Heat fluctuations in quantum spin chains

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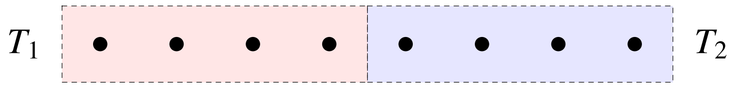
Introduction

- In collaboration with Dragi Karevski, Université de Lorraine.
- Idea: to study the heat flux exchanged between two XX quantum spin chains.
  - Prepare the system in two halves at different temperatures (quantum quench).



- At $t = 0$ we turn on the two halves and monitor the flow of heat between the two bodies.
  - Unitary dynamics.

- According to classical thermodynamics:
  - Heat should flow from the hot to the cold body.
  - The flow should continue until both bodies acquire the same temperature.
  - The total heat flow after a long time will be

$$Q = \frac{U(T_2) - U(T_1)}{2}$$

The Jarzynski-Wójcik fluctuation theorem

- In mesoscopic and microscopic systems, fluctuations become relevant.
  - We must now speak of Q as a random variable with a probability density $P_t(Q)$
- C. Jarzynski and D. K. Wójcik, *PRL*. 92, 230602 (2004)
  - Exchange fluctuation theorem (*valid for weak coupling*)

$$\frac{P_t(Q)}{P_t(-Q)} = e^{\Delta\beta\, Q}, \quad \Delta\beta = \frac{1}{T_1} - \frac{1}{T_2}$$

  - *"It is exponentially more likely to observe the flow of heat in the 'right' direction."*

- Consequences:

$$\langle e^{-\Delta\beta\, Q} \rangle = 1 \qquad \Rightarrow \qquad \langle Q \rangle \geq 0 \qquad (T_2 > T_1)$$

  - *"On average, heat always flows in the 'right' direction."*
- In practice, it is easier to study the characteristic function:

$$F_t(r) = \langle e^{i\,r\,Q} \rangle = \text{tr}\,\{e^{i\,r\,H_1(t)}\, e^{-i\,r\,H_1(0)}\, \rho_{\text{th}}\}$$

- Then the distribution of heat is found from the inverse Fourier transform

$$P_t(Q) = \frac{1}{2\,\pi} \int e^{-i\,r\,Q}\, F_t(r)\, \text{dr}$$

Goal of this work

- To study $P_t(Q)$ for a many-body model.
  - Observe the transition *micro* → *meso* → *macro*.
  - Study the influence of a quantum phase transition.

GTL, D. Karevski, *PRE* **93** 032122 (2016)

The XX chain

- We consider two XX chains weakly coupled to each other

$$H_1 = \frac{h}{2} \sum_{i=1}^{L} \sigma_i^z - \frac{1}{2} \sum_{i=1}^{L-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)$$

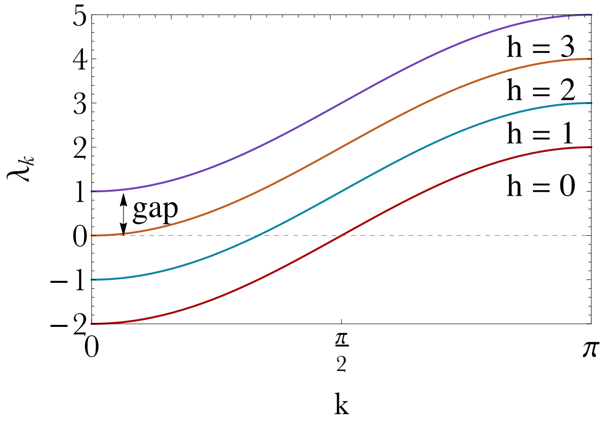
$$H_2 = \frac{h}{2} \sum_{i=L+1}^{2L} \sigma_i^z - \frac{1}{2} \sum_{i=L+1}^{2L-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)$$

$$V = \frac{g_0}{2} (\sigma_L^x \sigma_{L+1}^x + \sigma_L^y \sigma_{L+1}^y)$$

- Each chain can be individually diagonalized with a Jordan-Wigner + sine transform

$$H_1 = \sum_k \lambda_k a_k^\dagger a_k$$
$$H_2 = \sum_k \lambda_k b_k^\dagger b_k$$
$$\lambda_k = h - 2\cos(k)$$

  - Here a_k and b_k are Fermionic operators.
- The chains undergo a quantum phase transition at $h_c = 2$.
  - A gap opens in the excitation spectrum.



This model allows numerically exact solutions

- The interaction potential becomes

$$V = \sum_{k,\,q} G_{k,q}\left(a_k^\dagger\, b_q + b_q^\dagger\, a_k\right),$$

$$G_{k,q} = g \sin(L\,k)\sin(q) \qquad\qquad g = \frac{2\,g_0}{L+1}$$

- The evolution after $t = 0$ will be unitary with

$$H = \sum_k \lambda_k\left(a_k^\dagger\, a_k + b_k^\dagger\, b_k\right) + \sum_{k,\,q} G_{k,q}\left(a_k^\dagger\, b_q + b_q^\dagger\, a_k\right)$$

  - The Hamiltonian is quadratic.
  - Time evolution is entirely determined by the covariance matrix (in momentum space):

$$\theta_{k,q} = \langle c_k^\dagger\, c_q\rangle \quad \text{where } c \in \{a,\, b\}$$

  - Or in position space

$$\theta_{i,j} = \langle c_i^\dagger\, c_j\rangle$$

  - They satisfy

$$\frac{\mathrm{d}\theta}{\mathrm{dt}} = i\,[W,\,\theta], \qquad W = \text{some matrix}$$

- Example: one fermion starting on the left.

t

```
MatrixPlot[Abs[θsol7[121.136]], ImageSize → 300]
```

Analytical calculations

- The exact Hamiltonian is

$$H = \sum_k \lambda_k \left(a_k^\dagger a_k + b_k^\dagger b_k\right) + \sum_{k,q} G_{k,q}\left(a_k^\dagger b_q + b_q^\dagger a_k\right)$$

$$G_{k,q} = g \sin(L\,k) \sin(q) \qquad\qquad g = \frac{2\,g_0}{L+1}$$

- The 2nd term is naturally weak since it depends $\sim 1/L$.
  - V is a “surface” term
  - H_1 and H_2 are “volume” terms.
- We may treat V as a perturbation. We find:

$$H = \sum_k \left\{\lambda_k \left(a_k^\dagger a_k + b_k^\dagger b_k\right) + G_k\left(a_k^\dagger b_k + b_k^\dagger a_k\right)\right\}$$

$$G_k = g \sin(L\,k) \sin(k) = (\pm 1)\, g \sin^2 k$$

- The entire problem factors into L independent subspaces, one for each pair of normal modes (a_k, b_k).
  - Only modes with the same momentum can exchange energy.

Characteristic function

- The heat exchanged by each mode are independent random variables.

$$Q = \sum_k Q_k$$

(like a random walk)

- Charac. Func. $F_t(r)$ will factor into the product of L independent functions

$$F_t(r) = \prod_k F_t(r, k)$$

$$F_t(r, k) = p_k^0 + e^{i r \lambda_k} p_k^+ + e^{-i r \lambda_k} p_k^-$$

- During the evolution, there are only 3 possible events for Q_k:

$$p_k^+ = n_k^2 \left(1 - n_k^1\right) \sin^2(G_k t)$$

$$p_k^- = n_k^1 \left(1 - n_k^2\right) \sin^2(G_k t)$$

$$p_k^0 = 1 - p_k^+ - p_k^-$$

$$n_k^{1,2} = \left(e^{\lambda_k / T_{1,2}} + 1\right)^{-1}$$

- These probabilities individually satisfy the fluctuation theorem

$$\frac{p_k^+}{p_k^-} = e^{\Delta\beta \lambda_k}$$

Average heat

- The average heat is

$$\langle Q \rangle_t = \sum_k \lambda_k (p_k^+ - p_k^-) = \sum_k \lambda_k \left(n_k^2 - n_k^1\right) \sin^2(G_k t)$$

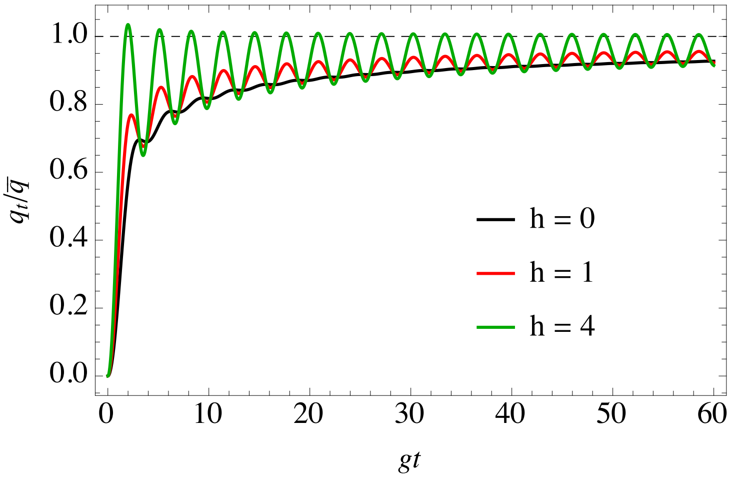
- If we set $T_2 = T$ and $T_1 = T + \Delta T$ and convert the sum to an integral (thermodynamic limit), we get

$$\langle Q \rangle_t = \frac{\Delta T\, L}{\pi} \int_0^\pi c_k(T) \sin^2\!\left(g\, t \sin^2 k\right) \mathrm{dk}$$

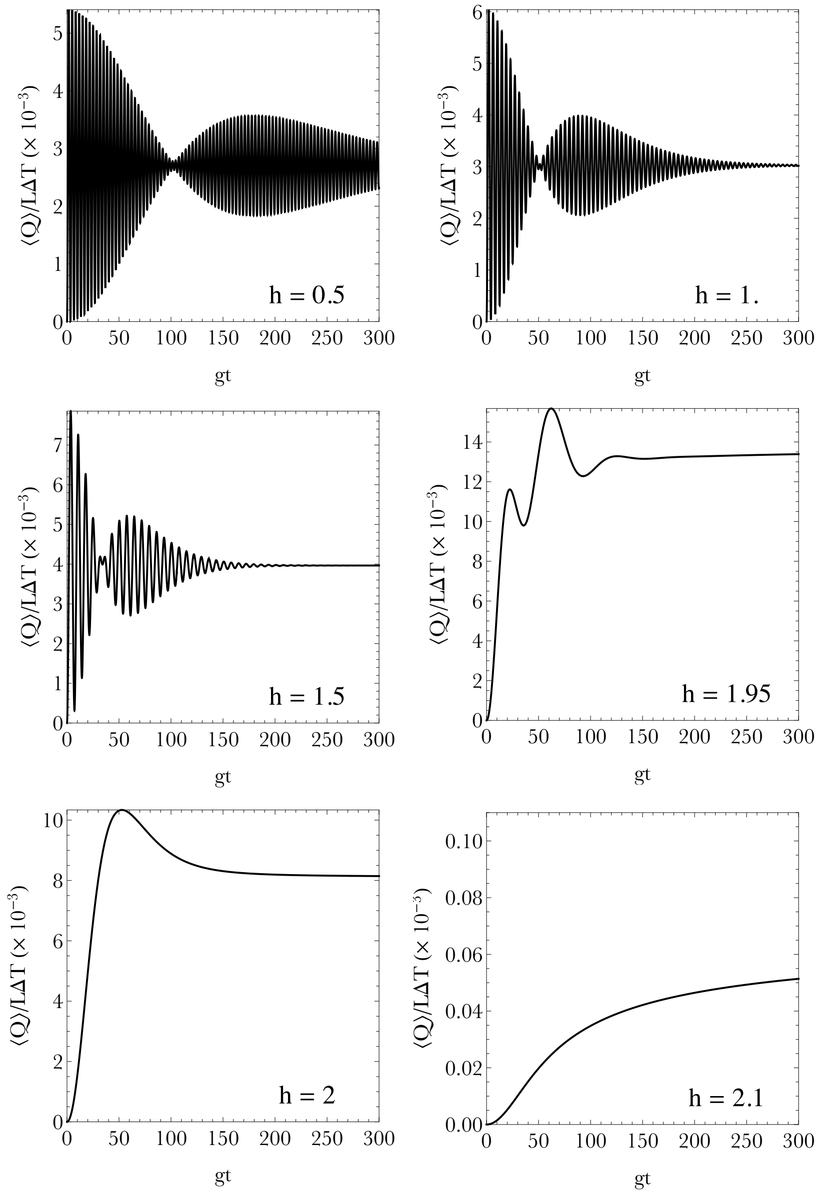
$$c_k(T) = \lambda_k \frac{\partial \bar{n}_k}{\partial T} = \text{specific heat of each mode}$$

- At high temperatures we obtain a somewhat uninteresting behavior:

High temp: T = 10



- At low temperatures we see a strong influence of the quantum phase transition.



- The average heat tends to the thermodynamic value

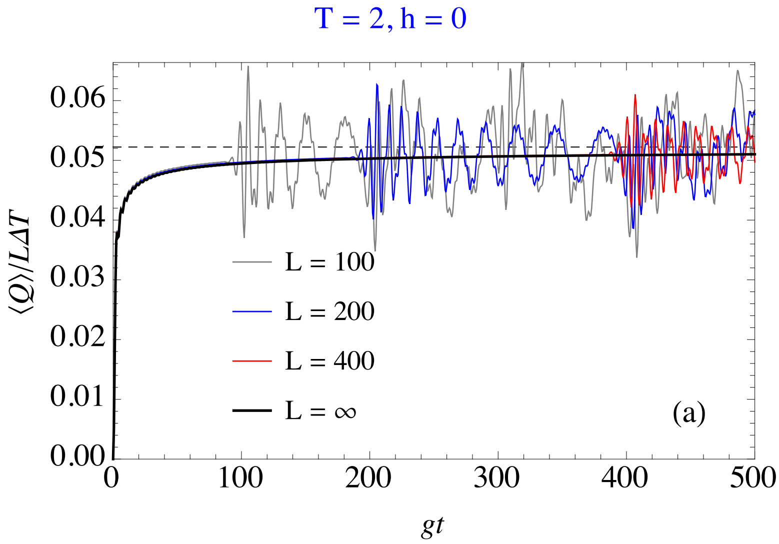
$$\lim_{t \to \infty} \langle Q \rangle_t = Q_{\text{thermo}} = \frac{U(T_2) - U(T_1)}{2}$$

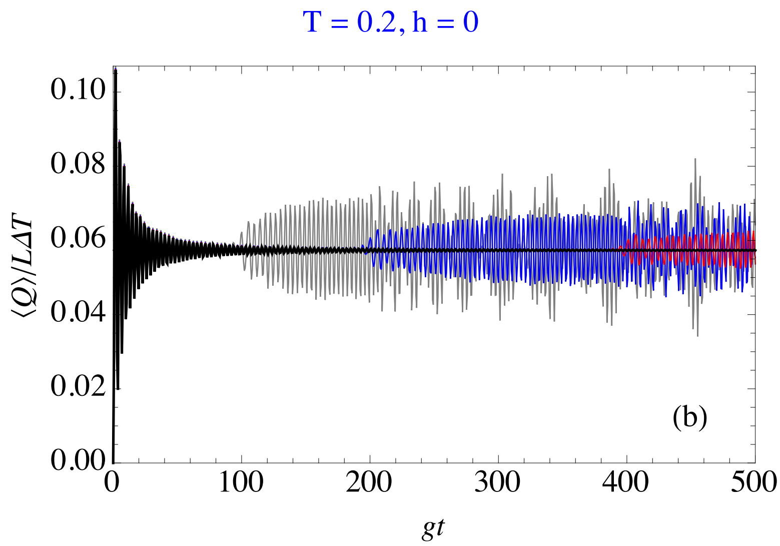
- But this does not mean that the system's density matrix will reach equilibrium.
  - It is widely expected for integrable systems that the system will tend to a generalized Gibbs state.

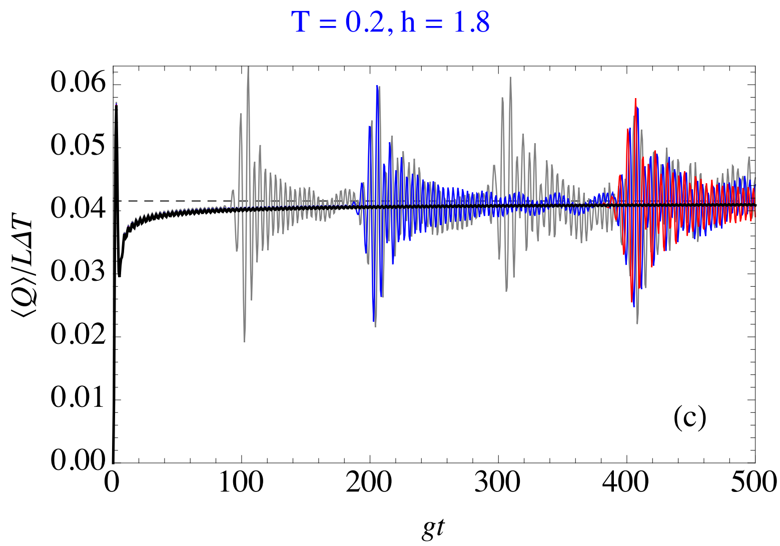
see: M. Collura & D. Karevski, *PRB*, **89**(21) (2014)

Finite size effects

- When the size of the system is fininte, there will be intereference from wavepackets that reflect at the boundaries of the sample.


T = 2, h = 0
⟨Q⟩/LΔT
gt
L = 100
L = 200
L = 400
L = ∞
(a)


T = 0.2, h = 0
⟨Q⟩/LΔT
gt
(b)

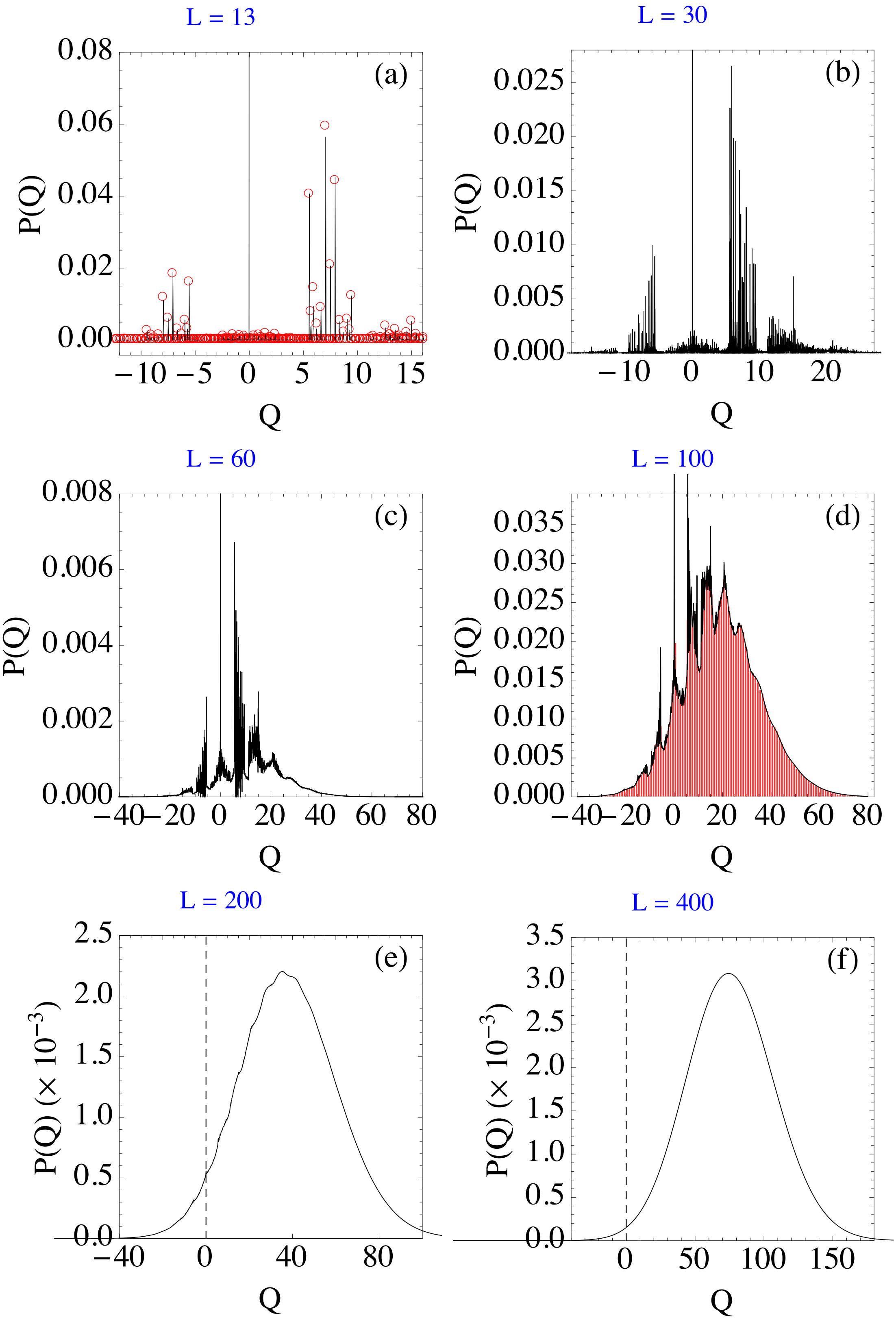

T = 0.2, h = 1.8
⟨Q⟩/LΔT
gt
(c)

The distribution of heat as a function of time

- We can find $P_t(Q)$ from an inverse Fourier transform of the characteristic functio

$$F_t(r) = \prod_k \{ p_k^0 + e^{i r \lambda_k} p_k^+ + e^{-i r \lambda_k} p_k^- \}$$

- This can be done using the FFT algorithm.


L = 13
(a)
P(Q)
Q
L = 30
(b)
P(Q)
Q
L = 60
(c)
P(Q)
Q
L = 100
(d)
P(Q)
Q
L = 200
(e)
P(Q) (× 10^−3)
Q
L = 400
(f)
P(Q) (× 10^−3)
Q

Influence of finite size effects on the time evolution

i

```
Show[frames1[[197]], ImageSize → 400]
```

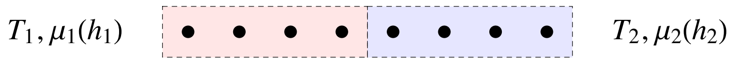
Instabilities due to reflections at the boundaries

i

```
Show[frames2⟦614⟧, ImageSize → 400]
```

Next step

- Couple the two halves to Lindblad baths



- In collaboration with Pedro Guimarães and Mario de Oliveira (USP).
  - Was discussed in poster session, 05/09.

P. H. Guimarães, GTL and M. J. de Oliveira, *submitted for publication* (2016)

Thank you all for your attention.

and thanks FAPESP for the financial support.

GTL, D. Karevski, *PRE* **93** 032122 (2016)

Particle and energy current

- The particle and energy currents in the steady-state and in the thermodynamic limit will be

$$\mathcal{J}_N = \frac{4\, g_0^2}{\pi} \int_0^{\pi} \sin^3 k \left(n_k^1 - n_k^2\right) \mathrm{dk}$$

$$\mathcal{J}_E = \frac{4\, g_0^2}{\pi} \int_0^{\pi} \lambda_k \sin^3 k \left(n_k^1 - n_k^2\right) \mathrm{dk}$$

- Now the currents depend on temperatures $T_{1,2}$ and chemical potentials $\mu_{1,2}$
- Expanding for infinitesimal unbalances, we obtain

$$\mathcal{J}_N = \delta\mu \frac{\partial F}{\partial \mu} + \delta \mathrm{T} \frac{\partial F}{\partial T}, \qquad F = \frac{4\, g_0^2}{\pi} \int n_k \sin^3 k \;\mathrm{dk}$$

$$\mathcal{J}_E = \delta\mu \frac{\partial G}{\partial \mu} + \delta \mathrm{T} \frac{\partial G}{\partial T}, \qquad G = \frac{4\, g_0^2}{\pi} \int \lambda_k\, n_k \sin^3 k \;\mathrm{dk}$$

```
L
lab[ plμ[160]  plT[160]
     pEμ[160]  pET[160] , L = 160]
```

Onsager reciprocal relations

- The heat flux is defined as

$$\mathcal{J}_Q = \mathcal{J}_E - \mu \mathcal{J}_N$$

- We found that $\mathcal{J}_N$ and $\mathcal{J}_Q$ can be put in Onsager's canonical form

$$\begin{pmatrix} \mathcal{J}_N \\ \mathcal{J}_Q \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} (\delta\mu)/T \\ -\delta(1/T) \end{pmatrix}$$

- The Onsanger coefficients are all obtained analytically:

$$L_{11} = T \frac{\partial F}{\partial \mu} \qquad L_{12} = T^2 \frac{\partial F}{\partial T}$$

$$L_{21} = T\left(\frac{\partial G}{\partial \mu} - \mu \frac{\partial F}{\partial \mu}\right) \qquad L_{22} = T^2\left(\frac{\partial G}{\partial T} - \mu \frac{\partial F}{\partial T}\right)$$

- Moreover, they satisfy the reciprocal relations

$$L_{21} = L_{12}$$

$$L_{11} L_{22} - L_{21} L_{12} \geq 0$$

- We attribute this to our choice of quantum master equation, which satisfies detailed balance.

P. H. Guimarães, GTL, M. J. de Oliveira, *submitted for publication (2016)*.

Funções auxiliares

```
(*Show[Import["","Image",ImageSize→600]]*)

SetDirectory[NotebookDirectory[]]
<< "LinLib`";
load[filename_, size_] := Show[Import[filename], ImageSize → Scaled[size]];
lab[img_, lbl_] :=
  Labeled[img, lbl, Top, LabelStyle → {FontFamily → "Times", 26, Blue}];

SetOptions[Plot,
  Frame → True,
  Axes → False,
  BaseStyle → {FontFamily → "Times", 20},
  ImageSize → 400];

SetOptions[InputNotebook[],
 DefaultNewCellStyle → "Item",
 ShowCellLabel → "False",
 CellGrouping → Manual,
 FontFamily → "Times",
 DefaultNewCellStyle → {"Text", FontFamily → "Times"},
 BaseStyle → {FontFamily → "Times"},
 MultiLetterItalics → False,
 SingleLetterItalics → Automatic
]
/Users/gtlandi/Dropbox/Presentations/2016_09 - Encontrao
Clear[ℐ];
ℐ[La_, γ_, k_, t_: 1] := Module[{a = γ^2 + t^2 Sin[k]^2, b = 2 γ t Cos[k], qr},
  qr = Range[π/(La + 1), π La/(La + 1), π/(La + 1)];
  Sin[k]^2/(La + 1) Sum[Sin[q]^2/(γ^2 + t^2 (Cos[k] - Cos[q])^2), {q, qr}]
 ]


Clear[ℐtl];
ℐtl[γ_, k_, t_: 1] := Module[{a = γ^2 + t^2 Sin[k]^2, b = 2 γ t Cos[k]},
  1/t^2 (1/(γ Sqrt[2]) Sqrt[a + Sqrt[a^2 + b^2]] - 1) Sin[k]^2
 ]


Clear[J];
J[La_, {μa_, μc_}, {Ta_, Tc_}, γ_: 1] := Module[{mr, e, n},

  mr = Range[π/(La + 1), π La/(La + 1), π/(La + 1)];
  e[k_] := -2 Cos[k];
  n[μ_, T_, k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k] - μ)/T] + 1)];
```

```
  4 γ (*g²*)
  ---------- Total@Flatten@Table[(Sin[k]² Sin[q]² (m[μa, Ta, k] - m[μc, Tc, k])) /
  (La + 1)²
        (γ² + (Cos[k] - Cos[q])²)   , {k, mr}, {q, mr}]
 ];

Clear[Jtl];
Jtl[{μa_, μc_}, {Ta_, Tc_}, γ_: 1] := Module[{mr, e, m, a, b, int},

  e[k_] := -2 Cos[k];
  m[μ_, T_, k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k]-μ)/T] + 1)];

  a = γ² + Sin[k]²;
  b = 2 γ Cos[k];
  (*int =( -1  + 1/(2γ) (Sqrt[a+ⅈ b] + Sqrt[a-ⅈ b]))Sin[k]²;*)
  int = (1/(γ Sqrt[2]) Sqrt[a + Sqrt[a² + b²]] - 1) Sin[k]²;

  4 γ (*g²*)
  ---------- NIntegrate[(m[μa, Ta, k] - m[μc, Tc, k]) (int), {k, 0, π}]
      π
 ];

Clear[F];
F[La_, μ_, T_, γ_: 1] := Module[{mr, e, m},

  mr = Range[π/(La + 1), π La/(La + 1), π/(La + 1)];
  e[k_] := -2 Cos[k];
  m[k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k]-μ)/T] + 1)] ;
  4 γ (*g²*)                        Sin[k]² Sin[q]² (m[k])
  ---------- Total@Flatten@Table[ --------------------------  , {k, mr}, {q, mr}]
  (La + 1)²                       γ² + (Cos[k] - Cos[q])²
 ];

Clear[Ftl];
Ftl[μ_, T_, γ_: 1] := Module[{mr, e, m, a, b, int},

  e[k_] := -2 Cos[k];
  m[k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k]-μ)/T] + 1)];

  a = γ² + Sin[k]²;
  b = 2 γ Cos[k];
  int = (1/(γ Sqrt[2]) Sqrt[a + Sqrt[a² + b²]] - 1) Sin[k]²;

  4 γ (*g²*)
  ---------- NIntegrate[(m[k]) (int), {k, 0, π}] // Chop
      π
```

```
  ];

ℐEtl[γ_, k_, t_: 1] := Module[{F, a, b},

   a = γ^2 + t^2 Sin[k]^2;
   b = 2 γ t Cos[k];

   F = 4/t Cos[k] - Sqrt[2]/(γ t^2) (t Cos[k] Sqrt[Sqrt[a^2 + b^2] + a] + γ Cos[k]/Sqrt[Cos[k]^2] Sqrt[Sqrt[a^2 + b^2] - a]);

   (*{-2t  Cos[k] ℐtl[γ,k,t] , Sin[k]^2F,-2t  Cos[k] ℐtl[γ,k,t] + Sin[k]^2F}*)
   -2 t Cos[k] ℐtl[γ, k, t] + Sin[k]^2 F
  ];
Clear[JE];
JE[La_, {μa_, μc_}, {Ta_, Tc_}, γ_: 1] := Module[{mr, e, n},

   mr = Range[π/(La + 1), π La/(La + 1), π/(La + 1)];
   e[k_] := -2 Cos[k];
   n[μ_, T_, k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k] - μ)/T] + 1)];
   (2 γ (*g^2*))/(La + 1)^2
    Total@Flatten@Table[(Sin[k]^2 Sin[q]^2 (n[μa, Ta, k] - n[μc, Tc, k]) (e[k] + e[q])) /
       (γ^2 + (Cos[k] - Cos[q])^2)  , {k, mr}, {q, mr}]
  ];

Clear[JEtl];
JEtl[{μa_, μc_}, {Ta_, Tc_}, γ_: 1] := Module[{mr, e, n, ie},

   e[k_] := -2 Cos[k];
   n[μ_, T_, k_] := If[T == 0, HeavisideTheta[μ - e[k]], 1/(Exp[(e[k] - μ)/T] + 1)];
   ie = ℐEtl[γ, k];

   (2 γ (*g^2*))/π NIntegrate[ie (n[μa, Ta, k] - n[μc, Tc, k]) , {k, 0, π}]
  ];

LLrange = {1, 4, 10, 20, 40, 60, 80, 100, 120, 160};
δμ = 0.001;
TT = 0.02;
Jtl =
  Chop@Quiet@Table[{μ, Jtl[{μ + δμ, μ}, {TT, TT}] / δμ}, {μ, linspace[-3, 3, 100]}];

Do[
 plμ[LL] = Show[
   Plot[Evaluate[{J[LL, {μ + δμ/2, μ - δμ/2}, {TT, TT}] / δμ}], {μ, -3, 3},
    PlotRange → {0, All},
```

```
      AspectRatio → 1,
      ImagePadding → {{50, 10}, {60, 10}},
      FrameLabel → {"μ", None},
      PlotLabel → "JN,μ",
      BaseStyle → {FontFamily → "Times", 20},
      ImageSize → 260,
      PlotStyle → Black,
      Frame → True,
      PlotStyle → Directive[Black]
     ],
     ListLinePlot[Jtl, PlotStyle → Directive[Red, Dashed]]
    ]; , {LL, LLrange}]

δT = 0.001;
TT = 0.02;
JtlT =
  Chop@Quiet@Table[{μ, 𝕁tl[{μ, μ}, {TT + δT, TT}] / δT}, {μ, linspace[-3, 3, 100]}];

Do[
 plT[LL] = Show[
     Plot[Evaluate[{𝕁[LL, {μ, μ}, {TT + δT/2, TT - δT/2}] / δT}], {μ, -3, 3},
      PlotRange → All,
      AspectRatio → 1,
      ImagePadding → {{50, 10}, {60, 10}},
      FrameLabel → {"μ", None},
      PlotLabel → "JN,T",
      BaseStyle → {FontFamily → "Times", 20},
      ImageSize → 260,
      PlotStyle → Black,
      Frame → True
     ],
     ListLinePlot[JtlT, PlotStyle → Directive[Red, Dashed]]
    ]; , {LL, LLrange}]


δμ = 0.001;
TT = 0.02;
JEtl =
  Chop@Quiet@Table[{μ, 𝕁Etl[{μ + δμ, μ}, {TT, TT}] / δμ}, {μ, linspace[-3, 3, 100]}];

Do[
 pEμ[LL] = Show[
     Plot[Evaluate[{𝕁E[LL, {μ + δμ/2, μ - δμ/2}, {TT, TT}] / δμ}], {μ, -3, 3},
      PlotRange → All,
      AspectRatio → 1,
      ImagePadding → {{50, 10}, {60, 10}},
      FrameLabel → {"μ", None},
      PlotLabel → "JE,μ",
      BaseStyle → {FontFamily → "Times", 20},
      ImageSize → 260,
      PlotStyle → Black,
      Frame → True,
      PlotStyle → Directive[Black]
```

```
    ],
    ListLinePlot[JEtl, PlotStyle → Directive[Red, Dashed]]
   ]; , {LL, LLrange}]


δT = 0.001;
TT = 0.02;
JEtlT =
  Chop@Quiet@Table[{μ, JEtl[{μ, μ}, {TT + δT, TT}] / δT}, {μ, linspace[-3, 3, 100]}];

Do[
 pET[LL] = Show[
    Plot[Evaluate[{JE[LL, {μ, μ}, {TT + δT/2, TT - δT/2}] / δT}], {μ, -3, 3},
     PlotRange → All,
     AspectRatio → 1,
     ImagePadding → {{50, 10}, {60, 10}},
     FrameLabel → {"μ", None},
     PlotLabel → "J_E,T",
     BaseStyle → {FontFamily → "Times", 20},
     ImageSize → 260,
     PlotStyle → Black,
     Frame → True,
     PlotStyle → Directive[Black]
    ],
    ListLinePlot[JEtlT, PlotStyle → Directive[Red, Dashed]]
   ]; , {LL, LLrange}]
DumpSave["plots.mx", {plμ, plT, pEμ, pET}];
LLrange = {1, 4, 10, 20, 40, 60, 80, 100, 120, 160};
<< "plots.mx";
fnames1 = FileNames["*tiff", "Frames_1"];
frames1 = Import /@ fnames1;
fnames2 = FileNames["*tiff", "Frames_2"];
frames2 = Import /@ fnames2;
DumpSave["θsol.mx", θsol7];
<< "θsol.mx";
```

```
Clear[AveQ];
AveQ[L_, h_, T_, t_] := Module[{λ, k, s},

    λ = h - 2 Cos[k];
    s = If[t === ∞, 1/2, Sin[t Sin[k]^2]^2];
    If[L === ∞,
     1/π NIntegrate[(λ/T)^2 ⅇ^(λ/T)/(ⅇ^(λ/T) + 1)^2 s,
       {k, 0, π}, Method -> {Automatic, "SymbolicProcessing" -> False}],
     1/L Total@Table[(λ/T)^2 ⅇ^(λ/T)/(ⅇ^(λ/T) + 1)^2 s, {k, π/(L + 1), L π/(L + 1), π/(L + 1)}]
    ]
   ];
```