Open quantum systems applied to condensed matter physics

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XXXIX Congresso Paulo Leal Ferreira
October 26th, 2016

Motivation: from *micro* to *macro*

- The main goal of condesed matter physics is to understand the *macroscopic properties of matter.* e.g.,
  - The conductivity of a metal.
  - The specific heat of a gas.
  - The viscosity of a fluid.
  - The magnetization of a piece of iron.
  - etc.
- Long ago we learned that, in order to do that, we must look at the *microscopic world.*
  - We now understand these properties as being **emergent properties** of the underlying microscopic interactions.
- Thus, we must learn how to obtain macroscopic results from a microscopic theory.
- In general that is a hard question:
  - The micro-world has $\sim 10^{23}$ particles, all interacting like crazy (Think, for a second, about how complicated a glass of water is).
- However, the great hero *Josiah Willard Gibbs,* continuing the work started by Maxwell and Boltzmann, found an answer for one specific class of systems: those in *thermal equilibrium.*
  - He found that the probability of finding the system at a quantum state $|n\rangle$ is

$$P_n = \frac{e^{-\beta E_n}}{Z}, \quad \beta = \frac{1}{k_B T}$$

- This formula represents a **bridge** between the two worlds:
  - It tells you how to compute macroscopic properties from knowledge of the microscopic energies.
- According to Robert Millikan,

" Gibbs did to statistical mechanics and thermodynamics what Laplace did for celestial mechanics and Maxwell for eletromagnetism."

- Please note: the Gibbs formula is **atemporal**: it does not matter how we arrived at equilibrium, all that matters is that we are there.

Example

nature physics
LETTERS
PUBLISHED ONLINE: 10 JANUARY 2012 | DOI: 10.1038/NPHYS2183

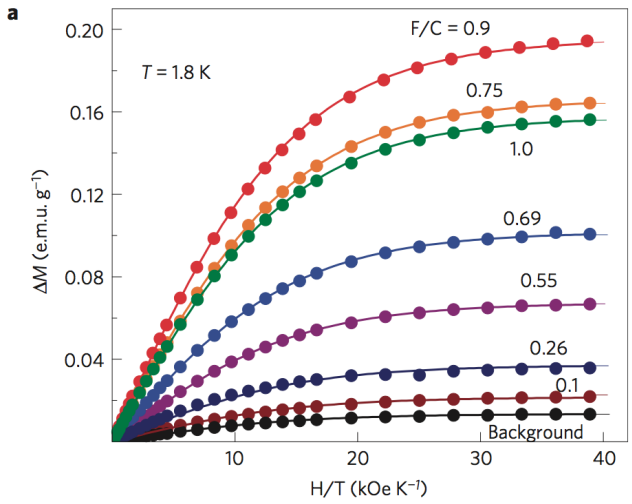
Spin-half paramagnetism in graphene induced by point defects

R. R. Nair[1], M. Sepioni[1], I-Ling Tsai[1], O. Lehtinen[2], J. Keinonen[2], A. V. Krasheninnikov[2,3], T. Thomson[1], A. K. Geim[1] and I. V. Grigorieva[1]*

- Prediction of the theory (this is a calculation any undergraduate student can do)

$$m = \tanh\left(\frac{\mu \mathrm{H}}{k_B \mathrm{T}}\right)$$

- Perfect agreement with experiment ($F/C := \mu$):



The Gibbs formula does not solve all problems, but... it tells you where to start.

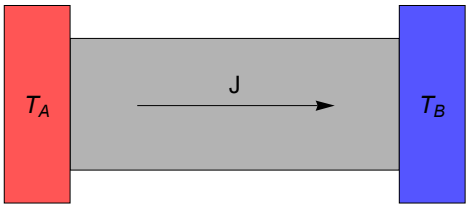
- All the information about the liquid-gas transition is contained within this integral.

$$Z = \int \exp\left[-\frac{1}{k_B T} \sum_{\text{pairs}} V(r_{i,j})\right] d^3 r_1 \, d^3 r_2 \ldots d^3 r_N$$

- We have no idea how to compute it, but that is not surprising:
  - The integral is difficult because *nature* is difficult.
- But at least we know *what* we should do.
- And now we can look for alternative ways to tackle the problem:
  - Monte Carlo, cluster expansions, mean-field theories, etc.

Non-equilibrium systems

- Now consider a physical system that is maintained in contact with two reservoirs at different temperatures.



- This system will never reach equilibrium, because the warmer reservoir will be constantly giving out heat to the colder reservoir.
- **NESS**: "Non-equilibrium steady-state".
  - Its a "steady-state" because things are no longer changing in time.
  - But its not thermal equilibrium.

What are the rules governing non-equilibrium systems?

What is the analog of the Gibbs formula for non-equilibrium systems?

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What is the analog of the Gibbs formula for non-equilibrium systems?

We have no idea!

- We do *not* have a general framework for handling non-equilibrium systems.
- If we want to study the NESS, we must go back to the fundamental laws (Newton, Schrödinger).
  - *Even though we are interested in something atemporal, we need to include the full dynamics!*

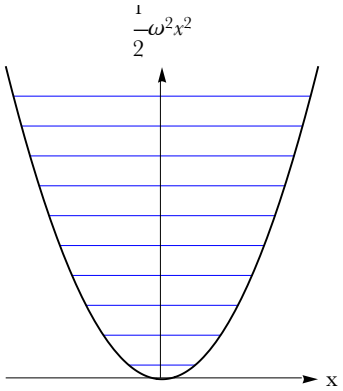
- There is no unified framework for dealing with non-equilibrium physics.
- Classical systems:
  - Stochastic processes: Langevin/Fokker-Planck equation
  - Molecular dynamics.
- Quantum systems:
  - Green-Kubo (linear response)
  - Landauer-Büttiker
  - Boltzmann equation.

My research interests: Lindblad dynamics

- My main research interest is in building a consistent framework to study (mostly) the NESS in condensed matter systems.
- And I do that by applying techniques initially developed in atomic physics and quantum optics.
  - In particular, today I want to focus on **Lindblad dynamics**
- This has applications in
  - Electron transport
  - Heat transport
  - Spin transport (magnon currents).

Motivation: the quantum harmonic oscillator

- $E_n = \hbar\omega(n + 1/2)$



- The contact with a heat bath will cause transitions between the different energy levels.
- Imagine that QHO = diatomic molecule and Heat Bath = Electromagnetic field.
  - The molecule can absorb and emit photons.
- The bath determines the average energy level $\overline{N}$.

t

$\overline{N}$ 0 0.5 1 2 4

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Lindblad dynamics

- Idea: to describe the contact with a bath in a fully quantum mechanical way.
- Extend von Neumann's equation with an additional term:

$$\frac{d\rho}{dt} = -i[H, \rho] + \mathcal{D}(\rho)$$

- $\mathcal{D}(\rho)$ is called the *dissipator* and describes the contact with the heat bath.
  - Must be *completely positive trace preserving*.
    - $\mathrm{tr}(\mathcal{D}(\rho)) = 0$
- Main work of Lindblad

$$\mathcal{D}(\rho) = \sum_\alpha \left(L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \{L_\alpha^\dagger L_\alpha, \rho\} \right)$$

- Constructing the dissipator may be a difficult task.
- We will discuss here two approaches:
  - Phenomenological dissipators.
  - Microscopic derivations.

The most famous example: the quantum harmonic oscillator

- The dissipator for a quantum harmonic oscillator with $H = \omega\, a^\dagger a$ is

$$\mathcal{D}(\rho) = \gamma(1+\bar{n})\left[a\,\rho\,a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right] + \gamma\,\bar{n}\left[a^\dagger\,\rho\,a - \frac{1}{2}\{a\,a^\dagger, \rho\}\right]$$

  where γ = *coupling strength to the bath* and

$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}$$

- This dissipator correctly thermalizes the system: it has only one fixed point:

$$\mathcal{D}\left(e^{-\beta H}\right) = 0$$

- It also satisfies **detailed balance**

$$\frac{\gamma(1+\bar{n})}{\gamma\,\bar{n}} = e^{\beta\,\omega}$$

- This is a physical property, related to the fact that the underlying dynamics (Schrödinger's equation for the system+bath) is time-reversal invariant.
- This dissipator produces

$$\frac{\mathrm{d}\,\langle a^\dagger a\rangle}{\mathrm{dt}} = \gamma(\bar{n} - \langle a^\dagger a\rangle)$$

- The average occupation of the oscillator relaxes toward its equilibrium value $\langle a^\dagger a\rangle_\infty = \bar{n}$.

Two coupled oscillators

- Now consider two coupled oscillators, with bosonic operators a and b. The Hamiltonian is taken to be

$$H = \omega(a^\dagger a + b^\dagger b) - g(a^\dagger b + b^\dagger a)$$

- Each system is now assumed to be connected to a dissipator, just like before:

$$\mathcal{D}_a(\rho) = \gamma(1+\bar{n}_a)\left[a\,\rho\,a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right] + \gamma\,\bar{n}_a\left[a^\dagger\,\rho\,a - \frac{1}{2}\{a\,a^\dagger, \rho\}\right]$$

$$\mathcal{D}_b(\rho) = \gamma(1+\bar{n}_b)\left[b\,\rho\,b^\dagger - \frac{1}{2}\{b^\dagger b, \rho\}\right] + \gamma\,\bar{n}_b\left[b^\dagger\,\rho\,b - \frac{1}{2}\{b\,b^\dagger, \rho\}\right]$$

- The complete dynamics of the system will then be governed by

$$\frac{d\rho}{dt} = -i[H, \rho] + \mathcal{D}_a(\rho) + \mathcal{D}_b(\rho)$$

- First problem: what should we take for $\bar{n}_{a,b}$? Let's leave them generic for now.
- Suppose first that the two baths are at the same temperature ($\bar{n}_a = \bar{n}_b$). Even in this case, these dissipators no longer take the system correctly to equilibrium!
  - Thermal equilibrium is $\rho = e^{-\beta H}$. But now the two oscillators interact so we cannot factor $e^{-\beta H}$ as a product.
- Moral of the story
  - If you want the dissipators to model Heat baths, then their shape will depend on H
    - Change any tiny detail on H and you should change your $\mathcal{D}$s
- The example above is what I call *"phenomenological dissipators"* or *"local dissipators"*
  - They should give reasonable answers when the two oscillators are weakly coupled.
  - Note: we no longer can define T_a and T_b. But we can still play with $\bar{n}_a$ and $\bar{n}_b$.

- Let's examine the NESS of this problem. We find

$$\langle a^\dagger a\rangle = \frac{\bar{n}_a + \bar{n}_b}{2} + \frac{\gamma^2}{\gamma^2 + g^2}\,\frac{(\bar{n}_a - \bar{n}_b)}{2}$$

$$\langle b^\dagger b\rangle = \frac{\bar{n}_a + \bar{n}_b}{2} - \frac{\gamma^2}{\gamma^2 + g^2}\,\frac{(\bar{n}_a - \bar{n}_b)}{2}$$

$$\langle a^\dagger b\rangle = \frac{2\,i\,\gamma\,g}{\gamma^2 + g^2}\,\frac{(\bar{n}_a - \bar{n}_b)}{2}$$

- The two oscillators are correlated: $\langle a^\dagger b\rangle \neq 0$.
  - This produces a flow of energy

$$\mathcal{J} \propto \langle a^\dagger b\rangle = \frac{\omega\,\gamma\,g}{\gamma^2 + g^2}\,\frac{(\bar{n}_a - \bar{n}_b)}{2}$$

- There will continue to be a flux as long as the bath occupations are different.
- We will come back to this problem later and compare with a microscopic model.
- Fun fact: this result for the current is actually the same for a 1D chain of N oscillators.
  - This defines a ballistic current (independent of size).
  - It is related to the fact that in these models the excitations propagate like waves.

Spin 1/2 chains

- Now I want to talk about spin chains.
- Consider a single spin 1/2 particle with $H = -\mu B \sigma_z$
- A local dissipator correctly thermalizing this particle is

$$\mathcal{D}(\rho) = \frac{\gamma}{2}(1+f)\left[\sigma_+ \rho \sigma_- - \frac{1}{2}\{\sigma_- \sigma_+, \rho\}\right] + \frac{\gamma}{2}(1-f)\left[\sigma_- \rho \sigma_+ - \frac{1}{2}\{\sigma_+ \sigma_-, \rho\}\right]$$

where

$$f = \tanh\left(\frac{\mu B}{k_B T}\right)$$

- This dissipator takes the system to the correct thermal state: $\mathcal{D}\left(e^{\beta \mu B \sigma_z}\right) = 0$.
- Moreover, it again satisfies detailed balance

$$\frac{\gamma(1+f)}{\gamma(1-f)} = e^{2\beta\mu B}$$

Quantum spin chains

- Now we apply this to a 1D quantum XXZ spin chain.

$$H = \frac{1}{2}\sum_{i=1}^{N-1}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \Delta\,\sigma_i^z\,\sigma_{i+1}^z)$$

- When $\Delta = 0$ (XX chain) the model is exactly solvable.
  - It maps into a model of free fermions.
- The Δ-term can be seen as an interaction between quasi-particles
- We use the local dissipators

$$\mathcal{D}_i(\rho) = \frac{\gamma}{2}(1+f_i)\left[\sigma_i^+\,\rho\,\sigma_i^- - \frac{1}{2}\{\sigma_i^-\,\sigma_i^+,\rho\}\right] + \frac{\gamma}{2}(1-f_i)\left[\sigma_i^-\,\rho\,\sigma_i^+ - \frac{1}{2}\{\sigma_i^+\,\sigma_i^-,\rho\}\right]$$

  with $i = 1$ or N.

- We are interested here in the *spin current*, defined from the continuity equation

$$\frac{\mathrm{d}\langle\sigma_i^z\rangle}{\mathrm{dt}} = \mathcal{J}_{i-1} - \mathcal{J}_i$$

- In this model it becomes

$$\mathcal{J}_i = \langle\sigma_i^x\,\sigma_{i+1}^y - \sigma_i^y\,\sigma_{i+1}^x\rangle$$

- In the NESS $\frac{\mathrm{d}\langle\sigma_i^z\rangle}{\mathrm{dt}} = 0 \longrightarrow \mathcal{J}_i = \mathcal{J}$ for all sites (the current is uniform through the chain).

XX chain (Δ =0)

- In the case of an XX chain the current becomes simply

$$\mathcal{J} = \frac{\gamma}{1+\gamma^2}\,\frac{(f_1 - f_N)}{2}$$

- It is almost identical to the case of the quantum harmonic oscillator.

  D. Karevski and P. Platini, *Phys. Rev. Lett.* **102**, 207207 (2009)
  GTL and D. Karevski, *Phys. Rev. E.* **93**, 032122 (2016)

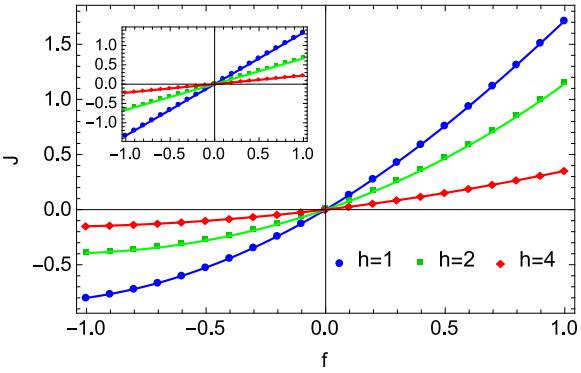
- Interpretation: the XX chain behaves like free fermions and the spin current is *ballistic*.
  - You inject particles on the left and collect on the right.
  - The particles just travel freely through the chain, so the total current does not depend on the size.

$\Delta \neq 0$: spin rectification

- We have carried out numerical studies of the current under non-uniform fields

$$H = \frac{1}{2}\sum_{i=1}^{\mathcal{N}-1}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta\,\sigma_i^z \sigma_{i+1}^z) + \sum_{i=1}^{\mathcal{N}} h_i \sigma_i^z$$

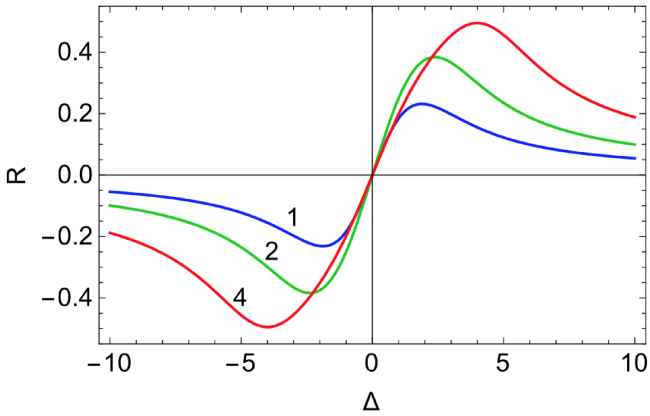
- We choose the field as a linear profile, varying linearly between -h and +h.
- This produces an asymmetry in the problem.



- The spin current is now *rectified*.
  - If you reverse the baths, you reverse the *sign* of the current but the *magnitude* does not necessarily remains the same.
- We may define the *rectification coefficient*

$$R = \frac{\mathcal{J}(f) + \mathcal{J}(-f)}{\mathcal{J}(f) - \mathcal{J}(-f)}$$

- It measures the asymmetry of the current.



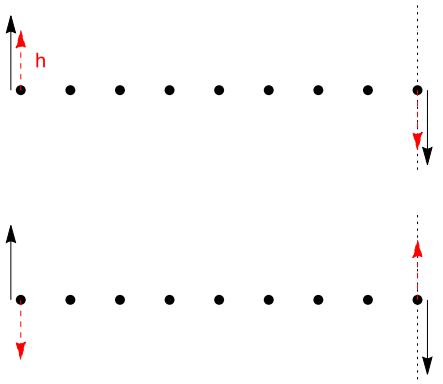
- The Rectification is zero when $\Delta = 0$, even if the system is assymetric.

GTL, *et. al.*, *Phys. Rev. E.* **90**, 042142 (2014)
L. Schuab, *et. al. Phys. Rev. E.* **94** 042122 (2016)

Heisenberg chain (Δ = 1)

- We have been able to obtain an *exact* solution, in the presence also of *boundary fields*.

$$H = \frac{1}{2}\sum_{i=1}^{\mathcal{N}-1}(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y + \sigma_i^z\,\sigma_{i+1}^z) + h(\sigma_1^z - \sigma_{\mathcal{N}}^z)$$



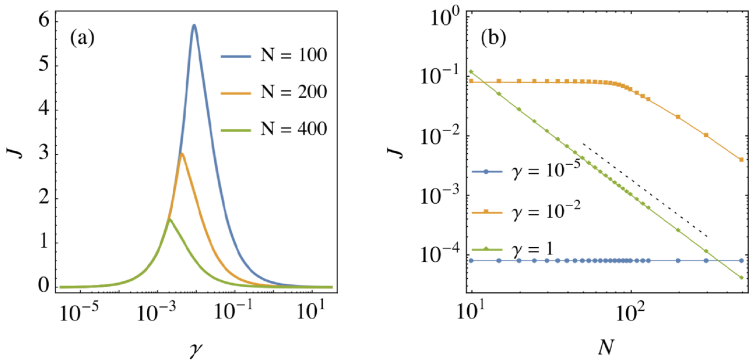
- The solution is based on the idea of **matrix product states**.

$$\rho = S\,S^{\dagger}$$
$$S = \langle 0 \,|\, \Omega_{\otimes}{}^{N} \,|\, 0\rangle$$
$$\Omega = S_z\,\sigma^z + S_+\,\sigma^+ + S_-\,\sigma^-$$

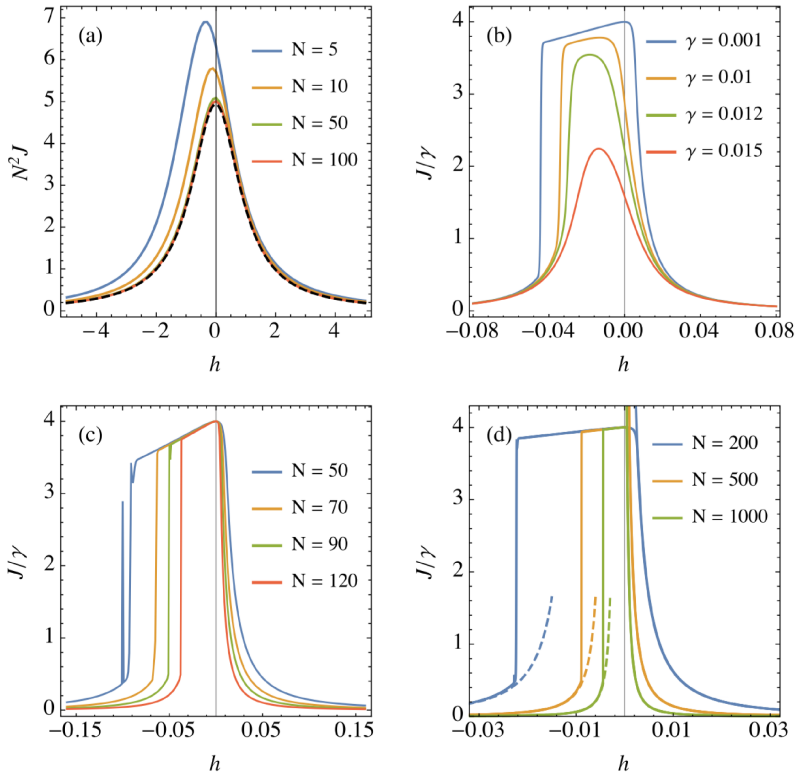
- Each spin site is augmented with an auxiliary space, modeled by operators S_i satisfying the SU(2) algebra.
- This allowed us to find an exact method to compute the current for arbitrary sizes.

D. Karevski, *et. al.*, *Phys. Rev. Lett.* **110**, 047201 (2013)
GTL and D. Karevski, *Phys. Rev. B.* **91**, 174422 (2015)

- Here are the results for h = 0



◆ Here are the results as a function of the boundary field h



"Semi-microscopic theories"

- Now I want to turn to *microscopic derivations*.
- Instead of using a phenomenological dissipator, we start with a *microscopic theory* of the system-bath interaction.
- To warm-up we start with a "semi-microscopic theory".
- Consider again the XX chain: it can be mapped into a fermionic chain

$$\begin{aligned} H &= \frac{1}{2}\sum_{i=1}^{N-1}\left(\sigma_i^x\,\sigma_{i+1}^x + \sigma_i^y\,\sigma_{i+1}^y\right) \\ &= \sum_{i=1}^{N-1}\left(\eta_i^\dagger\,\eta_{i+1} + \eta_{i+1}^\dagger\,\eta_i\right) \end{aligned}$$

- We ask what is the dissipator that would
  - Take this chain to the correct thermal equilibrium state $e^{-\beta H}$ and
  - Do so while satisfying detailed balance
- We can construct this by hand. First we diagonalize the chain in Fourier space

$$c_k = \sum_{i=1}^{N} S_{i,k}\,\eta_i, \qquad S_{i,k} = \sqrt{\frac{2}{N+1}}\,\sin\left(\frac{\pi\,i\,k}{N+1}\right)$$

- The Hamiltonian then becomes

$$H = \sum_k \epsilon_k\,c_k^\dagger\,c_k, \qquad \epsilon_k = \cos(k)$$

- This is now a problem of uncoupled Fermions. We know the dissipator which does the job for a single fermion. It reads

$$\mathcal{D}_k(\rho) = \gamma\,(1-f_k)\left[c_k\,\rho\,c_k^\dagger - \frac{1}{2}\{c_k^\dagger\,c_k,\rho\}\right] + \gamma\,f_k\left[c_k^\dagger\,\rho\,c_k - \frac{1}{2}\{c_k\,c_k^\dagger,\rho\}\right]$$

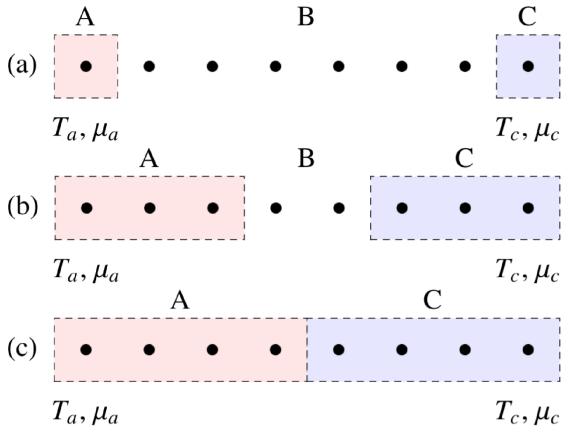
$$f_k = \frac{1}{e^{(\epsilon_k-\mu)/T}+1}$$

- So a way to thermalize the total chain would be through the master equation

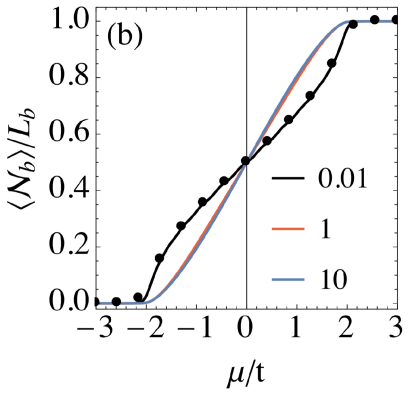
$$\frac{d\rho}{dt} = -i\,[H,\rho] + \sum_k \mathcal{D}_k(\rho)$$

Two coupled chains

- But we want to study transport so we divide a chain in two or three parts and couple the different parts to a bath in this way.



- This problem can be solved exactly if we assume that the different chains are weakly coupled.
- The profile of the inner chain correctly reproduces those of the outside chains when γ is small



Particle and energy current

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

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

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

- They have the structure of the Landauer-Büttiker formula.
  - Both depend on temperatures $T_{1,2}$ and chemical potentials $\mu_{1,2}$
  - Expanding for infinitesimal unbalances, we obtain

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

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

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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

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

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

- Reciprocal relations are related to detailed balance.
  - The original dissipators satisfy detailed balance.
  - But when we couple the two chains, DB is violated.
  - It only continues to hold approximately when γ is small.

P. H. Guimarães, GTL and M. J. de Oliveira, *Phys. Rev. E.* **94** 032139 (2016)

Full microscopic theory for a many-body theory

- We have just been able to construct a full microscopic derivation for a many-body theory.
- We consider the 1D bosonic tight-binding chain

$$H = \epsilon \sum_{i=1}^{\mathcal{N}} a_i^\dagger a_i - g \sum_{i=1}^{\mathcal{N}-1} \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \right)$$

- The first and last sites are coupled to heat baths ($i = 1$ or $\mathcal{N}$)

$$H_{B,i} = \sum_\ell \Omega_\ell \, b_{\ell,i}^\dagger \, b_{\ell,i}$$

$$H_{\text{int},i} = \sum_\ell c_\ell \left(a_i + a_i^\dagger \right) \left(b_{\ell,i} + b_{\ell,i}^\dagger \right)$$

- Even though the coupling is local (only at the first and last sites), we find that the Lindblad dissipator will be intrinsically *non-local*, affecting all normal modes of the system:

$$\mathcal{D}_i(\rho) =$$

$$\sum_k S_{i,k}^2 \, \gamma_{i,k} \, (1 + \bar{n}_{i,k}) \left[a_k \, \rho \, a_k^\dagger - \frac{1}{2} \{ a_k^\dagger \, a_k, \rho \} \right] + S_{i,k}^2 \, \gamma_{i,k} \, \bar{n}_{i,k} \left[a_k^\dagger \, \rho \, a_k - \frac{1}{2} \{ a_k \, a_k^\dagger, \rho \} \right]$$

  where γ_k is the bath spectral density

$$\gamma_k = 2 \pi \sum_\ell c_\ell^2 \, \delta(\epsilon_k - \Omega_\ell)$$

- This dissipator correctly thermalizes the entire system while satisfying detailed balance.
- Moreover, it has information about the position of which site is coupled to the bath.
- Therefore, it allows us to study the currents through the system.
  - They again have the form of Landauer's formula

$$\mathcal{J}_N = \frac{1}{2} \sum_k \gamma_k \, (\bar{n}_{1,k} - \bar{n}_{N,k})$$

$$\mathcal{J}_E = \frac{1}{2} \sum_k \epsilon_k \, \gamma_k \, (\bar{n}_{1,k} - \bar{n}_{N,k})$$

  - The transfer integral is now γ_k, the system-bath spectral density

J. P. Santos and GTL, arXiv:1610.05126 (2016)

Conclusions

- Main goal of condensed matter is to go from *micro* to *macro*.
- For systems in thermal equilibrium, Gibbs told us the answer:
  - $P_n = \frac{e^{-\beta E_n}}{Z}$
  - This formula is amazing: working with non-equilibrium physics has taught me to value the equilibrium formalism.
- NESS:
  - Much more complicated: must start with stochastic dynamics.
  - Enormous number of applications in condensed matter.
- Lindblad dynamics:
  - Offer a rich platform for fully quantum mechanical studies.
  - Phenomenological theories give reasonable results, but are of limited extent.
  - Microscopic derivations are more difficult, but now I think we got it!
- Next steps:
  - Full microscopic theory for the XX spin chain and the Ising model in a transverse field.
    - Study effects of quantum phase transition.
  - Magnons (modeled as bosons): study the magnon current.
  - Quantum field theory description and path integrals.
  - Microscopic theory for electrons: much harder because baths are usually bosonic.

Thank you all for your attention.

Funções auxiliares

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

SetDirectory[NotebookDirectory[]];
<< "LinLib.wl";
<< "CustomTicks`";
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 → 20, ImageSize → 400, PlotStyle → {Black}];

SetOptions[InputNotebook[],
 DefaultNewCellStyle → "Item",
 ShowCellLabel → "False",
 CellGrouping → Manual,
 FontFamily → "Times",
 DefaultNewCellStyle → {"Text", FontFamily → "Times"},
 BaseStyle → {FontFamily → "Times"},
 MultiLetterItalics → False,
 SingleLetterItalics → Automatic
]
```

Get::noopen: Cannot open LinLib.wl. >>

```
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 √2) √(a + √(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 (*g^2*)/(La + 1)^2 Total@Flatten@Table[(Sin[k]^2 Sin[q]^2 (m[μa, Ta, k] - m[μc, Tc, k]))/
          (γ^2 + (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 = γ^2 + 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[a^2 + b^2]] - 1) Sin[k]^2;

   4 γ (*g^2*)/π NIntegrate[(m[μa, Ta, k] - m[μc, Tc, k]) (int), {k, 0, 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 (*g^2*)/(La + 1)^2 Total@Flatten@Table[Sin[k]^2 Sin[q]^2 (m[k])/(γ^2 + (Cos[k] - Cos[q])^2)  , {k, mr}, {q, mr}]
  ];

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

   4 γ (*g^2*)/π NIntegrate[(m[k]) (int), {k, 0, π}] // Chop
```

```
  ];

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]^2 F,-2t  Cos[k] ℐtl[γ,k,t] + Sin[k]^2 F}*)
   -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, m},

   mr = Range[π/(La + 1), π La/(La + 1), π/(La + 1)];
   e[k_] := -2 Cos[k];
   m[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 (m[μa, Ta, k] - m[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, m, ie},

   e[k_] := -2 Cos[k];
   m[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 (m[μa, Ta, k] - m[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 → "J_N,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 → "J_N,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 → "J_E,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";
```