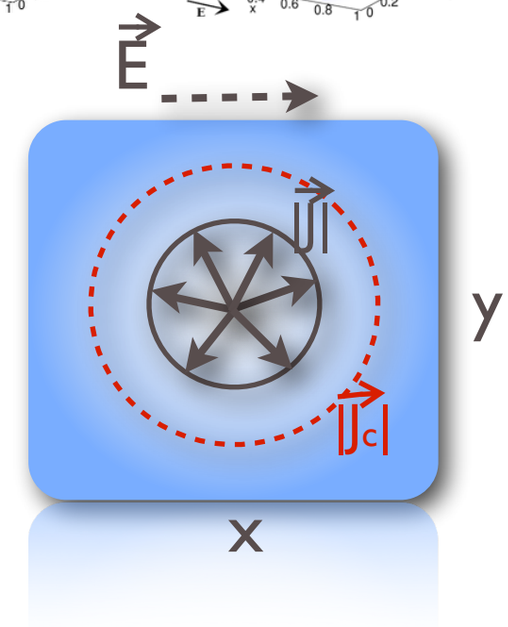
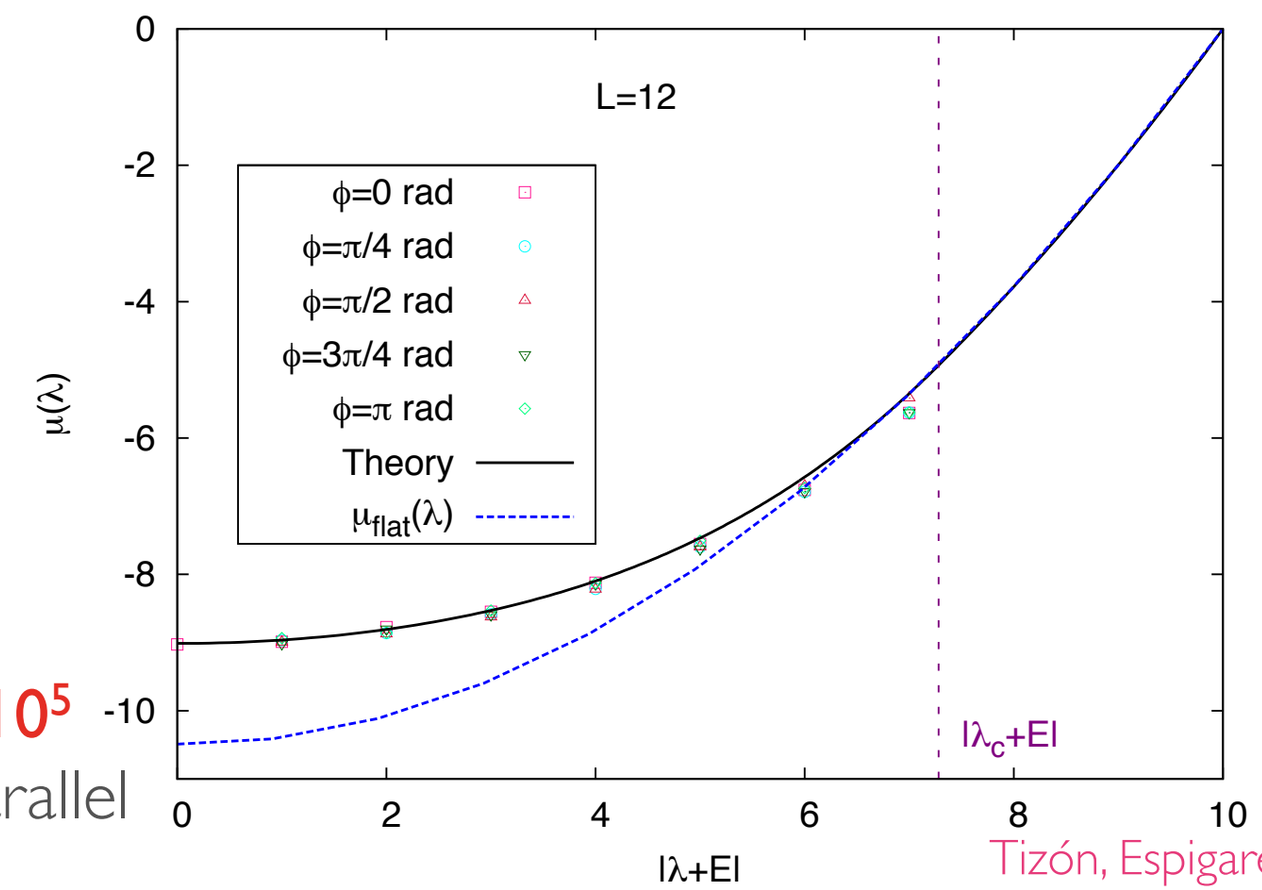


- **Questions:** Dynamic phase transitions in high-d? Traveling wave structure? Other symmetry-breaking solutions? ...
- **DPT in 2d:** way more complex!! PDE, multiple solutions, ...
- **Essential role of large-scale simulations** to ellucidate the nature of this phenomenon in more complex situations
- Extensive simulations of current statistics in **2d WASEP**: **SSB at the fluctuating level in 2d!!**





World record!?? 5×10^5 **clones** evolving in parallel

Tizón, Espigares, Garrido & Hurtado, preprint (2015)

DYNAMIC PHASE TRANSITION IN 2D

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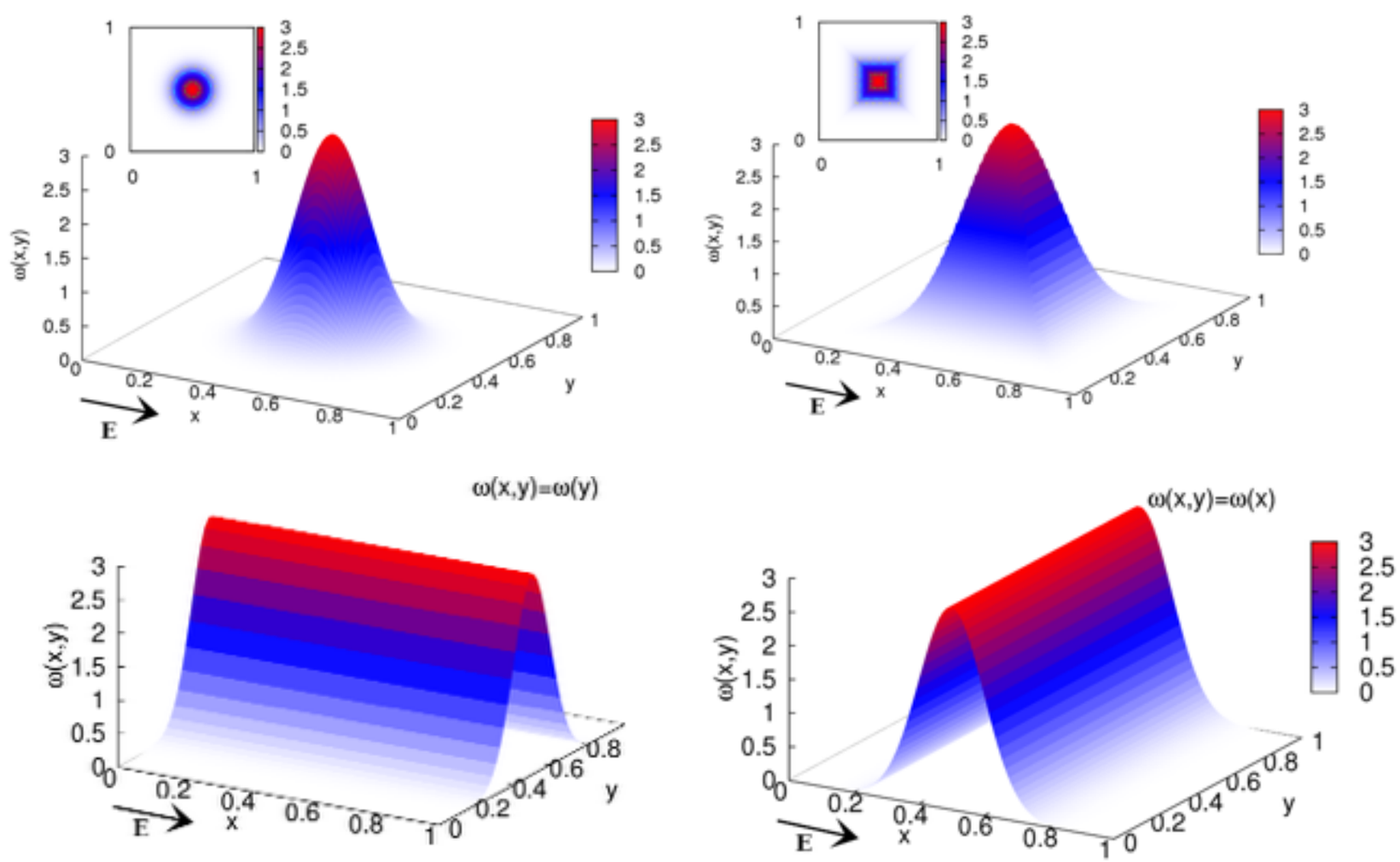

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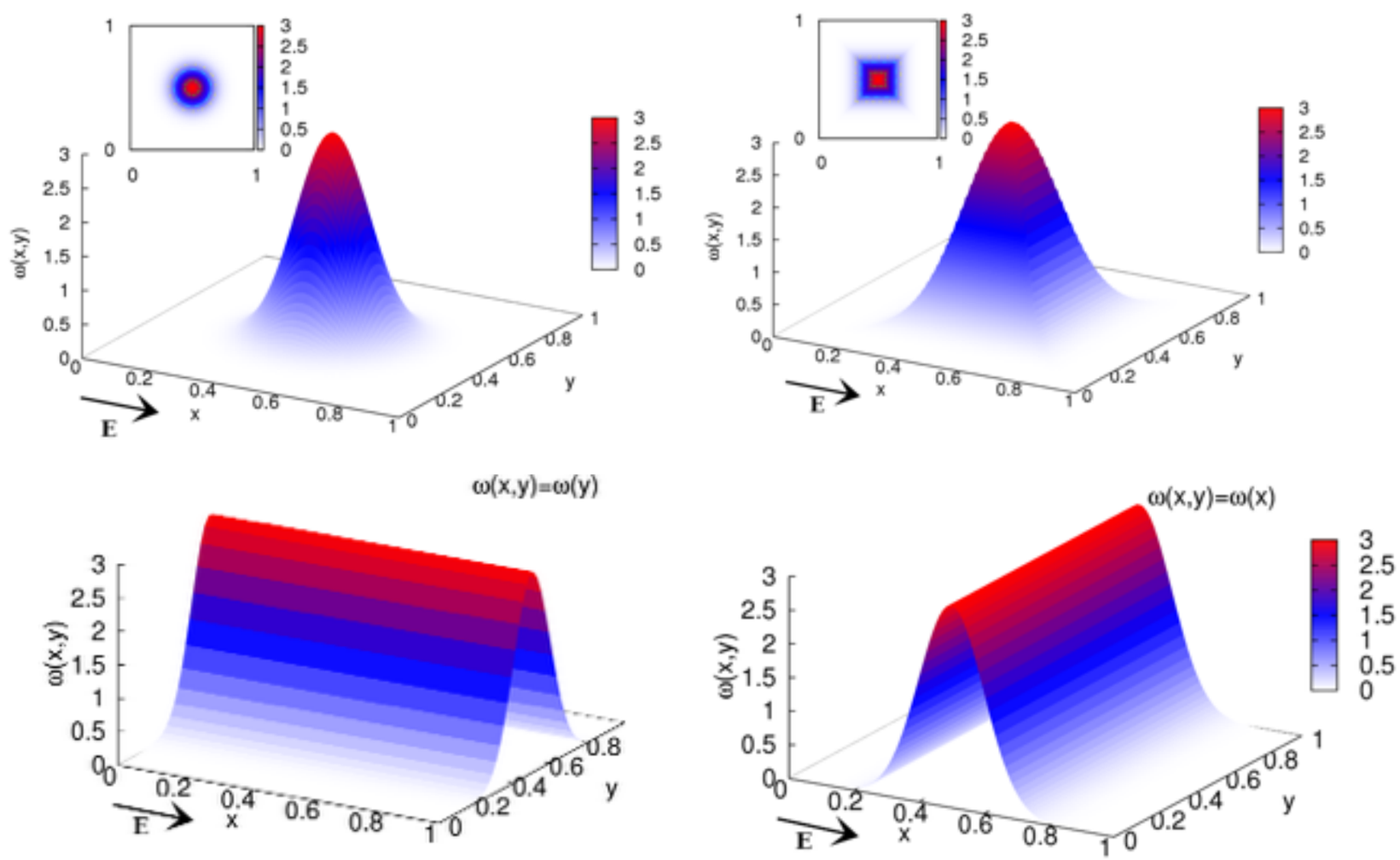

- Measure the **dispersion of the instantaneous center of mass position** for different slices of the system in the x- and y-directions

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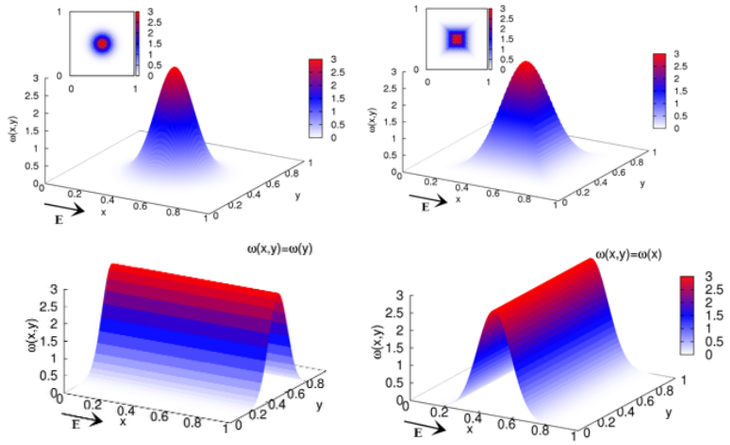

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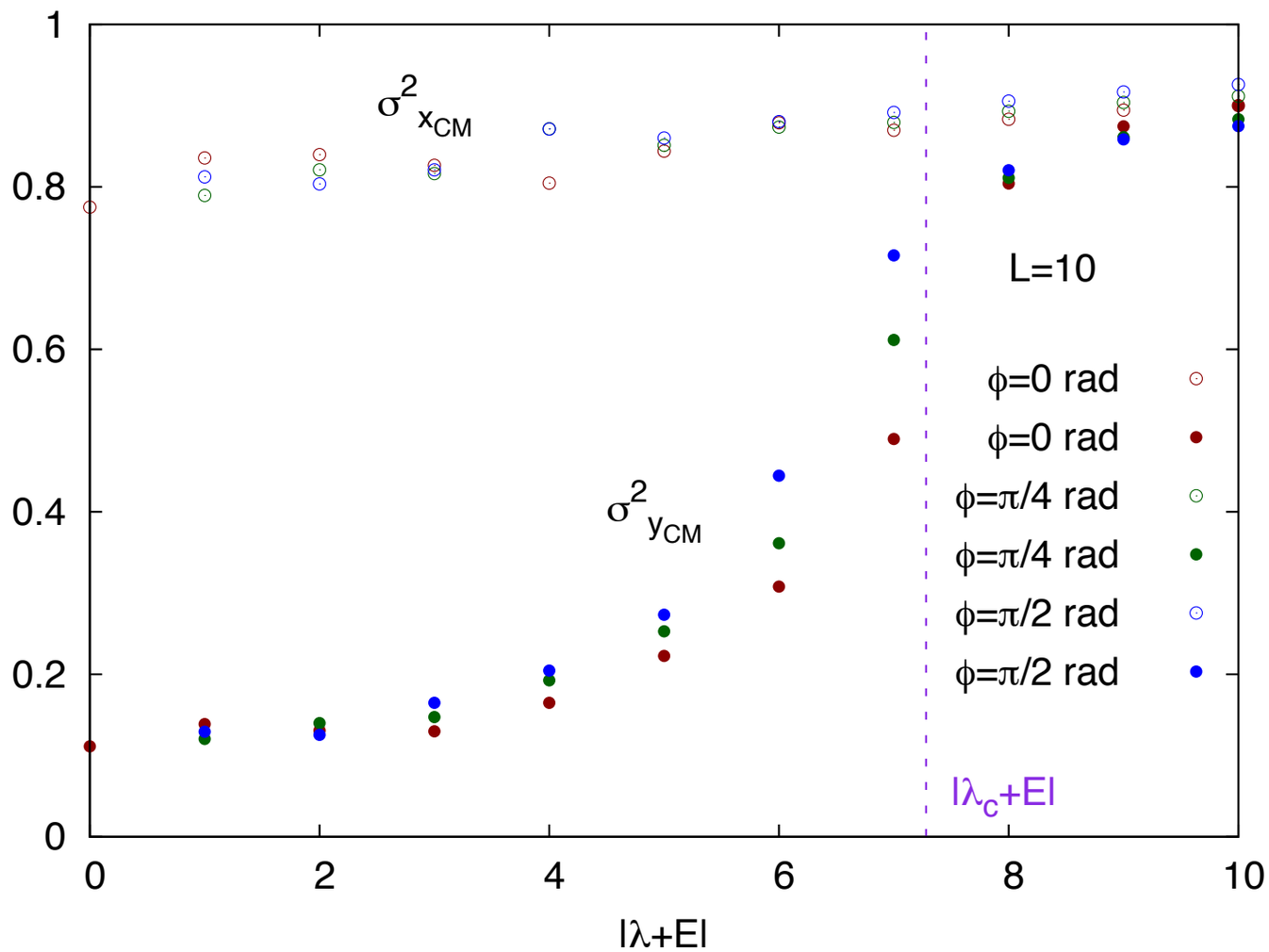

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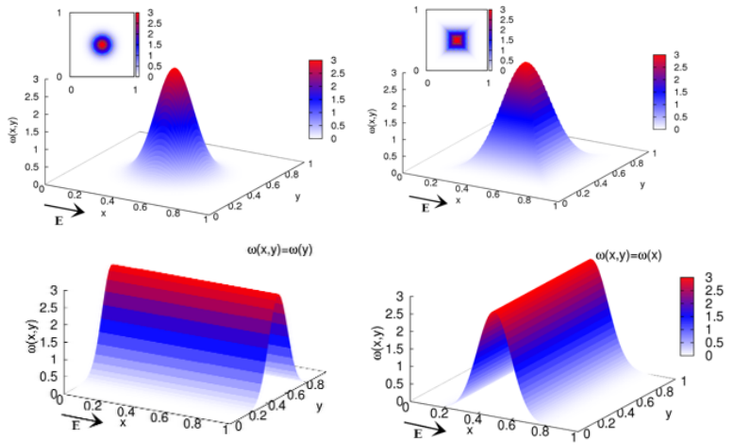

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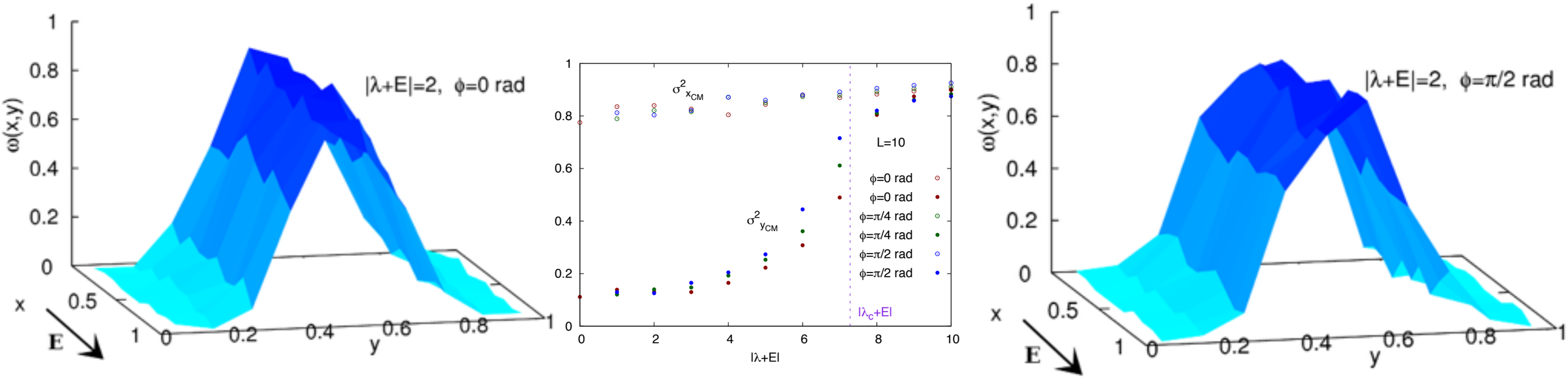

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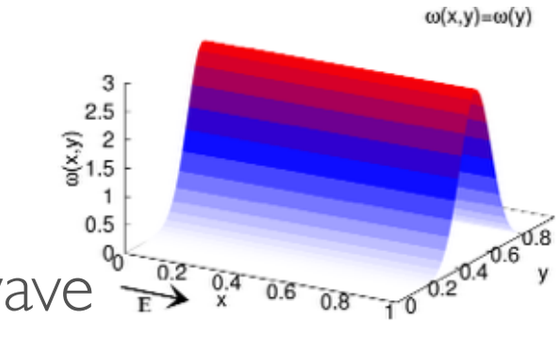
DYNAMIC PHASE TRANSITION IN 2D: MFT PREDICTIONS

- **General stability analysis in 2d** shows that flat (homogeneous) solution becomes unstable against small space-time perturbations whenever

$$\sigma''(\rho_0)\left(\frac{\mathbf{J}^2}{\sigma(\rho_0)^2}-\mathbf{E}^2\right) > 8\pi^2\frac{D(\rho_0)^2}{\sigma(\rho_0)}$$



- The first instability to kick in has the form of a 1d-type traveling wave
- The variational problems looks ugly but can be solved (numerically) for the 1d-projection case

$$\min_{\omega(\mathbf{r}),\varphi(\mathbf{r}),\mathbf{v}}\int_\Lambda d\mathbf{r}\frac{1}{2\sigma(\omega)}\Big[\big(\mathbf{J}-\mathbf{v}(\rho_0-\omega(\mathbf{r}))\big)^2+\varphi(\mathbf{r})\cdot\big(\varphi(\mathbf{r})+2\mathbf{J}-2\mathbf{v}(\rho_0-\omega(\mathbf{r}))$$
$$+2D(\omega)\nabla\omega(\mathbf{r})\big)+\sigma^2(\omega)\mathbf{E}^2+D^2(\omega)(\nabla\omega(\mathbf{r}))^2\Big]$$

$$\nabla\cdot\varphi(\mathbf{r})=0$$
$$\int_\Lambda\varphi(\mathbf{r})d\mathbf{r}=0$$
$$\rho_0=\int_\Lambda\omega(\mathbf{r})d\mathbf{r}$$

- Violations of additivity happen in d-dimensional periodic systems via a **dynamic phase transition to a traveling-wave phase with broken symmetries**, for which **divergence-free but structured current fields** also play a key role.

Tizón, Espigares, Garrido & Hurtado, preprint (2015)

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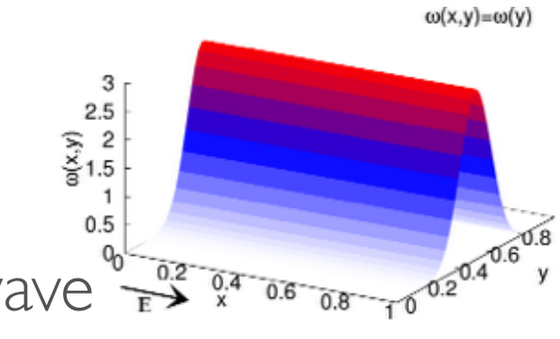

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- Crucial role of divergence-free but structured field φ(r)

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Tizón, Espigares, Garrido & Hurtado, preprint (2015)

Hurtado, C. Espigares, Pozo, Garrido, PNAS **108**, 7704 (201

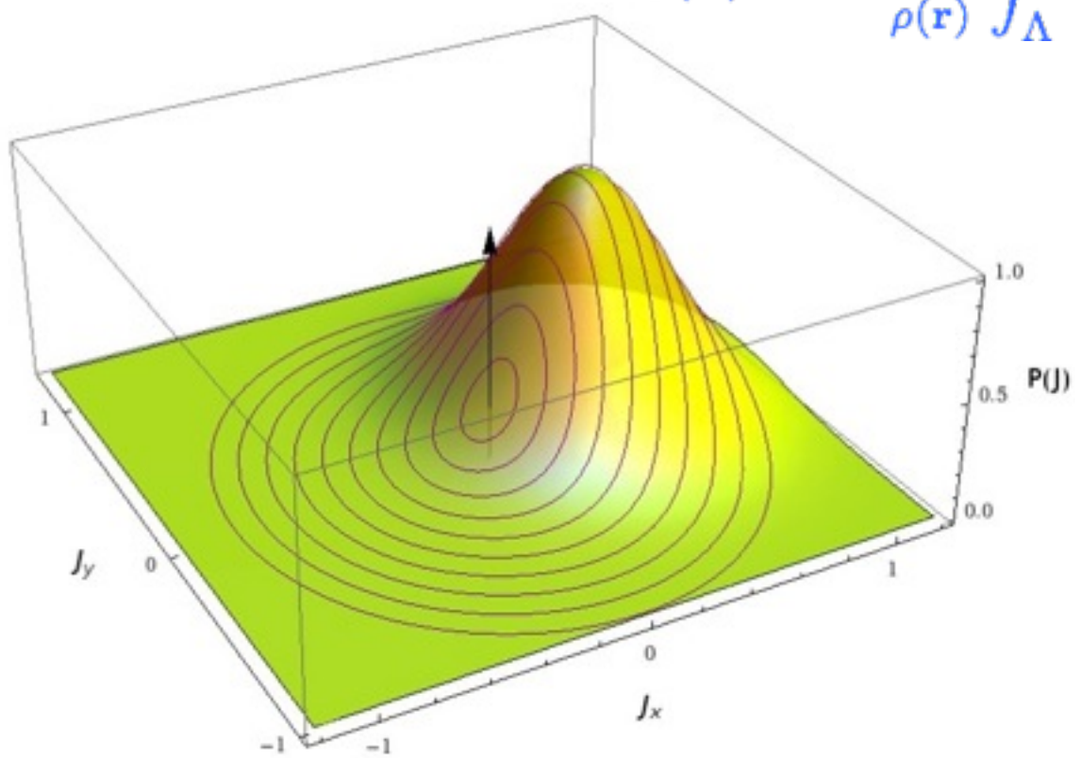
THE ISOMETRIC FLUCTUATION RELATION

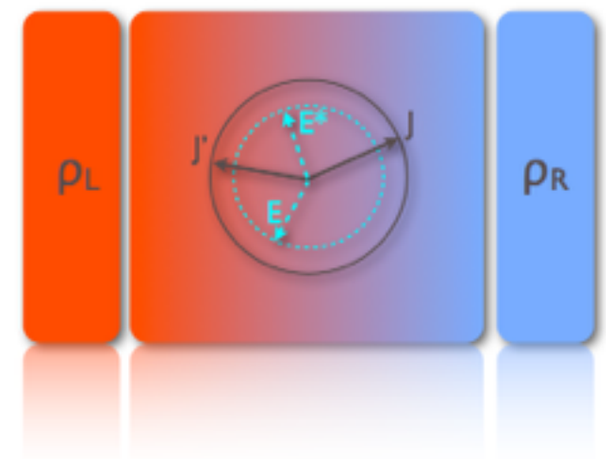
- Within **MFT + sAP**, invariance of optimal paths leads to **Isometric Fluctuation Relation (IFR)**

$$G_s(\mathbf{J}) = -\min_{\rho(\mathbf{r})} \int_\Lambda d\mathbf{r} \frac{\left[\mathbf{J} - \mathbf{Q}_\mathbf{E}(\rho)\right]^2}{2\sigma(\rho)} \xrightarrow{\text{reversivility}} \rho_\mathbf{J}(\mathbf{r}) \equiv \rho_{|\mathbf{J}|}(\mathbf{r})$$

$$\lim_{\tau\to\infty} \frac{1}{\tau L^d} \ln\left[\frac{\mathrm{P}_\tau(\mathbf{J})}{\mathrm{P}_\tau \mathbf{J}'}\right] = \boldsymbol{\epsilon}\cdot(\mathbf{J}-\mathbf{J}')$$

$$\mathbf{J}' = \hat{\mathcal{R}}_d \mathbf{J} \Rightarrow |\mathbf{J}'| = |\mathbf{J}|$$





Hurtado, C. Espigares, Pozo, Garrido, PNAS **108**, 7704 (201

THE ISOMETRIC FLUCTUATION RELATION

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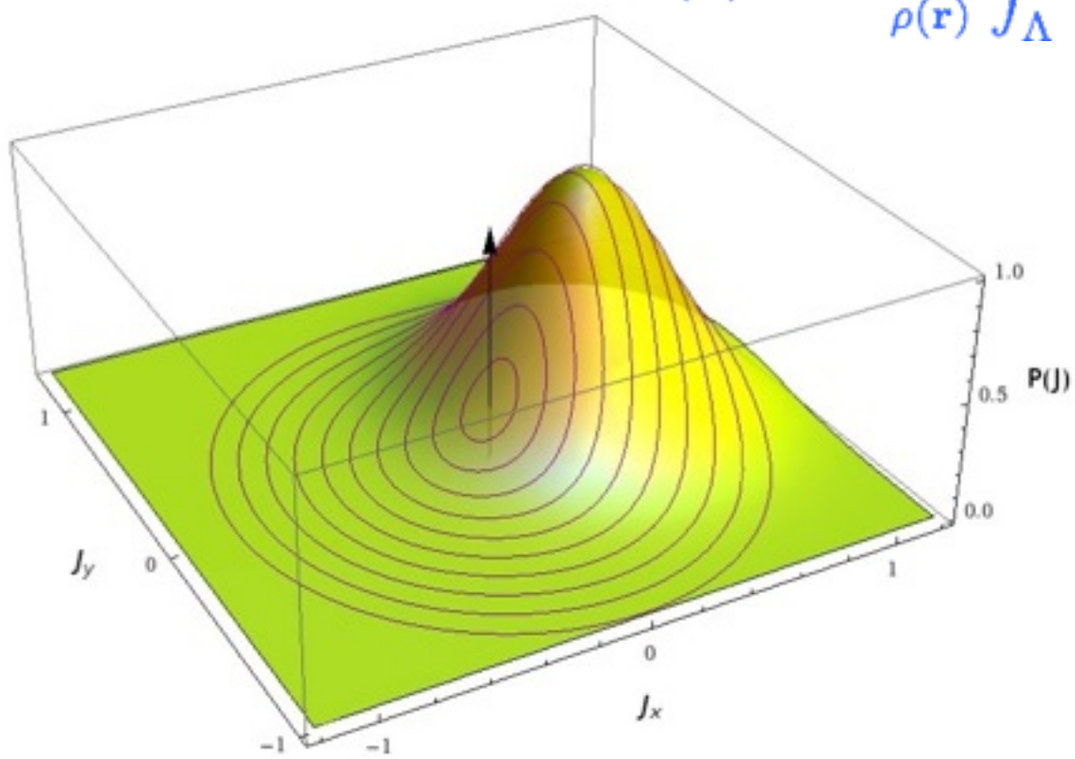
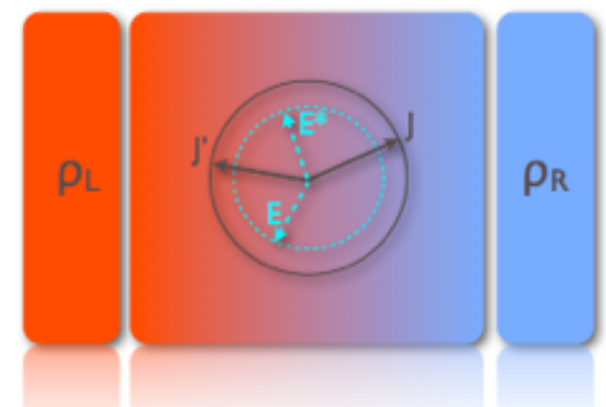




P.H., C. Espigares, Pozo, Garrido, JSP **154,** 214 (2014)
Villavicencio, Harris & Touchette, EPL, **105**, 30009 (2014)
Kumar et al, PRE **91**, 030102(2015)
Lacoste & Gaspard, PRL **113**, 240602 (2014)

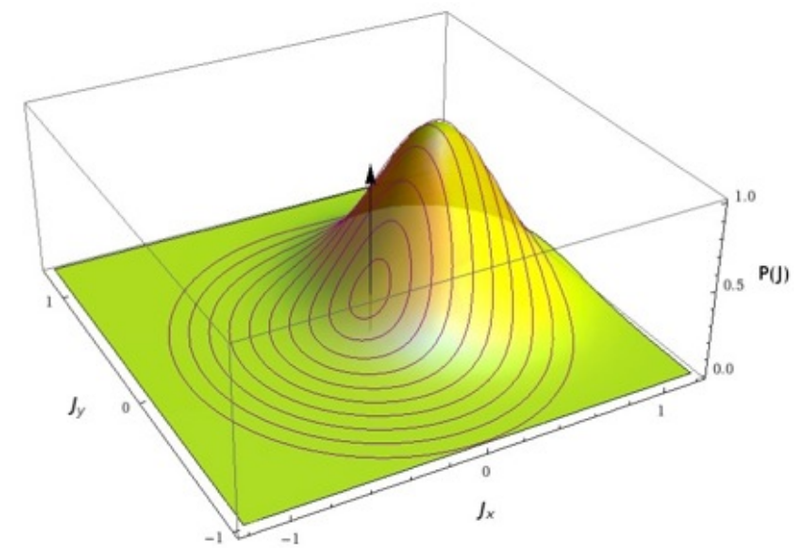
- **Tested in simulations of rare events** for different stochastic lattice gases, **exact matrix computations and even experiments**. **Generalized to anisotropic systems** and various **equilibrium systems with broken symmetries**

- **Small deviations from IFR** observed for large current fluctuations are related to the presence of the **structured, divergence-free optimal current vector field**. However, generalized IFR

$$\lim_{\tau\to\infty} \frac{1}{\tau L^d} \ln\left[\frac{\mathrm{P}_\tau[\mathcal{J}(\mathbf{r})]}{\mathrm{P}_\tau[\mathcal{J}'(\mathbf{r})]}\right] = \int_{\partial\Lambda} d\Gamma \frac{\delta\mathcal{H}[\rho]}{\delta\rho} \hat{n}\cdot[\mathcal{J}'(\mathbf{r}) - \mathcal{J}(\mathbf{r})]$$

SYMMETRIES IN NONEQUILIBRIUM FLUCTUATIONS

- Time-reversibility sets **strong constraints** on nonequilibrium current fluctuations



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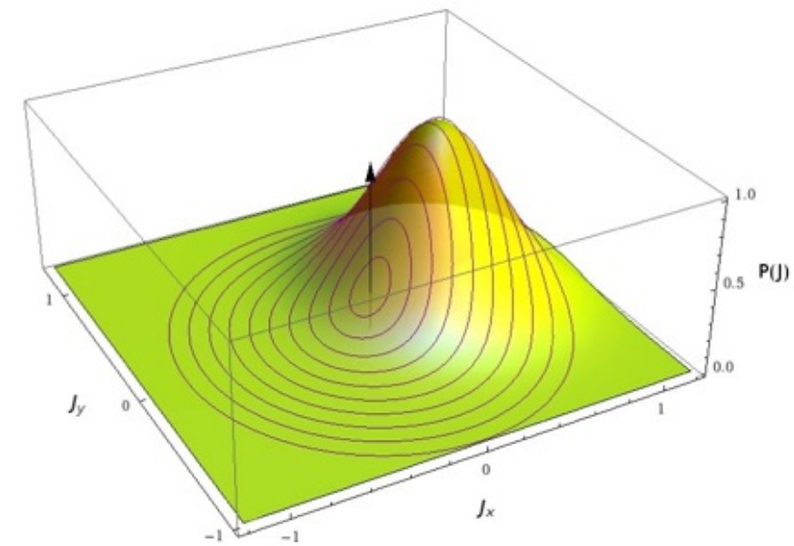
P.H., Espigares, Pozo, Garrido, PNAS 108, 7704 (2011)

SYMMETRIES IN NONEQUILIBRIUM FLUCTUATIONS

- Time-reversibility sets **strong constraints** on nonequilibrium current fluctuations

- **Hierarchy of equations for the cumulants of the current distribution**, coupled via the generators $\mathscr{L}$ of d-dimensional rotations

$$\sum_{i=1}^{n} \mu^{(n)}_{\alpha_1 \ldots \alpha_{i-1} \beta_i \alpha_{i+1} \ldots \alpha_n} \mathcal{L}_{\beta_i \alpha_i} + \mathcal{L}_{\gamma\nu} \epsilon_\nu \mu^{(n+1)}_{\gamma \alpha_1 \ldots \alpha_n} = 0$$



$$\lim_{\tau\to\infty} \frac{1}{\tau L^d} \ln \left[\frac{P_\tau(\boldsymbol{J})}{P_\tau(\boldsymbol{J}')} \right] = \boldsymbol{\epsilon} \cdot (\boldsymbol{J} - \boldsymbol{J}')$$

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- Example in **d=2** (def. $\Delta J_\alpha \equiv J_\alpha - \langle J_\alpha \rangle_\epsilon$)

$$\begin{aligned}
\langle J_x \rangle_\epsilon &= \tau L^2 \left[\epsilon_x \langle \Delta J_y^2 \rangle_\epsilon - \epsilon_y \langle \Delta J_x \Delta J_y \rangle_\epsilon \right] \\
\langle J_y \rangle_\epsilon &= \tau L^2 \left[\epsilon_y \langle \Delta J_x^2 \rangle_\epsilon - \epsilon_x \langle \Delta J_x \Delta J_y \rangle_\epsilon \right]
\end{aligned}$$

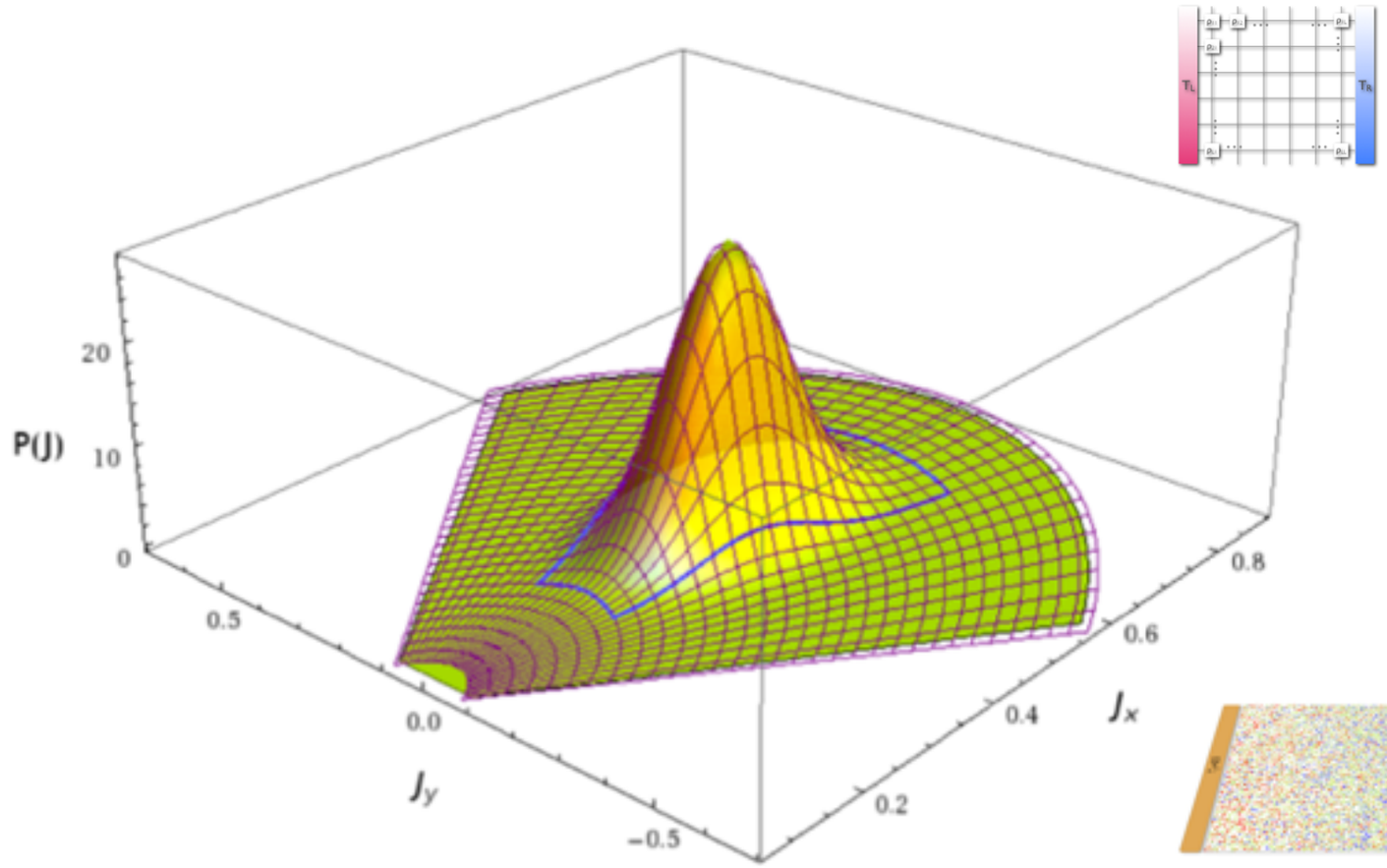
$$\begin{aligned}
2\langle \Delta J_x \Delta J_y \rangle_\epsilon &= \tau L^2 \left[\epsilon_y \langle \Delta J_x^3 \rangle_\epsilon - \epsilon_x \langle \Delta J_x^2 \Delta J_y \rangle_\epsilon \right] \\
&= \tau L^2 \left[\epsilon_x \langle \Delta J_y^3 \rangle_\epsilon - \epsilon_y \langle \Delta J_x \Delta J_y^2 \rangle_\epsilon \right] \\
\langle \Delta J_x^2 \rangle_\epsilon - \langle \Delta J_y^2 \rangle_\epsilon &= \tau L^2 \left[\epsilon_x \langle \Delta J_x \Delta J_y^2 \rangle_\epsilon - \epsilon_y \langle \Delta J_x^2 \Delta J_y \rangle_\epsilon \right]
\end{aligned}$$

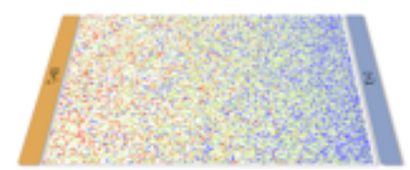
- **Further consequences**: Green-Kubo integrals, hierarchy for nonlinear response coefficients, etc

Test the IFT!! ... Simulation of rare events

P.H., Espigares, Pozo, Garrido, PNAS 108, 7704 (2011)

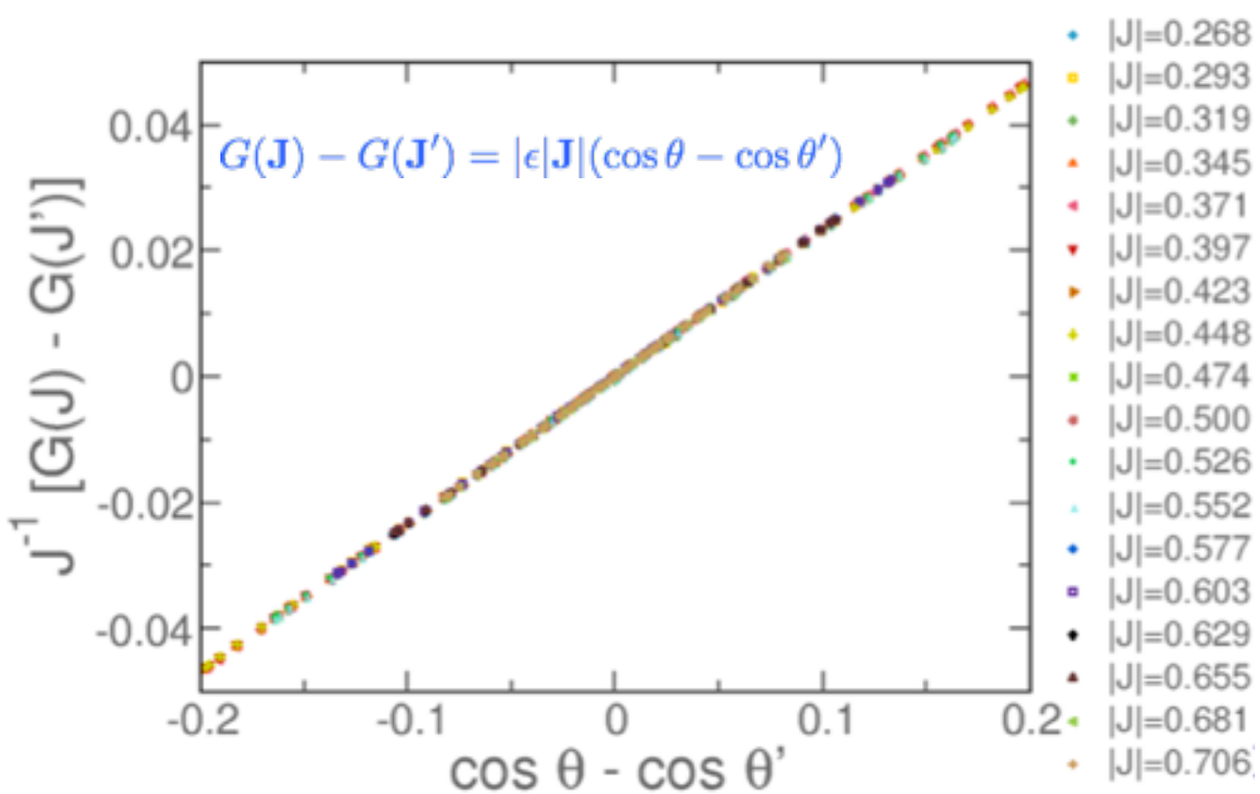
SYMMETRY IN FLUCTUATIONS: TESTING THE IFT

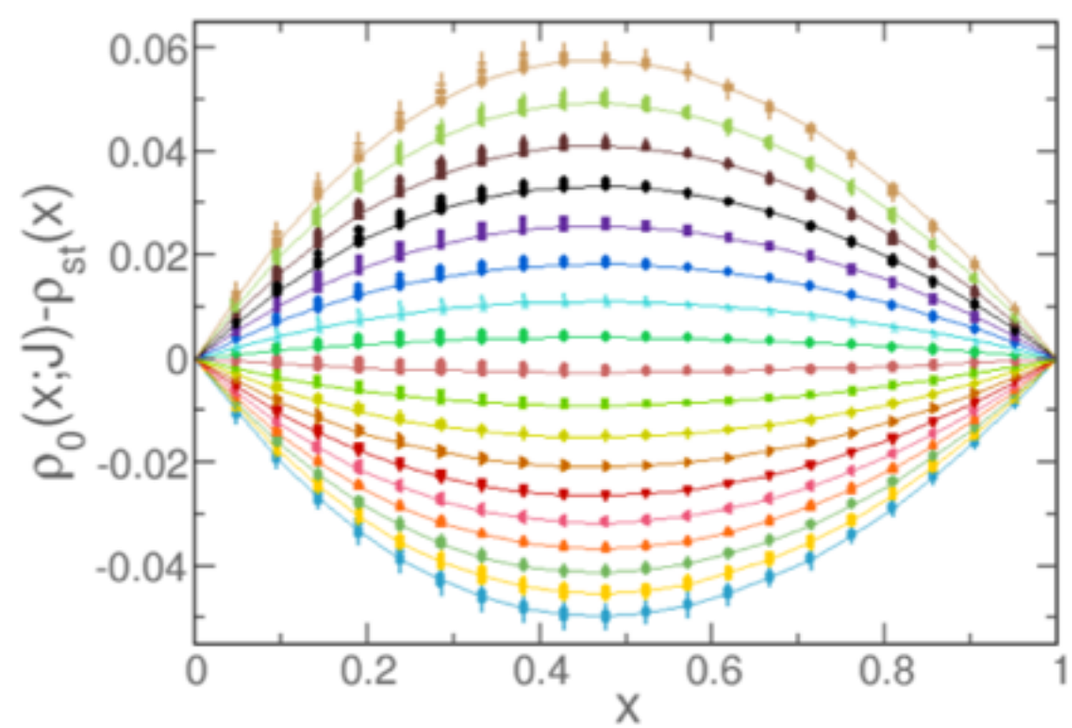




- **IFT is numerically confirmed with high precission**
- **Optimal profiles** remain invariant under current rotations
- Also confirmed for hard-disks: **IFT valid for hydrodynamic systems**

$$\lim_{\tau\to\infty} \frac{1}{\tau L^d} \ln\left[\frac{P_\tau(\boldsymbol{J})}{P_\tau(\boldsymbol{J}')}\right] = \boldsymbol{\epsilon}\cdot(\boldsymbol{J}-\boldsymbol{J}')$$





WHAT ARE LARGE DEVIATION FUNCTIONS?

Examples

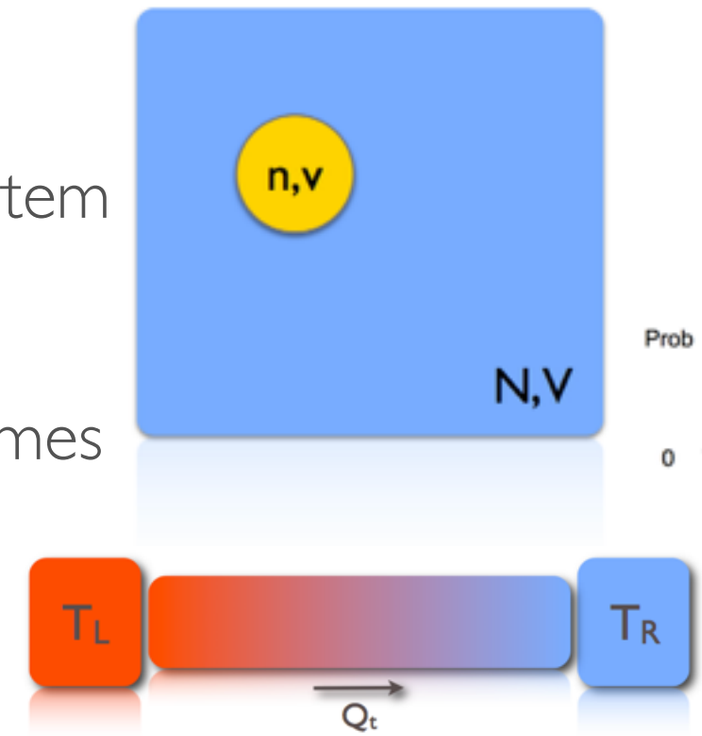
- Density distribution in large subsystem

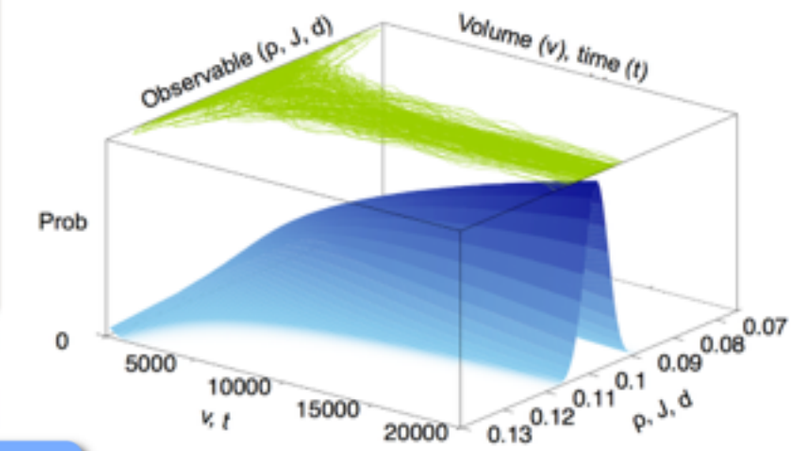
$$\mathrm{P}(n/v = \rho) \asymp \mathrm{e}^{v\mathcal{I}(\rho)}$$

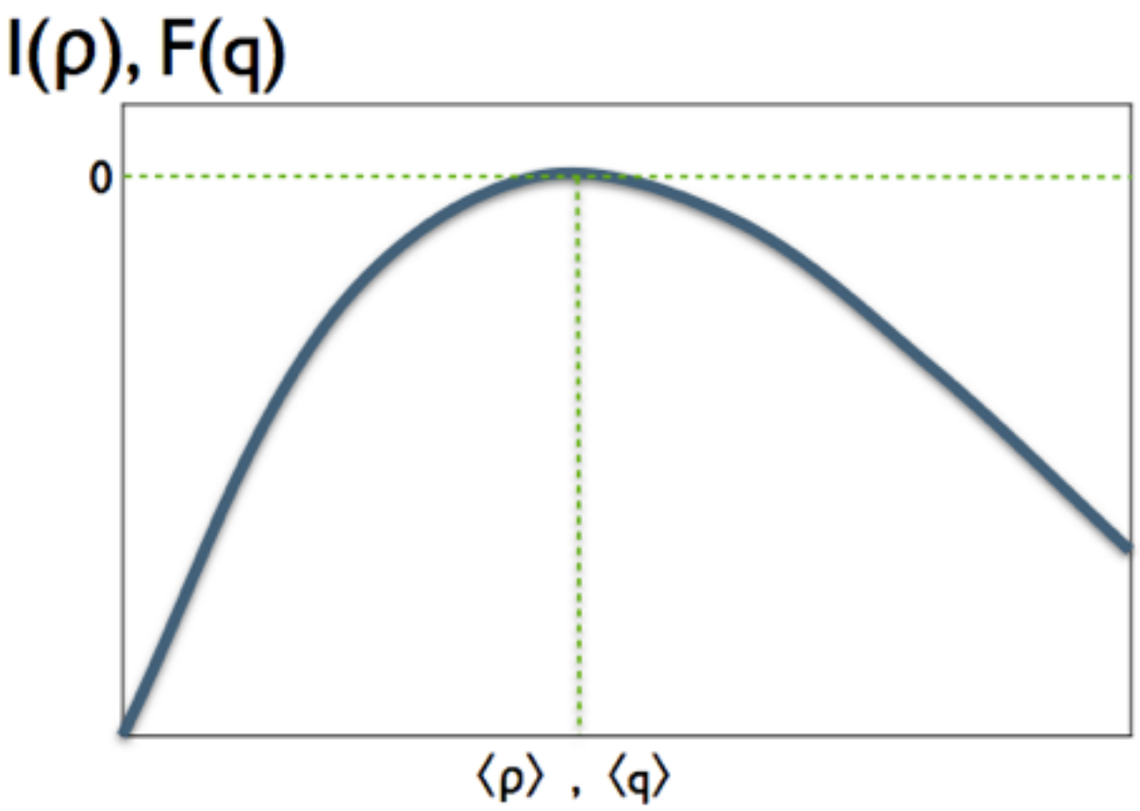
- Time-integrated current for long times

$$\mathrm{P}\left(Q_t/t = q\right) \asymp \mathrm{e}^{t\mathcal{F}(q)}$$

- LDFs have a typical shape







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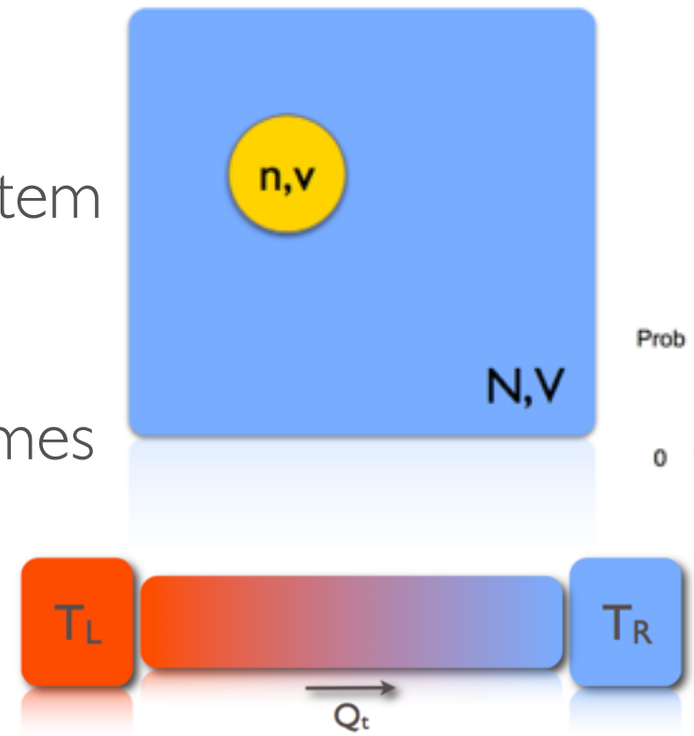
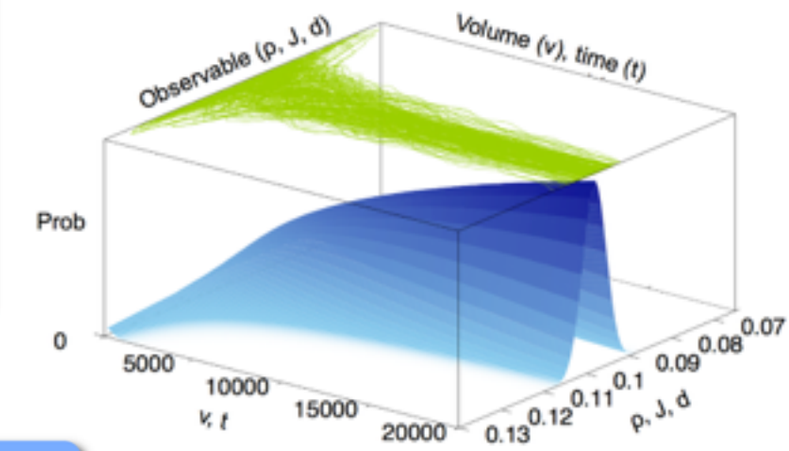
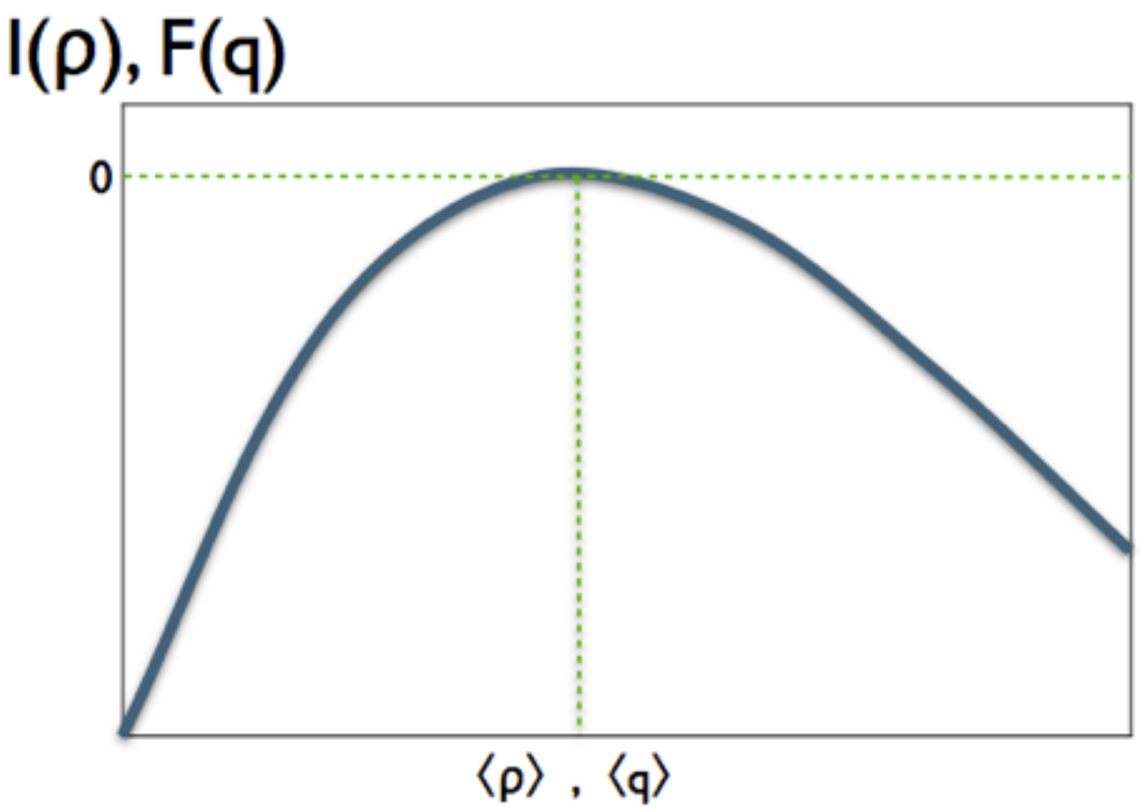






Why LDFs are important?

- Rate of convergence toward average
- **Equilibrium**: LDFs = entropy/free energy

$$P[\rho(\vec{x})] \sim \exp\left(-L^d \mathcal{I}[\rho(\vec{x})]\right)$$

$$\mathcal{I}[\rho(\vec{x})] = \frac{1}{k_B T}\int d\vec{x}\left(f[\rho(\vec{x})] - f(\rho^*)\right)$$

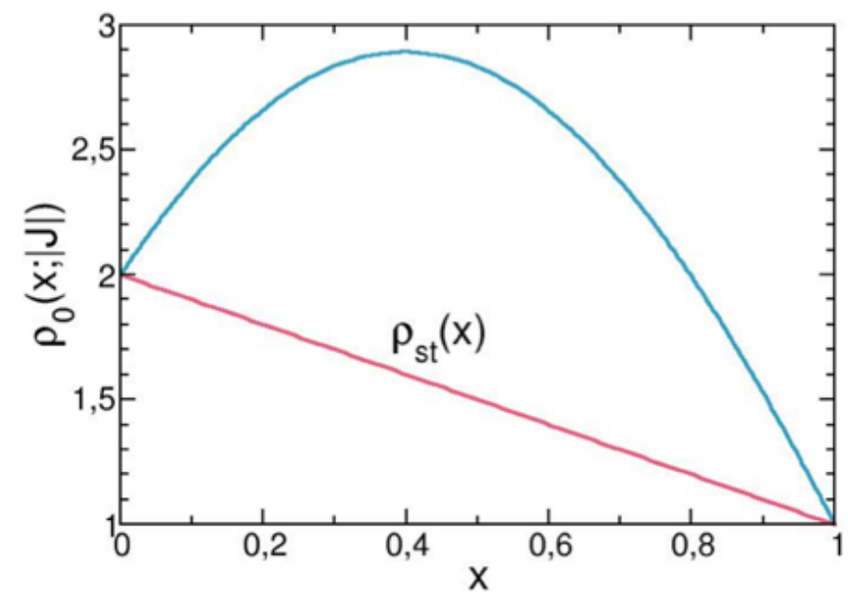
- **Nonequilibrium**: LDFs extend the notion of **free energy out of equilibrium**

MACROSCOPIC FLUCTUATION THEORY (II)

- Fluctuations of **space&time-averaged current** $\longrightarrow q = \frac{1}{\tau}\int_0^\tau dt \int_0^1 dx\, j(x,t)$

$$\mathrm{P}_\tau(q) \sim \mathrm{e}^{+\tau N G(q)} \qquad G(q) = \frac{1}{\tau}\max_{\{\rho,j\}_0^\tau} \mathcal{I}_\tau[\rho,j]$$

$$\mathcal{I}_\tau[\rho,j] = -\int_0^\tau dt \int_0^1 dx \frac{(j + D[\rho]\partial_x\rho)^2}{2\sigma[\rho]}$$



- **Optimal profiles≠steady profiles**: Typical path to sustain a given fluctuation

- **Additivity principle** (Bodineau&Derrida, PRL 2004): time-independent optimal profiles

$$\rho_q(x,t) = \rho_q(x)\ ;\ j_q(x,t) = q$$

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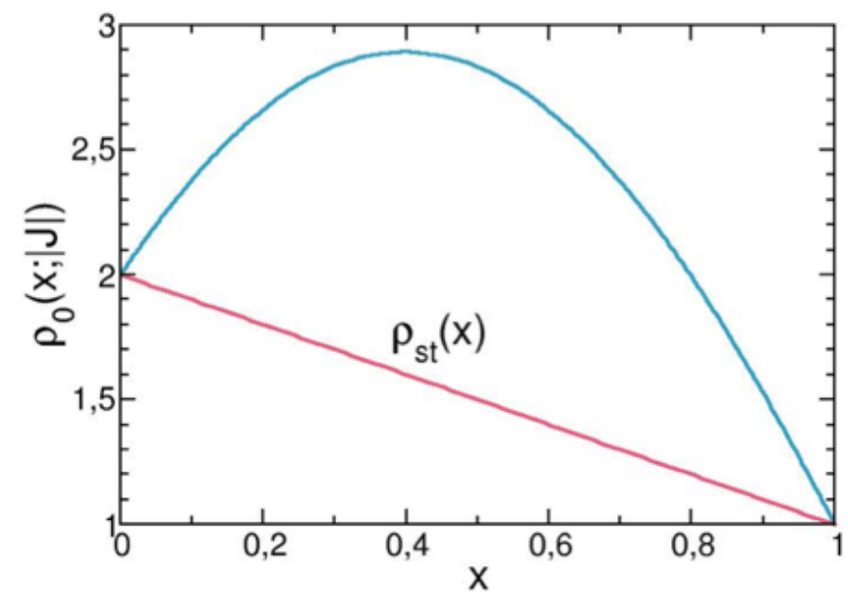

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- For **isolated systems**, flat profiles are always solution ...

$$\rho_q(x,t) = \rho_0\ ;\ j_q(x,t) = q$$

$$G(q) = -q^2/2$$

- Is this the whole story? ... **NO!!**

Gaussian statistics!

- Additivity scenario eventually breaks down for large fluctuations (**|q| > q_c**): **spontaneous symmetry breaking at the fluctuation level**

Bodineau&Derrida, PRE 2005

PHASE TRANSITION IN MFT

- Local stability of flat profiles against small perturbation

Instability

$$|q_c| = 2\pi D(\rho_0)\sqrt{2\sigma(\rho_0)/\sigma''(\rho_0)}$$

- For $|q|>q_c$ → **traveling wave:** $\rho_q(x,t) = \omega_q(x-vt) \Rightarrow j_q(x,t) = q - v\rho_0 + v\omega_q(x-vt)$

$$G(q) = -\min_{\omega_q(x),v} \int_0^1 \frac{\left[q - v\rho_0 + v\omega_q(x)\right]^2 + \omega_q'(x)^2 D[\omega_q]^2}{2\sigma[\omega_q]}\, dx$$

Bodineau&Derrida, PRE 2005

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- Equation for optimal wave profile

$$\left[q - v\rho_0 + v\omega_q(x)\right]^2 - \omega_q'(x)^2 D[\omega_q]^2 = 2\sigma[\omega_q]\Big\{C_1 + C_2\omega_q(x)\Big\}$$

- $\omega_q(x)$ symmetric with **single minimum $\omega_1=\omega(x_1)$ and maximum $\omega_2=\omega(x_2)$** such that $|x_2-x_1|=1/2$

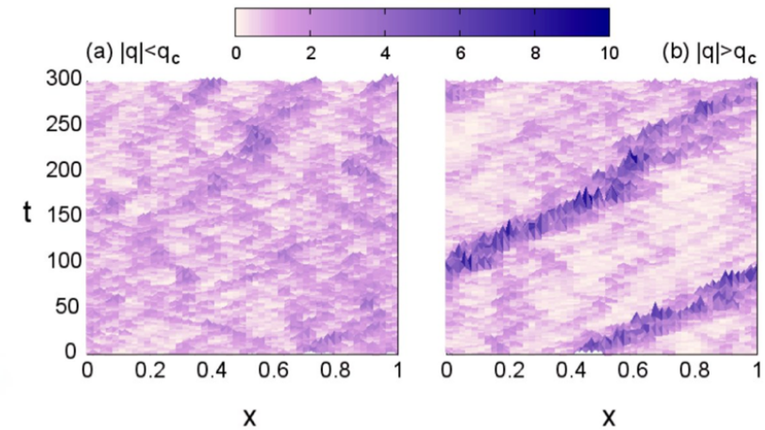
- These constraints fix constants C_1 and C_2: $\frac{\rho_0}{2} = \int_{\omega_1}^{\omega_2} \frac{\omega D(\omega)}{Z_v(\omega)} d\omega \quad ; \quad \frac{1}{2} = \int_{\omega_1}^{\omega_2} \frac{D(\omega)}{Z_v(\omega)} d\omega$

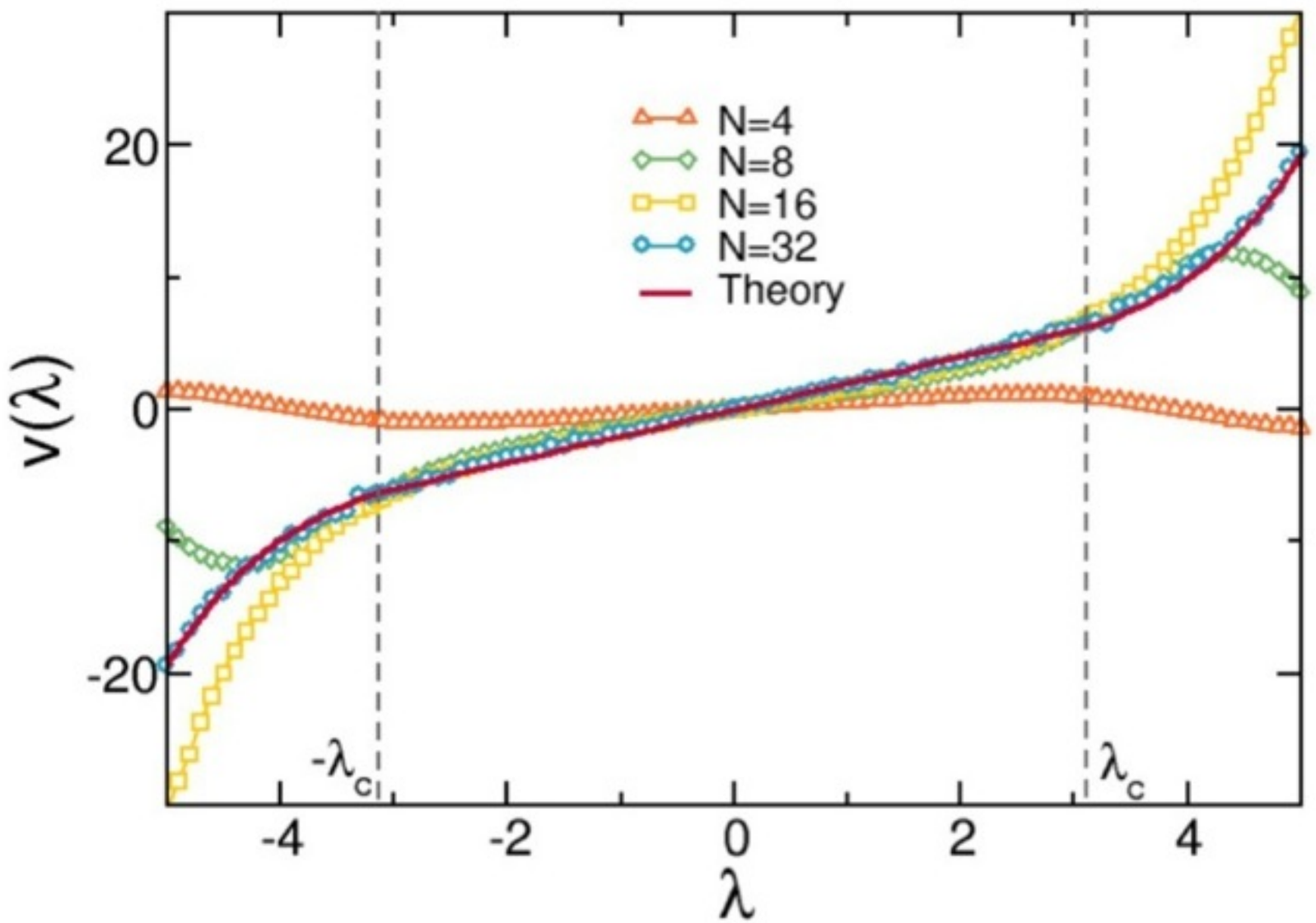
$$Z_v(\omega) = \left[(q - v\rho_0 + v\omega)^2 - 2\sigma(\omega)(C_1 + C_2\omega)\right]^{1/2}$$

- Optimal wave velocity:

$$v = -q\frac{\nu_1^{(v)}}{\nu_2^{(v)}} \qquad\qquad \nu_n^{(v)} \equiv \int_{\omega_1}^{\omega_2} \frac{D(\omega)\big(\omega - \rho_0\big)^n}{\sigma(\omega)Z_v(\omega)}\, d\omega$$

TRAVELING WAVE VELOCITY





- Average wave velocity as a function of λ and different sizes N
- Agreement with MFT very good for large enough N
- For $|q| < q_c \longrightarrow v=2q$. However, above q_c the relation becomes nonlinear