

Hey físicos e físicas! Vocês têm um  
minutinho para ouvir a pylavra da serpente  
quântica?

Caipyra 2018

Krissia Zawadzki

[krissia.zawadzki@gmail.com](mailto:krissia.zawadzki@gmail.com)

09 de Junho, 2018



## Motivação

Aventuras no mundo da Mecânica Quântica

Python em pesquisas envolvendo física quântica

## Aventuras com férnions interagentes

O dímero de Hubbard e trabalho quântico

Modelo e tratamento analítico

Formulação numérica

Usando o Python para a simulação

## Resultados da aventura

Resultados exatos

Resultados aproximados

# Motivação

Aventuras no mundo da Mecânica Quântica



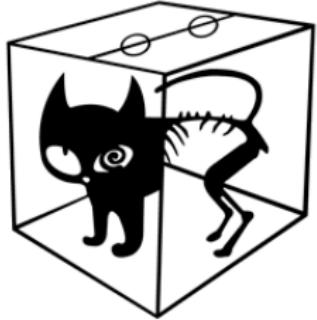
- Mecânica quântica e o mundo subatômico

$$H|\Psi(\mathbf{r}, t)\rangle = i\hbar \frac{\partial}{\partial t} |\Psi(\mathbf{r}, t)\rangle$$

função  
de onda  
 $\Psi$

Hamiltoniano  $H$

SCHRÖDINGER'S CAT IS  
**A L E A V I E**



# Motivação

Aventuras no mundo da Mecânica Quântica

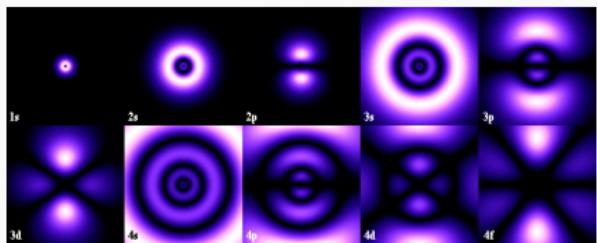


- Mecânica quântica e o mundo subatômico

$$H|\Psi(\mathbf{r}, t)\rangle = i\hbar \frac{\partial}{\partial t} |\Psi(\mathbf{r}, t)\rangle$$

função  
de onda  
 $\Psi$

Hamiltoniano  $H$



SCHRÖDINGER'S CAT IS  
**A L E A V I E**



# Motivação

Aventuras no mundo da Mecânica Quântica

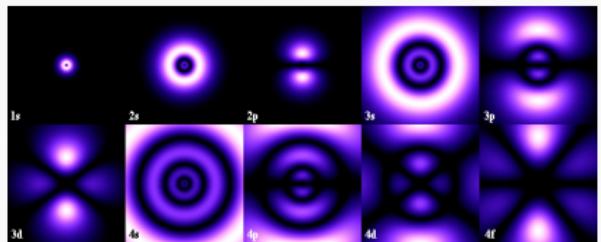


► Mecânica quântica e o mundo subatômico

$$H|\Psi(\mathbf{r}, t)\rangle = i\hbar \frac{\partial}{\partial t} |\Psi(\mathbf{r}, t)\rangle$$

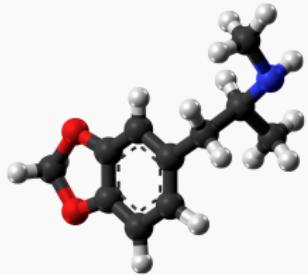
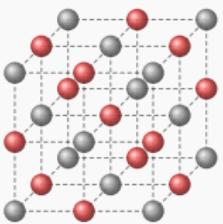
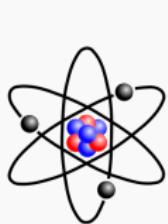
função  
de onda  
 $\Psi$

Hamiltoniano  $H$



fenômenos em  
escalas  
 $\mu\text{m}$ ,  $\text{nm}$ ,  $\text{\AA}$

SCHRÖDINGER'S CAT IS  
**A L E A V I E**



# Motivação

O problema de partículas quânticas interagentes

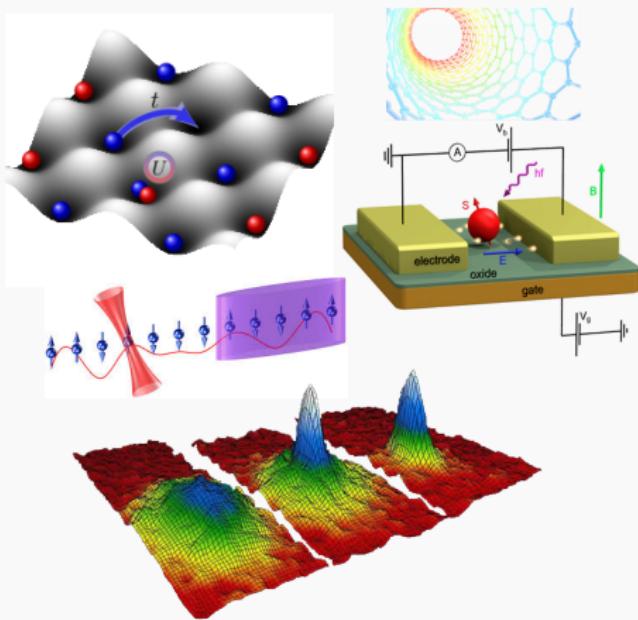


MQ: linhas de pesquisa



### MQ: linhas de pesquisa

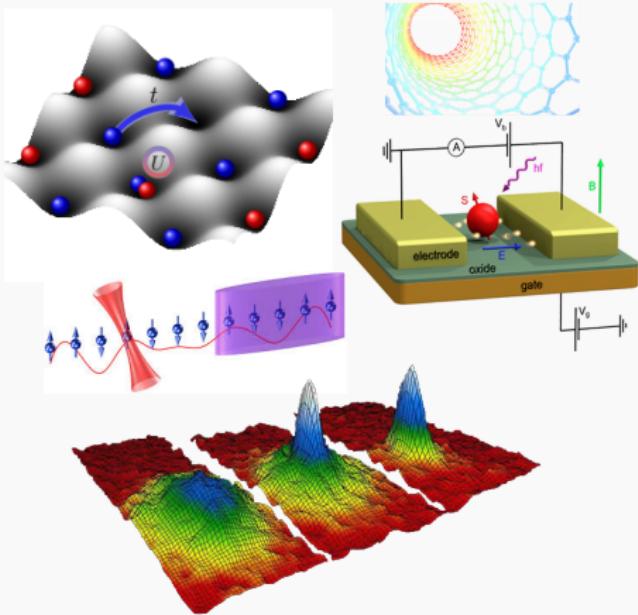
#### Matéria Condensada



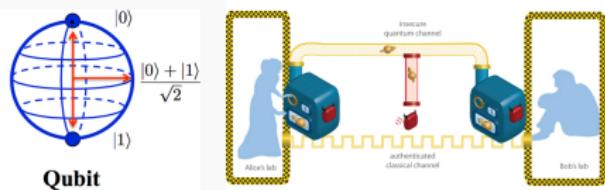


### MQ: linhas de pesquisa

#### Matéria Condensada



#### Informação Quântica



# Motivação

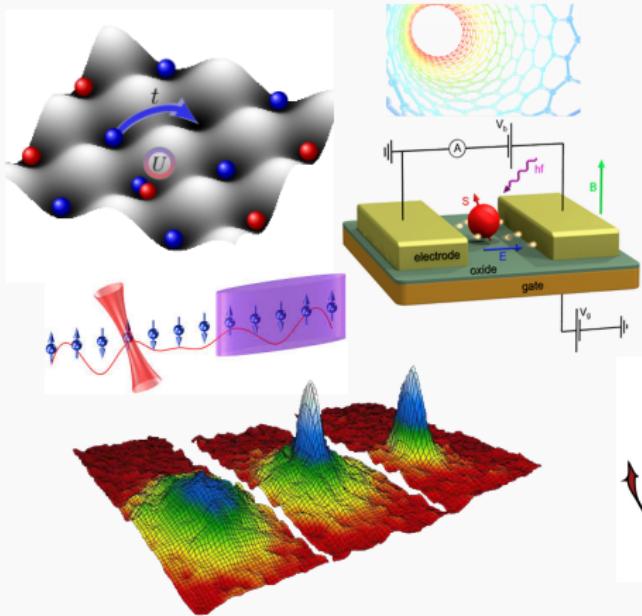
O problema de partículas quânticas interagentes



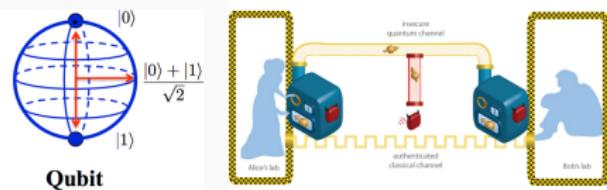
3

## MQ: linhas de pesquisa

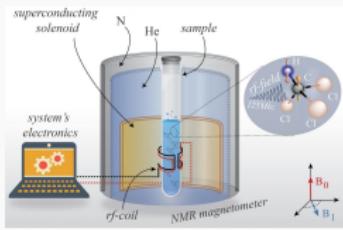
### Matéria Condensada



### Informação Quântica

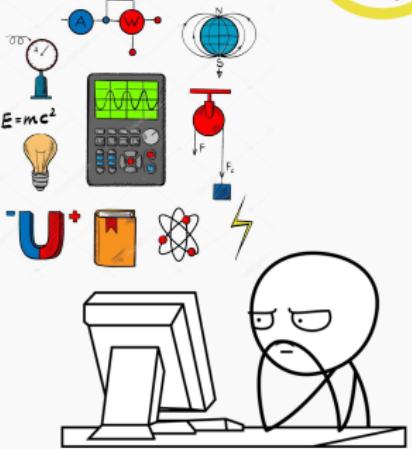


### Thermodinâmica Quântica



# Motivação

Simulações em Mecânica Quântica e Python



# Motivação

Simulações em Mecânica Quântica e Python



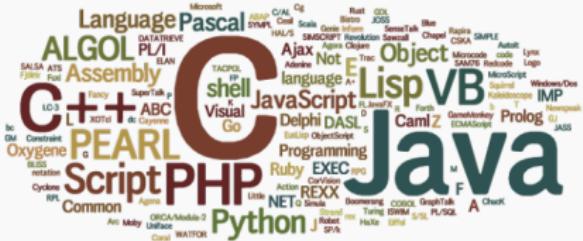
# Motivação

Simulações em Mecânica Quântica e Python



Quantum Mechanics  
@github

## Languages



Python	34
C++	32
TeX	24
Jupyter Notebook	19
Java	9
Matlab	9
JavaScript	7
Fortran	6
Julia	5
Mathematica	4

# Motivação

Simulações em Mecânica Quântica e Python



## Languages

Python

C++

TeX

Jupyter Notebo

Java

Matlab

Fortran

Julia

Mathematica



# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, ranging from the simplest single electron transistor to molecular junctions. The physics being the same of that in a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transfer (SET) and a site-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{s=L,R} f_{ks}^\dagger f_{ks} + \sum_{s=L,R} V_s (f_{ks}^\dagger c_0 + H.c.) + H_d \quad (1)$$

where  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ ,  $R$  (right) Fermi gases (metallic leads),  $\mu$  is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{ks}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{ks} = \frac{1}{\sqrt{N}} \sum_l \alpha_{k,l} \quad (2)$$

$V_s = V = \sqrt{\frac{E}{2\pi}}$  is the coupling amplitude between the quantum dot and the metallic leads with tunneling width  $\Gamma$ ,  $c_{k,\sigma}^\dagger c_{k,\sigma}$  are creation (annihilation) operators describing the quantum dot,  $\alpha_{k,l}$  is the operator associated with the occupation in the quantum dot, and, finally,  $H_d$  is defined as

$$H_d = V_G n_d + U n_d n_{d\downarrow} \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\begin{aligned} \sum_{n_{0m}} \frac{1}{\epsilon_F - \Delta} &= \sum_{l=1}^L \frac{1}{\cos(\frac{\pi(l-1)\Delta}{2})} \frac{1}{\epsilon_F - \Delta} \\ &= \frac{1}{-2i \cos(\arccos(\ell_{0m})) - \Delta} + \frac{1}{2i \cos(\arccos(\ell_{0m}+1)) - \Delta} + \\ &\quad + \frac{1}{-2i \cos(\arccos(\ell - \ell_{0m})) - \Delta} \end{aligned} \quad (30)$$

Since  $\cos(\arccos(x)) = x$ , the last term in the sum of eq (30) can be expressed as

$$\frac{1}{-2i \cos(\arccos(\ell_{0m})) - \Delta} = \frac{1}{D\lambda^{-1} + \Delta - \Delta} = \frac{1}{D\lambda^{-1}} \quad (31)$$

The second is

$$\begin{aligned} \frac{1}{-2i \cos(\arccos(\ell_{0m}+1)) - \Delta} &= \frac{1}{-2i \cos(\arccos(\frac{\pi(l-1)\Delta}{2}) + \frac{\pi}{2}) - \Delta} \\ &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi l}{2}) + 2i\sqrt{1 - (D\lambda^{-1} + \Delta)^2} \sin(\frac{\pi l}{2}) - \Delta} \end{aligned} \quad (32)$$

It is possible to verify that for all the remaining  $l$ 's belonging to  $\ell_{0m}$ , we can write

$$\begin{aligned} \frac{1}{-2i \cos(\arccos(\ell_{0m}+l')) - \Delta} &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi l'}{2}) + 2i\sqrt{1 - (D\lambda^{-1} + \Delta)^2} \sin(\frac{\pi l'}{2}) - \Delta} \\ \frac{1}{c_{k,\sigma}^\dagger} &= \frac{1}{\cos\left(\frac{\pi l}{L+1} + \delta_l(\lambda, z)\right) - \cos\left(\frac{\pi L}{2(L+1)}\right)} \end{aligned} \quad (33)$$

# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, including from the simplest single electron transistor to molecular junctions. The physics being the same that of a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transistor (SET) and a side-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{s=L,R} f_{ks}^\dagger f_{ks} + \sum_{s=L,R} V_s (f_{ks}^\dagger c_0 + H.c.) + H_E \quad (1)$$

where  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ ,  $R$  (right) Fermi gases (metallic leads),  $\mu$  is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{ks}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{ks} = \frac{1}{\sqrt{N}} \sum_n \phi_{kn} \quad (2)$$

$V_s = V = \sqrt{\frac{e}{2\pi}}$  is the coupling amplitude between the quantum dot and the metallic leads with tunneling width  $\Gamma$ ,  $c_{k,\sigma}^\dagger c_{k,\sigma}$  are creation (annihilation) operators describing the quantum dot,  $v_d = c_d^\dagger c_d$  is the operator associated with the occupation in the quantum dot, and, finally,  $H_E$  is defined as

$$H_E = V_G n_d + U n_d v_d \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\begin{aligned} \sum_{n,k} \frac{1}{\epsilon_k - \Delta} &= \sum_{l=\frac{L+1}{2}\cos(\frac{(2k+1)\pi}{2L})}^L \frac{1}{\epsilon_k - \Delta} \\ &= \frac{1}{-2i\cos(\arcsin(\ell_{nm})) - \Delta} + \frac{1}{-2i\cos(\arcsin(\ell_{nm}+1)) - \Delta} + \\ &\quad + \dots + \frac{1}{-2i\cos(\arcsin(L - \ell_{nm})) - \Delta} \end{aligned} \quad (30)$$

Since  $\cos(\arcsin(x)) = x$ , the last term in the sum of eq. (30) can be expressed as

$$\frac{1}{-2i\cos(\arcsin(\ell_{nm})) - \Delta} = \frac{1}{D\lambda^{-1} + \Delta - \Delta} = \frac{1}{D\lambda^{-1}} \quad (31)$$

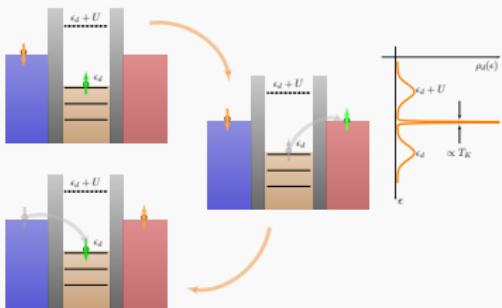
The second is

$$\begin{aligned} \frac{1}{-2i\cos(\arcsin(\ell_{nm}+1)) - \Delta} &= \frac{1}{-2i\cos(\arcsin(\frac{\partial \lambda^{-1}}{2} + \frac{\pi}{2L})) - \Delta} \\ &= \frac{1}{(D\lambda^{-1} + \Delta)\cos(\frac{\pi i}{2L}) + 2i\sqrt{1 - (\frac{\partial \lambda^{-1}}{2})^2}\sin(\frac{\pi i}{2L}) - \Delta} \end{aligned} \quad (32)$$

It is possible to verify that for all the remaining  $\ell'$  belonging to  $\ell_{nm}$ , we can write

$$\begin{aligned} \frac{1}{-2i\cos(\arcsin(\ell_{nm}+\ell')) - \Delta} &= \frac{1}{(D\lambda^{-1} + \Delta)\cos(\frac{\pi i}{2L}) + 2i\sqrt{1 - (\frac{\partial \lambda^{-1}}{2})^2}\sin(\frac{\pi i}{2L}) - \Delta} \\ \frac{1}{c_d^\dagger} &= \frac{1}{\cos\left(\frac{\pi i}{L+1} + \delta_0(\lambda, z)\right) - \cos\left(\frac{\pi i L}{2(L+1)}\right)} \end{aligned} \quad (33)$$

### ► desenhos



# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, including from the simplest single electron transistor to molecular junctions. The physics being the same that in a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transistor (SET) and a side-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{s=L,R} f_{ks}^\dagger f_{ks} + \sum_{s=L,R} V_s (f_{ks}^\dagger c_0 + H.c.) + H_E \quad (1)$$

where  $c_{k,\sigma}^\dagger (c_{k,\sigma})$  operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ .  $R$  (right) Fermi gases (metallic leads),  $\mu$  is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{ks}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{ks} = \frac{1}{\sqrt{N}} \sum_l c_{k+Ll,\sigma} \quad (2)$$

$V_s = V/\sqrt{\pi T}$  is the coupling amplitude between the quantum dot and the metallic leads with tunneling width  $\Gamma$ ,  $c_{k,\sigma}^\dagger c_{k,\sigma}$  are creation (annihilation) operators describing the quantum dot,  $v_d = c_{k,\sigma}^\dagger c_k$  is the operator associated with the occupation in the quantum dot, and finally,  $H_E$  is defined as

$$H_E = V_G n_d + U n_d n_{d\bar{d}} \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\begin{aligned} \sum_{k,k'} \frac{1}{\epsilon_k - \Delta} &= \sum_{l=1}^L \frac{1}{\cos(\frac{\pi k}{L} + \frac{(2l-1)\pi}{2L}) - \Delta} \\ &= \frac{1}{-2i \cos(\cos^{-1}(\theta_{m0})) - \Delta} + \frac{1}{-2i \cos(\cos^{-1}(\theta_{m0} + 1)) - \Delta} + \\ &\quad + \dots + \frac{1}{-2i \cos(\cos^{-1}(L - \theta_{m0})) - \Delta} \end{aligned} \quad (30)$$

Since  $\cos(\cos^{-1}(x)) = x$ , the last term in the sum of eq (30) can be expressed as

$$\frac{1}{-2i \cos(\cos^{-1}(\theta_{m0})) - \Delta} = \frac{1}{D\lambda^{-1} + \Delta - \Delta} = \frac{1}{D\lambda^{-1}} \quad (31)$$

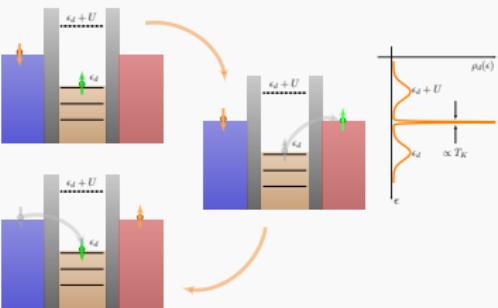
The second is

$$\begin{aligned} \frac{1}{-2i \cos(\cos^{-1}(\theta_{m0} + 1)) - \Delta} &= \frac{1}{-2i \cos(\cos^{-1}(\frac{D\lambda^{-1} + \Delta}{2} + \frac{\pi}{2L})) - \Delta} \\ &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi}{L+1}) + 2i\sqrt{1 - (\frac{D\lambda^{-1} + \Delta}{2})^2} \sin(\frac{\pi}{L+1}) - \Delta} \end{aligned} \quad (32)$$

It is possible to verify that for all the remaining  $\ell$ 's belonging to  $\ell_{m+1}$ , we can write

$$\begin{aligned} \frac{1}{-2i \cos(\cos^{-1}(\theta_{m0} + \ell)) - \Delta} &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi \ell}{L+1}) + 2i\sqrt{1 - (\frac{D\lambda^{-1} + \Delta}{2})^2} \sin(\frac{\pi \ell}{L+1}) - \Delta} \\ \frac{1}{v_d} &= \frac{1}{\cos(\frac{\pi L}{L+1} + \delta_L(\lambda, z)) - \cos(\frac{\pi L}{2(L+1)})} \end{aligned} \quad (33)$$

### ► desenhos



### ► programação



# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, including from the simplest single electron transistor to molecular junctions. The physics being the same that in a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transistor (SET) and a side-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{s=L,R} f_{ks}^\dagger f_{ks} + \sum_{s=L,R} V_s (f_{ks}^\dagger c_0 + H.c.) + H_E \quad (1)$$

where  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ .  $R$  (right) Fermi gases (metallic leads),  $\mu$  is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{ks}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{ks} = \frac{1}{\sqrt{2\pi}} \sum_n \phi_{kn} \quad (2)$$

$V_s = V = \sqrt{\frac{e}{2\pi}}$  is the coupling amplitude between the quantum dot and the metallic leads with tunneling width  $\Gamma$ ,  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) are creation (annihilation) operators describing the quantum dot,  $v_d = c_{k,\sigma}^\dagger c_k$  is the operator associated with the occupation in the quantum dot, and finally,  $H_E$  is defined as

$$H_E = V_G n_d + U n_d n_{d\bar{d}} \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\begin{aligned} \sum_{k,L} \frac{1}{\epsilon_k - \Delta} &= \sum_{l=1}^L \frac{1}{\cos(\frac{(2l-1)\pi}{2L}) \sin(\frac{(2l-1)\pi}{2L})} \frac{1}{\epsilon_l - \Delta} \\ &= \frac{1}{-2i \cos(\arcsin(\theta_{lm})) - \Delta} + \frac{1}{2i \cos(\arcsin(\theta_{lm})) - \Delta} \\ &\quad + \dots + \frac{1}{-2i \cos(\arcsin(L - \theta_{lm})) - \Delta} \end{aligned} \quad (30)$$

Since  $\cos(\arcsin(x)) = |x|$  the last term in the sum of eq (30) can be expressed as

$$\frac{1}{-2i \cos(\arcsin(\theta_{lm})) - \Delta} = \frac{1}{D\lambda^{-1} + \Delta - \Delta} = \frac{1}{D\lambda^{-1}} \quad (31)$$

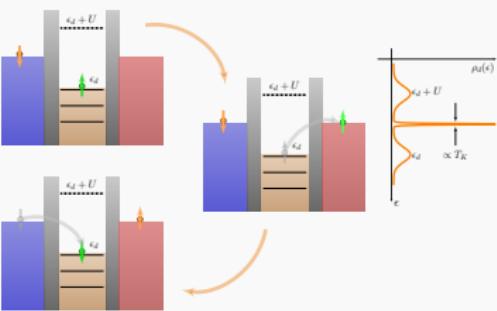
The second is

$$\begin{aligned} \frac{1}{-2i \cos(\arcsin(\theta_{lm} + 1)) - \Delta} &= \frac{1}{-2i \cos(\arcsin(\frac{2l+1}{2L}) + \frac{\pi}{2L}) - \Delta} \\ &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi l}{L}) + 2i\sqrt{1 - (\frac{2l+1}{2L})^2} \sin(\frac{\pi l}{L})} - \Delta \end{aligned} \quad (32)$$

It is possible to verify that for all the remaining  $l'$  belonging to  $\ell_{m+1}$ , we can write

$$\begin{aligned} \frac{1}{-2i \cos(\arcsin(\theta_{lm} + l')) - \Delta} &= \frac{1}{(D\lambda^{-1} + \Delta) \cos(\frac{\pi l'}{L}) + 2i\sqrt{1 - (\frac{2l'+1}{2L})^2} \sin(\frac{\pi l'}{L})} - \Delta \\ \frac{1}{v_d} &= \frac{1}{\cos(\frac{\pi l'}{L+1} + \delta_l(\lambda, z)) - \cos(\frac{\pi l}{2(L+1)})} \end{aligned} \quad (33)$$

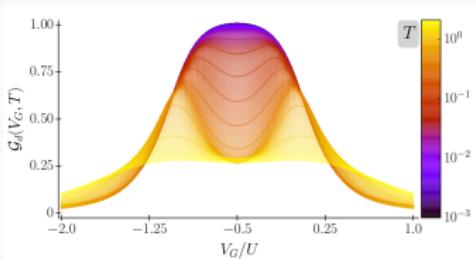
### ► desenhos



### ► programação



### ► gráficos bonitos



# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, including from the simplest single electron transistor to molecular junctions. The physics being the same that in a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transistor (SET) and a side-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{s=L,R} f_{ks}^\dagger f_{ks} + \sum_{s=L,R} V_s (f_{ks}^\dagger c_0 + H.c.) + H_E \quad (1)$$

where  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ .  $R$  (right) Fermi gases (metallic leads),  $\mu$  is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{ks}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{ks} = \frac{1}{\sqrt{N}} \sum_l c_{k+L,l} \quad (2)$$

$V_s = V = \sqrt{\frac{E}{2\pi}}$  is the coupling amplitude between the quantum dot and the metallic leads (coupling width),  $\Gamma_c$  ( $\Gamma_d$ ) are creation (annihilation) operators describing the quantum dot,  $v_d = c_d^\dagger c_d$  is the operator associated with the occupation in the quantum dot, and finally,  $H_E$  is defined as

$$H_E = V_G n_d + U n_d v_d \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\sum_{n_{kz}} \frac{1}{\epsilon_k - \Delta} \sum_{l=0,2,4, \dots}^L \frac{1}{\cos(\theta(l)) \sin(\frac{\pi k l}{L+1})} \frac{1}{\cos(\theta(m)) \sin(\frac{\pi k m}{L+1})} - \Delta \quad (30)$$

$$\rightarrow + \frac{1}{-2i \cos(\theta(m)) \sin(\frac{\pi k m}{L+1})} \quad (31)$$

Since  $\cos(\theta(z)) = \pm 1$ , the last term in the sum of eq. (30) can be expressed as

$$\frac{1}{-2i \cos(\theta(m)) \sin(\frac{\pi k m}{L+1})} = \frac{1}{\Delta - \Delta + \Delta - \Delta} = \frac{1}{\Delta} \quad (32)$$

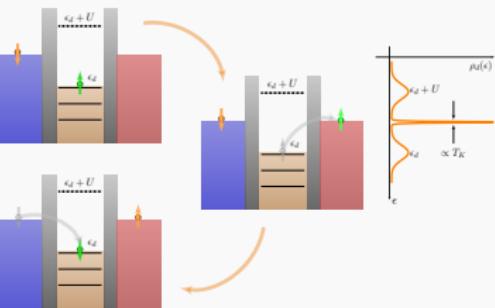
The second term is

$$\begin{aligned} & -2i \cos(\theta(m)) \sin(\frac{\pi k m}{L+1}) - \Delta = \\ & = -2i \cos\left[\theta\left(\frac{m}{L+1}\right)\right] \frac{\pi k}{L+1} - \Delta \\ & = \frac{1}{\left(\frac{m}{L+1} + \Delta\right) \cos\left(\frac{\pi k}{L+1}\right) + 2i\sqrt{1 - \left(\frac{m}{L+1} + \Delta\right)^2} \sin\left(\frac{\pi k}{L+1}\right)} - \Delta \end{aligned} \quad (33)$$

It is possible to note that for all the remaining  $l$  belonging to  $\ell_m$ , we can write

$$\begin{aligned} & -2i \cos(\theta(m) + \ell_m) \sin(\frac{\pi k (m+\ell_m)}{L+1}) - \Delta = \\ & = -2i \cos\left[\theta\left(\frac{m+\ell_m}{L+1}\right)\right] \frac{\pi k}{L+1} - \Delta \\ & = \frac{1}{\cos\left(\frac{\pi k}{L+1} + \theta\left(\frac{m+\ell_m}{L+1}\right)\right) - \cos\left(\frac{\pi k \ell_m}{L+1}\right)} - \Delta \end{aligned} \quad (34)$$

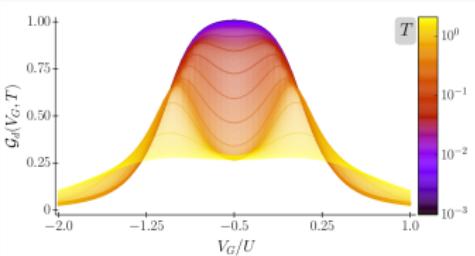
### ► desenhos



### ► programação



### ► gráficos bonitos



# Vida de uma pesquisadora

## Em matéria condensada computacional



### ► muita teoria

#### I Model Hamiltonian

The Anderson model has served as a basis on the fundamental understanding of transport properties in nanosystems, including from the simplest single electron transistor to molecular junctions. The physics being the same that in a metallic band coupled to a magnetic impurity, allowed for an accurate description of many-body phenomena arising in quantum dots.

In particular, the Anderson model for a single electron transistor (SET) and a side-coupled quantum dot is formulated as

$$H = \sum_{\sigma=L,R} \sum_k (\epsilon_k - \mu) c_{k,\sigma}^\dagger c_{k,\sigma} + W \sum_{i=L,R} f_{k,i}^\dagger f_{k,i} + \sum_{i=L,R} V_i (f_{k,i}^\dagger c_k + H.c.) + H_E \quad (1)$$

where  $c_{k,\sigma}^\dagger$  ( $c_{k,\sigma}$ ) operates that create (annihilate) one electron in the energy level  $\epsilon_k$  of the conduction band on the  $y = U(k)$ . Right (left) Fermi gases (metallic leads), is the chemical potential that shifts the Fermi level  $\epsilon_F$  of the conduction band  $\epsilon_k$ ,  $W$  is a scattering potential applied to the conduction band,  $f_{k,i}$  represents the Wannier state to which the quantum dot is coupled and is defined as

$$f_{k,i} = \frac{1}{\sqrt{N}} \sum_l c_{l,i} \quad (2)$$

$V_d = V = \sqrt{\frac{E}{2\pi}}$  is the coupling amplitude between the quantum dot and the metallic leads (coupling width  $\Gamma$ ),  $c_{k,i}^\dagger$  ( $c_{k,i}$ ) are creation (annihilation) operators describing the quantum dot,  $v_d = c_{k,i}^\dagger c_{k,i}$  is the operator associated with the occupation in the quantum dot, and finally,  $H_E$  is defined as

$$H_E = V_G n_d + U n_d n_{d\bar{d}} \quad (3)$$

where  $V_G$  is the applied gate voltage and  $U$  is the charging energy accounting for the Coulomb repulsion when the dot is doubly occupied.

### ► contas analíticas

For the integrals in eq(28), a simplification is made possible. Consider, for instance, the interval labeled by  $m = 0$

$$\sum_{n_{k,i}} \frac{1}{\epsilon_k - \Delta} \sum_{l=0}^L \frac{1}{2\cos(\pi \frac{l+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta} + \dots - 2\cos(\pi \frac{L+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta \quad (30)$$

Since  $\cos(\pi \frac{l+1}{L+1} \sin(\frac{\theta k}{2})) = 1$  the first term in the sum of eq (30) can be expressed as

$$-\frac{1}{2\cos(\pi \frac{L+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta} = \frac{1}{\Delta - D\Lambda + \Delta - \Delta} = \frac{1}{D\Lambda - \Delta} \quad (31)$$

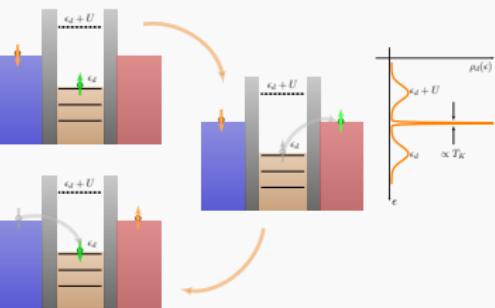
The second term is

$$-\frac{1}{2\cos(\pi \frac{L+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta} = -\frac{1}{2\cos(\pi \frac{L+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta} = \frac{1}{(D\Lambda - \Delta) \cos(\frac{\theta k}{2}) + 2\sqrt{1 - (D\Lambda - \Delta)^2} \sin(\frac{\theta k}{2}) - \Delta} \quad (32)$$

It is possible to show that for all the remaining  $\ell$  belonging to  $\ell_{m+1}$ , we can write

$$-\frac{1}{2\cos(\pi \frac{L+1}{L+1} \sin(\frac{\theta k}{2})) - \Delta} = -\frac{1}{\cos(\frac{\theta k}{2} + \ell\pi + \Delta) \cos(\frac{\theta k}{2}) + 2\sqrt{1 - (\cos(\frac{\theta k}{2} + \ell\pi + \Delta))^2} \sin(\frac{\theta k}{2}) - \Delta} = \frac{1}{\cos(\frac{\theta k}{2} + \ell\pi + \Delta, z)} - \cos(\frac{\theta k}{2(L+1)}) \quad (33)$$

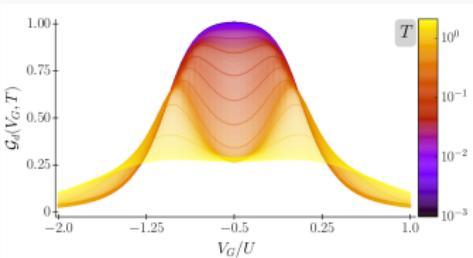
### ► desenhos



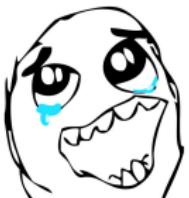
### ► programação



### ► gráficos bonitos



### ► aventuras



# Aventuras com férmiões interagentes

## Derretendo o dímero



Cornell University  
Library

arXiv.org > quant-ph > arXiv:1803.06724

Search or Article

(Help | Advanced search)

Quantum Physics

## Melting a Hubbard dimer: benchmarks of 'ALDA' for quantum thermodynamics

Marcela Herrera



Krissia Zawadzki



Irene D'Amico



The competition between evolution time, interaction strength, and temperature challenges our understanding of many-body quantum systems out-of-equilibrium. Here we consider a benchmark system, the Hubbard dimer, which allows us to explore all the relevant regimes and calculate exactly the related average quantum work. At difference with previous studies, we focus on the effect of increasing temperature, and show how this can turn competition between many-body interactions and driving field into synergy. We then turn to use recently proposed protocols inspired by density functional theory to explore if these effects could be reproduced by using simple approximations. We find that, up to and including intermediate temperatures, a method which borrows from ground-state adiabatic local density approximation improves dramatically the estimate for the average quantum work, including, in the adiabatic regime, when correlations are strong. However at high temperature and at least when based on the pseudo-LDA, this method fails to capture the counterintuitive qualitative dependence of the quantum work with interaction strength, albeit getting the quantitative estimates relatively close to the exact results.

Subjects: Quantum Physics (quant-ph); Materials Science (cond-mat.mtrl-sci); Strongly Correlated Electrons (cond-mat.str-el)

Cite as: arXiv:1803.06724 [quant-ph]

(or arXiv:1803.06724v1 [quant-ph] for this version)

### Submission history

From: Krissia Zawadzki [[view email](#)]

[v1] Sun, 18 Mar 2018 19:38:09 GMT (5917kb,D)

# Aventuras com férmiões interagentes

## Derretendo o dímero



Cornell University  
Library

arXiv.org > quant-ph > arXiv:1803.06724

Search or Article

(Help | Advanced search)

Quantum Physics

## Melting a Hubbard dimer: benchmarks of 'ALDA' for quantum thermodynamics

Marcela Herrera



Krissia Zawadzki



Irene D'Amico



The competition between evolution time, interaction strength, and temperature challenges our understanding of many-body quantum systems out-of-equilibrium. Here we consider a benchmark system, the Hubbard dimer, which allows us to explore all the relevant regimes and calculate exactly the related average quantum work. At difference with previous studies, we focus on the effect of increasing temperature, and show how this can turn competition between many-body interactions and driving field into synergy. We then turn to use recently proposed protocols inspired by density functional theory to explore if these effects could be reproduced by using simple approximations. We find that, up to and including intermediate temperatures, a method which borrows from ground-state adiabatic local density approximation improves dramatically the estimate for the average quantum work, including, in the adiabatic regime, when correlations are strong. However at high temperature and at least when based on the pseudo-LDA, this method fails to capture the counterintuitive qualitative dependence of the quantum work with interaction strength, albeit getting the quantitative estimates relatively close to the exact results.

Subjects: Quantum Physics (quant-ph); Materials Science (cond-mat.mtrl-sci); Strongly Correlated Electrons (cond-mat.str-el)

Cite as: arXiv:1803.06724 [quant-ph]

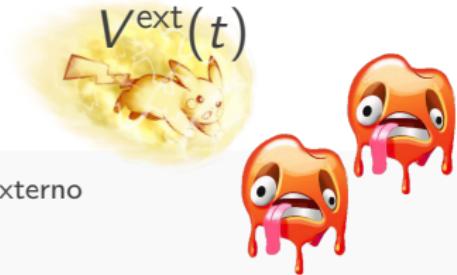
(or arXiv:1803.06724v1 [quant-ph] for this version)

### Submission history

From: Krissia Zawadzki [view email]

[v1] Sun, 18 Mar 2018 19:38:09 GMT (5917kb,D)

- Simulação de dois elétrons interagentes sob campo externo



# Aventuras com férmiões interagentes

## Derretendo o dímero



Cornell University  
Library

arXiv.org > quant-ph > arXiv:1803.06724

Search or Article

(Help | Advanced search)

### Quantum Physics

## Melting a Hubbard dimer: benchmarks of 'ALDA' for quantum thermodynamics

Marcela Herrera

Krissia Zawadzki

Irene D'Amico

The competition between evolution time, interaction strength, and temperature challenges our understanding of many-body quantum systems out-of-equilibrium. Here we consider a benchmark system, the Hubbard dimer, which allows us to explore all the relevant regimes and calculate exactly the related average quantum work. At difference with previous studies, we focus on the effect of increasing temperature, and show how this can turn competition between many-body interactions and driving field into synergy. We then turn to use recently proposed protocols inspired by density functional theory to explore if these effects could be reproduced by using simple approximations. We find that, up to and including intermediate temperatures, a method which borrows from ground-state adiabatic local density approximation improves dramatically the estimate for the average quantum work, including, in the adiabatic regime, when correlations are strong. However at high temperature and at least when based on the pseudo-LDA, this method fails to capture the counterintuitive qualitative dependence of the quantum work with interaction strength, albeit getting the quantitative estimates relatively close to the exact results.

Subjects: Quantum Physics (quant-ph); Materials Science (cond-mat.mtrl-sci); Strongly Correlated Electrons (cond-mat.str-el)

Cite as: arXiv:1803.06724 [quant-ph]

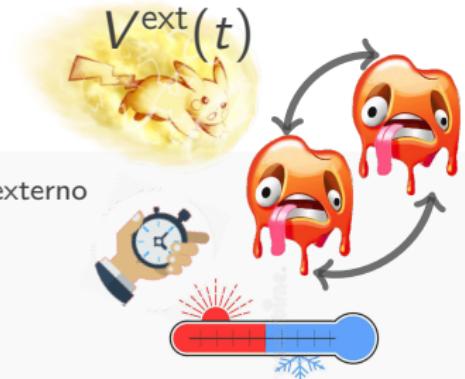
(or arXiv:1803.06724v1 [quant-ph] for this version)

### Submission history

From: Krissia Zawadzki [[view email](#)]

[v1] Sun, 18 Mar 2018 19:38:09 GMT (5917kb,D)

- Simulação de dois elétrons interagentes sob campo externo
  - escalas: tempo, temperatura, interação



# Aventuras com férmiões interagentes

## Derretendo o dímero



Cornell University  
Library

arXiv.org > quant-ph > arXiv:1803.06724

Search or Article

(Help | Advanced search)

### Quantum Physics

## Melting a Hubbard dimer: benchmarks of 'ALDA' for quantum thermodynamics



Marcela Herrera



Krissia Zawadzki



Irene D'Amico

The competition between evolution time, interaction strength, and temperature challenges our understanding of many-body quantum systems out-of-equilibrium. Here we consider a benchmark system, the Hubbard dimer, which allows us to explore all the relevant regimes and calculate exactly the related average quantum work. At difference with previous studies, we focus on the effect of increasing temperature, and show how this can turn competition between many-body interactions and driving field into synergy. We then turn to use recently proposed protocols inspired by density functional theory to explore if these effects could be reproduced by using simple approximations. We find that, up to and including intermediate temperatures, a method which borrows from ground-state adiabatic local density approximation improves dramatically the estimate for the average quantum work, including, in the adiabatic regime, when correlations are strong. However at high temperature and at least when based on the pseudo-LDA, this method fails to capture the counterintuitive qualitative dependence of the quantum work with interaction strength, albeit getting the quantitative estimates relatively close to the exact results.

Subjects: Quantum Physics (quant-ph); Materials Science (cond-mat.mtrl-sci); Strongly Correlated Electrons (cond-mat.str-el)

Cite as: arXiv:1803.06724 [quant-ph]

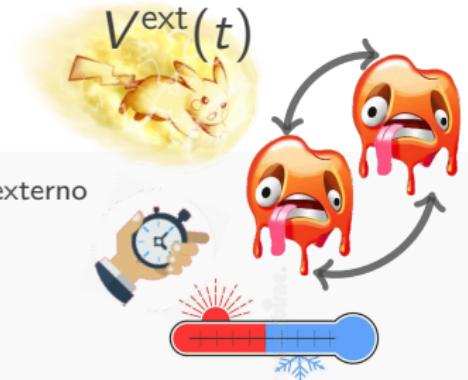
(or arXiv:1803.06724v1 [quant-ph] for this version)

### Submission history

From: Krissia Zawadzki [view email]

[v1] Sun, 18 Mar 2018 19:38:09 GMT (5917kb,D)

- Simulação de dois elétrons interagentes sob campo externo
  - escalas: tempo, temperatura, interação
  - exato vs aproximado (DFT)



# Aventuras com férmiões interagentes

## Derretendo o dímero



# Aventuras com férnions interagentes

## Derretendo o dímero



# Derretendo o dímero

## Formulação analítica



- Modelo de Hubbard para férmions interagentes

$$\hat{H}(t) = -J(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}) + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + \hat{V}^{\text{ext}}(t)$$

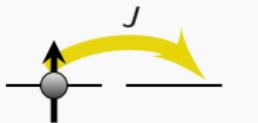
# Derretendo o dímero

Formulação analítica



- Modelo de Hubbard para férmions interagentes

$$\hat{H}(t) = \underbrace{-J(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma})}_{\text{cinético "hopping"} } + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + \hat{V}^{\text{ext}}(t)$$



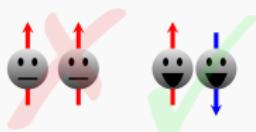
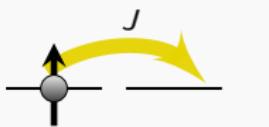
# Derretendo o dímero

Formulação analítica



- Modelo de Hubbard para férmions interagentes

$$\hat{H}(t) = \underbrace{-J(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma})}_{\text{cinético "hopping"} } + \underbrace{U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}}_{\text{repulsão Coulombiana}} + \hat{V}^{\text{ext}}(t)$$



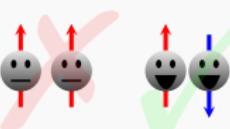
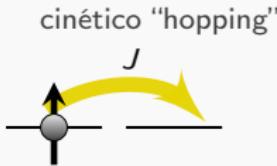
# Derretendo o dímero

Formulação analítica

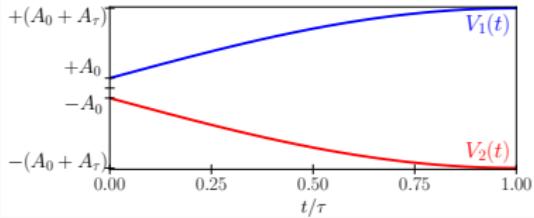


- Modelo de Hubbard para férmions interagentes

$$\hat{H}(t) = \underbrace{-J(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma})}_{\text{cinético "hopping"} } + \underbrace{U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}}_{\text{repulsão Coulombiana}} + \underbrace{\hat{V}^{\text{ext}}(t)}_{\text{potencial "driven"}}$$



$$V_j(t) = (-1)^j [A_0 + A_\tau \sin(\omega_\tau t)]$$



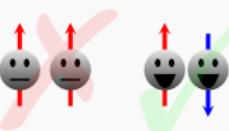
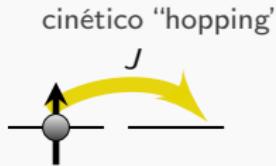
# Derretendo o dímero

Formulação analítica

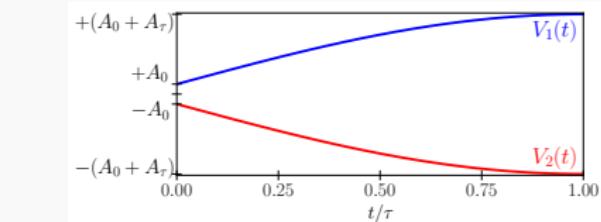
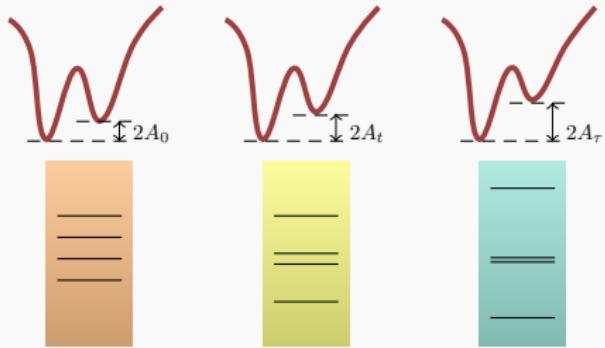


- Modelo de Hubbard para férmitons interagentes

$$\hat{H}(t) = \underbrace{-J(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma})}_{\text{cinético "hopping"} } + \underbrace{U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}}_{\text{repulsão Coulombiana}} + \underbrace{\hat{V}^{\text{ext}}(t)}_{\text{potencial "driven"}}$$



$$V_j(t) = (-1)^j [A_0 + A_\tau \sin(\omega_4 \tau t)]$$

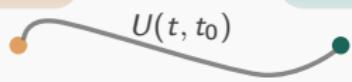


estado inicial

$$\rho(t=0)$$

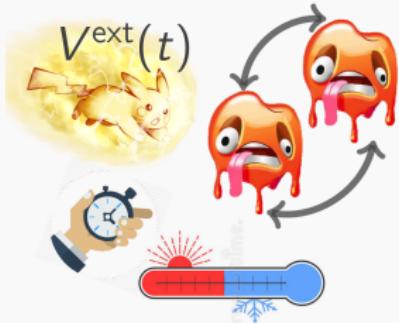
estado final

$$\rho(t=\tau)$$



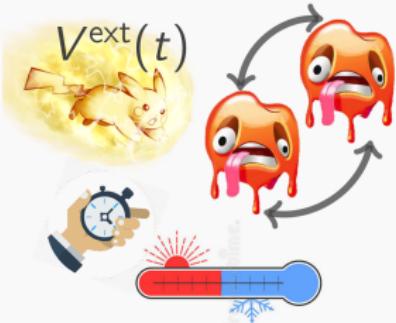
# Derretendo o dímero

## Formulação analítica

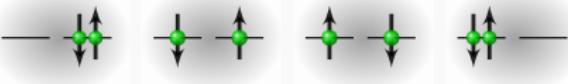


# Derretendo o dímero

## Formulação analítica

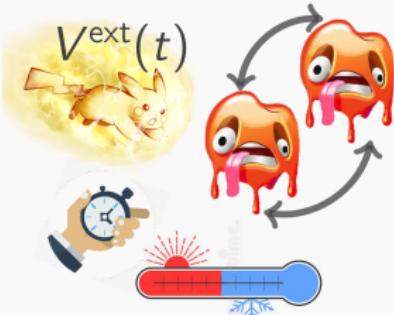


► base de estados

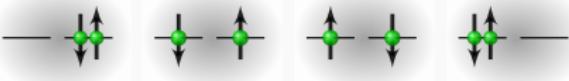


# Derretendo o dímero

Formulação analítica



► base de estados

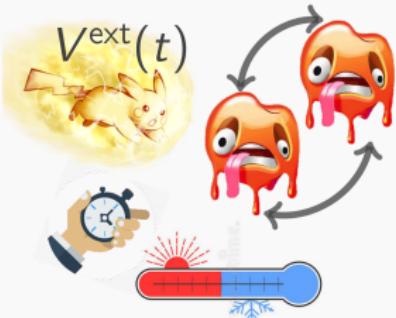


► operador Hamiltoniano

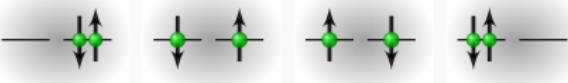
$$H(t) = \begin{pmatrix} 2V_2(t) + U & -J & J & 0 \\ -J & V_1(t) + V_2(t) & 0 & -J \\ J & 0 & V_1(t) + V_2(t) & J \\ 0 & -J & J & 2V_1(t) + U \end{pmatrix}$$

# Derretendo o dímero

Formulação analítica



► base de estados

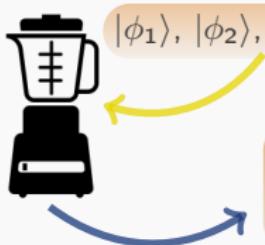


► operador Hamiltoniano

$$H(t) = \begin{pmatrix} 2V_2(t) + U & -J & J & 0 \\ -J & V_1(t) + V_2(t) & 0 & -J \\ J & 0 & V_1(t) + V_2(t) & J \\ 0 & -J & J & 2V_1(t) + U \end{pmatrix}$$

► estado inicial

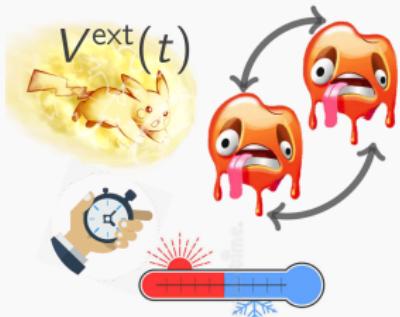
$|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle$



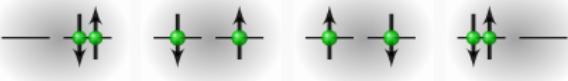
$$\rho(t=0) = \sum_{i=1}^4 \frac{e^{-\frac{\epsilon_i}{kT}}}{Z}$$

# Derretendo o dímero

Formulação analítica



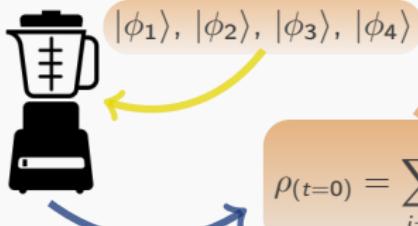
► base de estados



► operador Hamiltoniano

$$H(t) = \begin{pmatrix} 2V_2(t) + U & -J & J & 0 \\ -J & V_1(t) + V_2(t) & 0 & -J \\ J & 0 & V_1(t) + V_2(t) & J \\ 0 & -J & J & 2V_1(t) + U \end{pmatrix}$$

► estado inicial



$$\rho(t=0) = \sum_{i=1}^4 \frac{e^{-\frac{\epsilon_i}{kT}}}{Z}$$

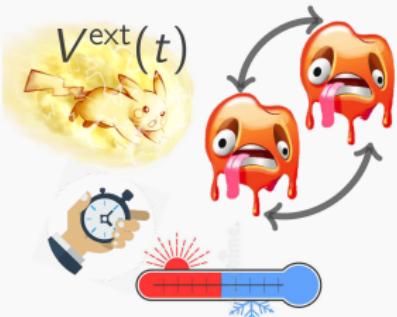
► evolução temporal

$$U(t, 0) = e^{-\frac{i}{\hbar} H(t)}$$

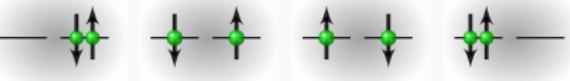
$$\rho(t = \tau)$$

# Derretendo o dímero

Formulação analítica



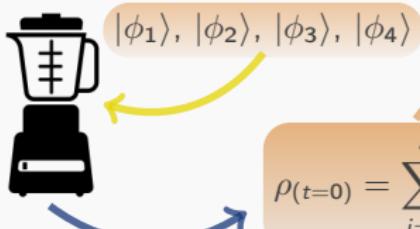
► base de estados



► operador Hamiltoniano

$$H(t) = \begin{pmatrix} 2V_2(t) + U & -J & J & 0 \\ -J & V_1(t) + V_2(t) & 0 & -J \\ J & 0 & V_1(t) + V_2(t) & J \\ 0 & -J & J & 2V_1(t) + U \end{pmatrix}$$

► estado inicial



$$\rho(t=0) = \sum_{i=1}^4 \frac{e^{-\frac{\epsilon_i}{kT}}}{Z}$$

► evolução temporal

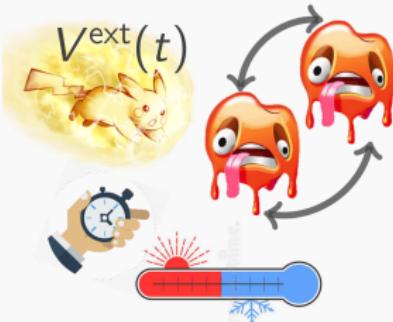
$$U(t, 0) = e^{-\frac{i}{\hbar} H(t)}$$

$$\rho(t = \tau)$$



# Derretendo o dímero

Simulando o problema



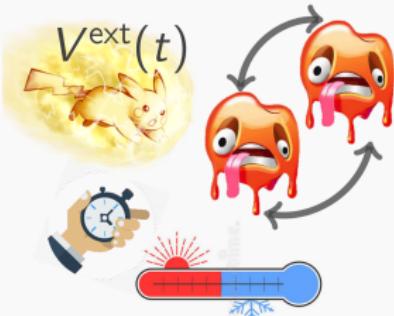
➤ cálculo de propriedades

$$\triangleright \mathcal{O}(t) = \text{Tr} [\hat{O} \cdot \rho(t)]$$

➤ densidades  
 $n_1(t), n_2(t)$

# Derretendo o dímero

Simulando o problema



➤ cálculo de propriedades

$$\triangleright \mathcal{O}(t) = \text{Tr} [\hat{O} \cdot \rho(t)]$$

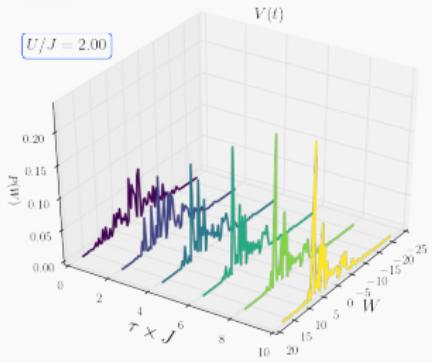
➤ densidades  
 $n_1(t), n_2(t)$

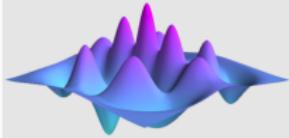


➤ trabalho extraído durante o processo

$$W = - \int w P(w) dw$$

$$P(w) = \sum_{n,m} p_n(t=0) p_m(t=\tau) |n(t=0)\rangle \delta(w - \Delta\epsilon_{m,n})$$





## QuTiP

Quantum Toolbox in Python

# QuTiP: Quantum Toolbox in Python 4.2

Search docs

Frontmatter  
Installation  
Users Guide  
API documentation  
Change Log  
Developers  
Bibliography

- Manipulating States and Operators
  - Introduction
  - State Vectors (kets or bras)
  - Density matrices
  - Qubit (two-level) systems
  - Expectation values
  - Superoperators and Vectorized Operators
  - Choi, Kraus, Stinespring and  $\chi$  Representations
  - Properties of Quantum Maps
- Using Tensor Products and Partial Traces
  - Tensor products
  - Example: Constructing composite Hamiltonians
  - Partial trace
  - Superoperators and Tensor Manipulations
- Time Evolution and Quantum System Dynamics
  - Dynamics Simulation Results
  - Lindblad Master Equation Solver
  - Monte Carlo Solver
  - Solving Problems with Time-dependent Hamiltonians
  - Bloch-Redfield master equation
  - Floquet Formalism
  - Setting Options for the Dynamics Solvers

<http://qutip.org>

- Um pacote completo para simular dinâmica de sistemas quânticos abertos
- suporte Windows, MacOSX, Linux
- interface amigável
- diversos exemplos em Jupyter notebooks!



### ► Hamiltoniano livre

```
from qutip import *

si = qeye(2)
sx = sigmax()
sy = sigmay()
sz = sigmaz()

def n2_operator():
    return tensor(si, si)+0.5*(tensor(sz, si)+tensor(si, sz))

def n1_operator():
    return tensor(si, si)-0.5*(tensor(sz, si)+tensor(si, sz))

def hopping_operator():
    return (tensor(sx, si)-tensor(si, sx))

def repulsionee_operator():
    return 0.5*(tensor(si, si)+tensor(sz, sz))
```

```
def dimer_Hamiltonian_free(J,U):
    H_hopping_Op = -J*hopping_operator()
    H_coulomb_Op = U * repulsionee_operator()
    return H_hopping_Op + H_coulomb_Op
```

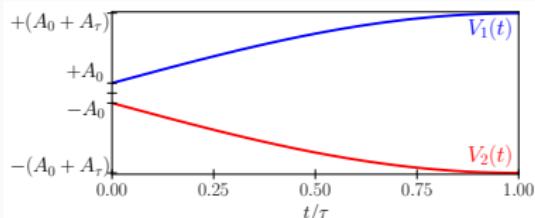
# Derretendo o dímero

Simulando o problema com o QuTip

13

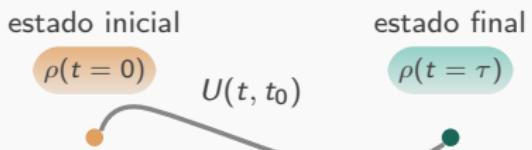
## ► Potencial dependente do tempo

```
def Vext_sin(A0+A, omega, tau, t, *args):
    return A0+A * sin(omega * t / tau)
```



## ► Estado inicial

```
def thermal_state(Ham, beta):
    bH = -beta * Ham
    Z = (bH.expm()).tr()
    rho_thermal = bH.expm() / Z
    return rho_thermal
```

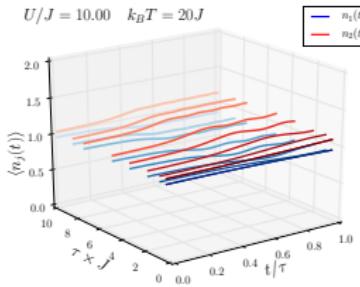
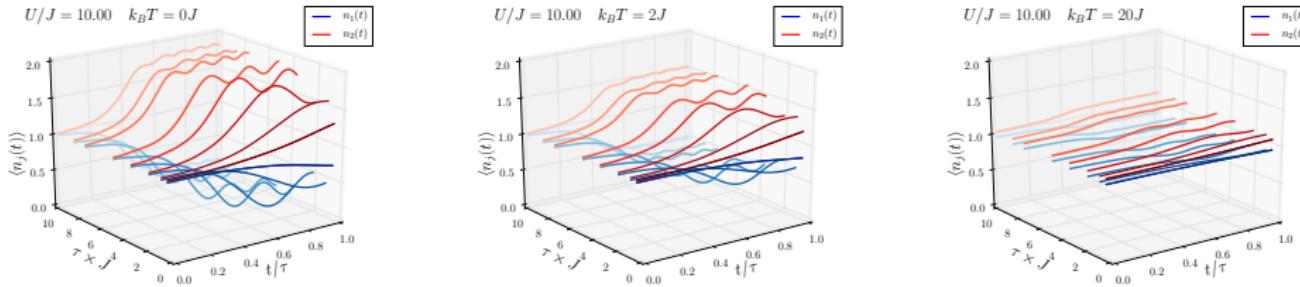
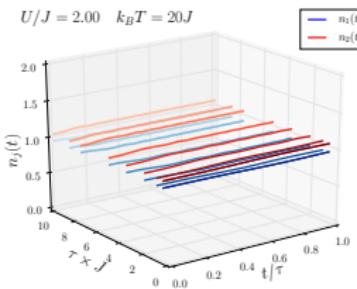
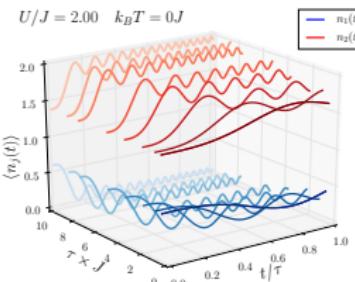
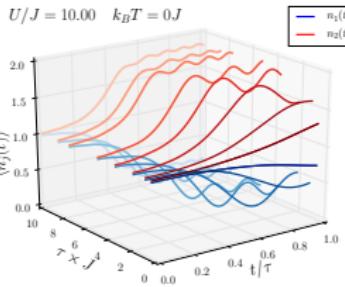
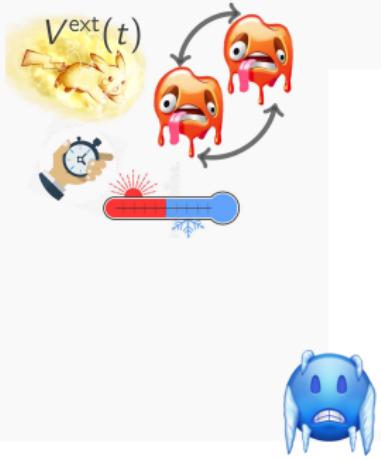


## ► Evolução temporal

```
Ht = [H0, [n1_Op, Vext_sin], [n2_Op, -Vext_sin]]
rho_t = qutip.mesolve(Ht, rho0, [0, tau], [], []).states
rho_tau = rho_t[-1]
```

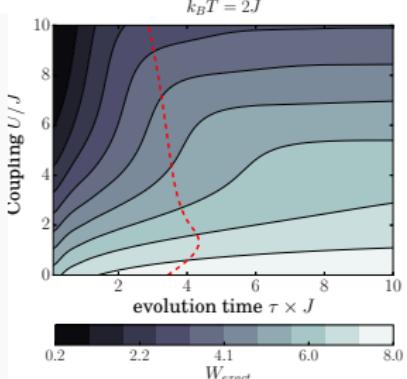
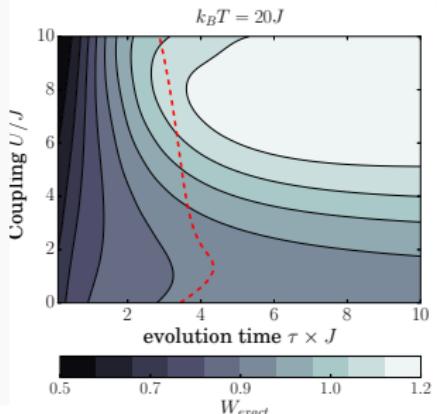
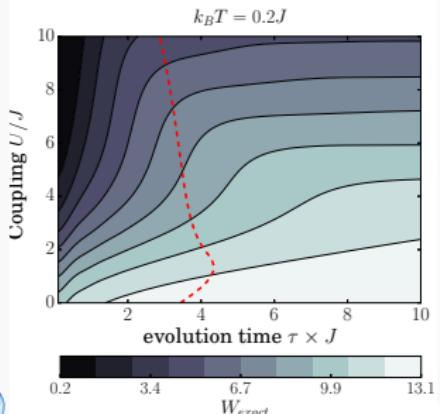
# Derretendo o dímero

## Analisando o problema: densidades



# Derretendo o dímero

## Analisando o problema: trabalho extraído

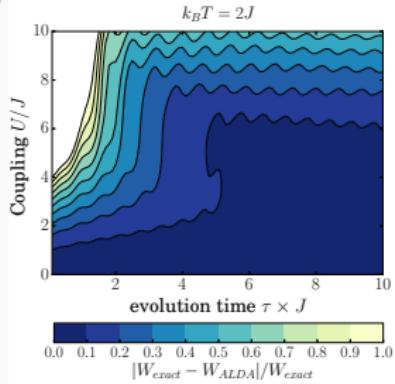
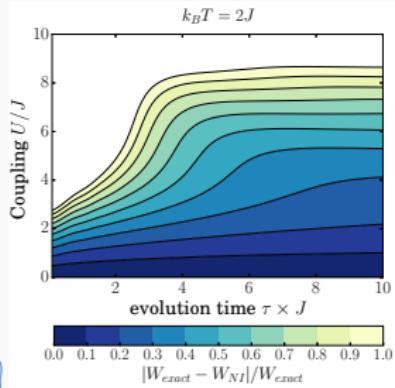


# Derretendo o dímero

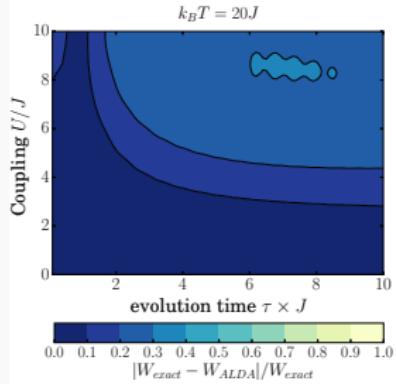
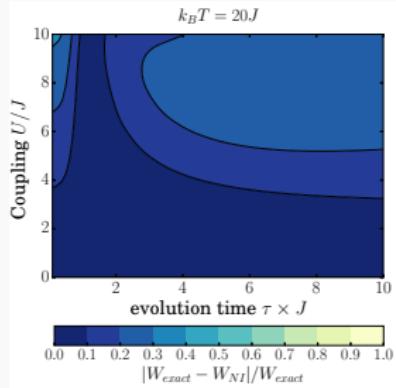
## Analisando o problema: aproximação



► não  
interagente



► LDA  
adiabática



The background features four large, rounded, abstract shapes resembling speech bubbles. There are two light blue shapes, one at the top and one on the left, and two yellow/orange shapes, one on the right and one at the bottom. Each shape has a small white horizontal bar near its base and a white circle near its top edge.

Obrigada pela atenção e pelas paçoquinhas!