“Ground states” of periodically driven systems

Le M. Cristian[1] Akashi Ryosuke[2] Shinji Tsuneyuki[2,3]

[1]Max Planck Institute for Structure and Dynamics of Matter

[2]Department of Physics, University of Tokyo

[3]Institute for Solid State Physics, University of Tokyo

NQS 2022
Nov 11, 2022

Contents

Contents

Amazing what we can achieve nowadays

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM
- **Exotic states of matter:** superconductors, topological material

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM
- **Exotic states of matter:** superconductors, topological material
- **Explore ultra-fast dynamics:** fs-lasers, TD-DFT

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM
- **Exotic states of matter:** superconductors, topological material
- **Explore ultra-fast dynamics:** fs-lasers, TD-DFT *-Is this what we really want?*

Holy grail of computational physics

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM
- **Exotic states of matter:** superconductors, topological material
- **Explore ultra-fast dynamics:** fs-lasers, TD-DFT *-Is this what we really want?*

Unsolved systems: Material + Laser

- Long time dynamics
- Many-body interaction
- Steady state with environment

Holy grail of Floquet physics

Amazing what we can achieve nowadays

- **Simulate materials just from composition:** DFT, CC-SD
- **Precise control of atoms:** optical tweezers, STM
- **Exotic states of matter:** superconductors, topological material
- **Explore ultra-fast dynamics:** fs-lasers, TD-DFT *-Is this what we really want?*

Unsolved systems: Material + Laser

- Time-periodic systems
- Many-body interaction
- Steady state with environment
- From first principles

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:**

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Just solve Schrodinger equation $\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle \qquad \left(e^{-iE_n t}\left|\Psi_n\right\rangle\right)$

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation *(Not for lasers)* $\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation $\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$
  (Not for lasers)
- **General time-dependent:**

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$
  (Not for lasers)
- **General time-dependent:** TD-Schrodinger equation $|\Psi(t+\delta_t)\rangle = |\Psi(t)\rangle - i\delta_t\hat{H}(t)|\Psi(t)\rangle$

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation *(Not for lasers)* $\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$
- **General time-dependent:** TD-Schrodinger equation *(Slow and inefficient - only laser pulses)* $|\Psi(t+\delta_t)\rangle = |\Psi(t)\rangle - i\delta_t\hat{H}(t)\,|\Psi(t)\rangle$

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation *(Not for lasers)* $\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$
- **General time-dependent:** TD-Schrodinger equation *(Slow and inefficient - only laser pulses)* $|\Psi(t+\delta_t)\rangle = |\Psi(t)\rangle - i\delta_t \hat{H}(t)\,|\Psi(t)\rangle$
- **Time-periodic:**

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation *(Not for lasers)* $\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$
- **General time-dependent:** TD-Schrodinger equation *(Slow and inefficient - only laser pulses)* $\left|\Psi(t+\delta_t)\right\rangle = \left|\Psi(t)\right\rangle - i\delta_t\hat{H}(t)\left|\Psi(t)\right\rangle$
- **Time-periodic:** Floquet solution[1] $[\hat{H}(t) - i\partial_t]\left|\Phi_n(t)\right\rangle = \epsilon_n\left|\Phi_n(t)\right\rangle$

[1] Shirley, J. H. (1965) *Physical Review*, **138**, B979; Sambe, H. (1973) *Physical Review A*, **7**, 2203 .

Why Floquet physics?

Dynamics in Quantum Mechanics

- **Static systems:** Schrodinger equation *(Not for lasers)* $$\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$
- **General time-dependent:** TD-Schrodinger equation *(Slow and inefficient - only laser pulses)* $$\left|\Psi(t+\delta_t)\right\rangle = \left|\Psi(t)\right\rangle - i\delta_t\hat{H}(t)\left|\Psi(t)\right\rangle$$
- **Time-periodic:** Floquet solution[1] *(Stable/slowly varying laser fields)* $$[\hat{H}(t) - i\partial_t]\left|\Phi_n(t)\right\rangle = \epsilon_n\left|\Phi_n(t)\right\rangle$$

[1] Shirley, J. H. (1965) *Physical Review*, **138**, B979; Sambe, H. (1973) *Physical Review A*, **7**, 2203 .

It works!

It works!

Key features:

- Energy Brillouin zone
- Stable eigenstates
- Adiabatic or Thermodynamic

It works!

Key features:

- Energy Brillouin zone
- Stable eigenstates
- Adiabatic or Thermodynamic

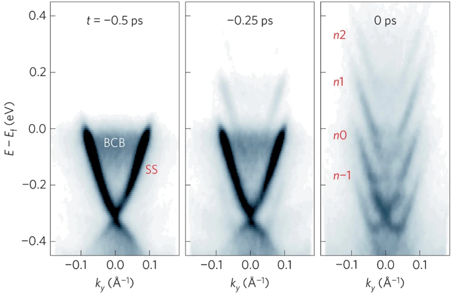

Figure: Floquet state in $\mathrm{Bi_2Se_3}$[2]

[2] Mahmood, F. et al. (2016) *Nature Physics*, **12**, 306 .

It works!

Key features:

- Energy Brillouin zone
- Stable eigenstates
- Adiabatic or Thermodynamic

Promising applications:

- Floquet engineering
- Topological material
- Quantum computing

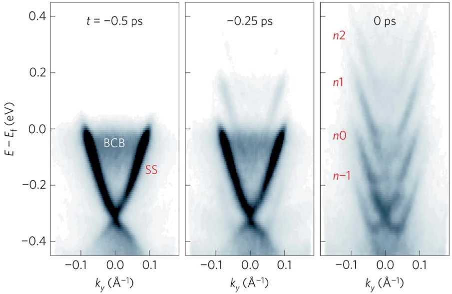

Figure: Floquet state in $\mathrm{Bi_2Se_3}$[2]

[2] Mahmood, F. et al. (2016) *Nature Physics*, **12**, 306 .

What's the issue?

Floquet + *ab-initio* = incompatible

Floquet + *ab-initio* = incompatible

First-principles methods:

- Derived from ground-state
  $\rightarrow$ Excited state, thermal, time-dependent...
- No assumption or prior experiment
- Self-consistent interaction

Floquet + *ab-initio* = incompatible

First-principles methods:

- Derived from ground-state
  → Excited state, thermal, time-dependent...
- No assumption or prior experiment
- Self-consistent interaction

Floquet systems:

- Energy Brillouin zone → No lowest "energy"[3]
- Models fitted to experiment or excited state calculations
- Unclear what's the target state
- No adiabatic continuation[4]

[3] Maitra, N. T. and Burke, K. (2007) *Chemical Physics Letters*, **441**, 167 .
[4] Hone, D. W. et al. (1997) *Physical Review A*, **56**, 4045 .

No Floquet ground state → No Floquet DFT

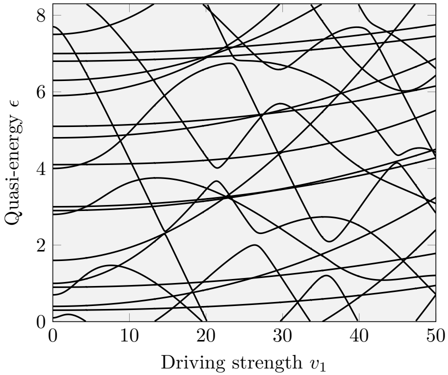

Figure: Typical Floquet picutre[5]

[5] Hone, D. W. et al. (1997) *Physical Review A*, **56**, 4045 .

No Floquet ground state → No Floquet DFT

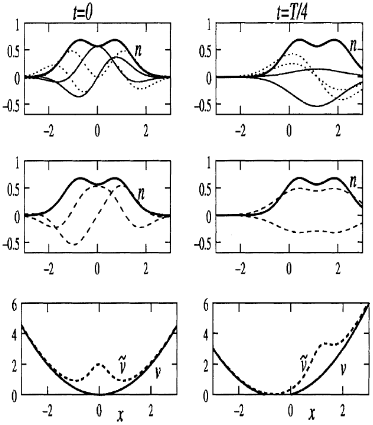

Figure: Floquet DFT breaking down[5]

[5] Maitra, N. T. and Burke, K. (2002) *Chemical Physics Letters*, **359**, 237 .

Floquet + *ab-initio* = incompatible

First-principles methods:

- Derived from ground-state
  → Excited state, thermal, time-dependent...
- No assumption or prior experiment
- Self-consistent interaction

Floquet systems:

- Energy Brillouin zone → No lowest "energy"[3]
- Models fitted to experiment or excited state calculations
- Unclear what's the target state
- No adiabatic continuation[4]

Due to quasi-energy formalism

[3] Maitra, N. T. and Burke, K. (2007) *Chemical Physics Letters*, **441**, 167 .
[4] Hone, D. W. et al. (1997) *Physical Review A*, **56**, 4045 .

Can we overcome this?

Contents

Why do we care about the energy?

Why do we care about the energy?

$$E[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle$$

Conserved quantum number

- Observable → Can be measured
- Does not change in time

Ehrenfest theorem

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \left\langle \frac{\partial\hat{\mathcal{O}}(t)}{\partial t} \right\rangle - i\left\langle [\hat{\mathcal{O}}(t), \hat{H}] \right\rangle$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left\langle \frac{\partial\hat{H}}{\partial t} \right\rangle = 0$$

Why do we care about the energy?

Conserved quantum number

- Observable $\to$ Can be measured
- Does not change in time

Observable of Hamiltonian

- Determines dynamics/conserved observables

$$E[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle$$

Ehrenfest theorem

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \left\langle \frac{\partial\hat{\mathcal{O}}(t)}{\partial t} \right\rangle - i\left\langle [\hat{\mathcal{O}}(t), \hat{H}] \right\rangle$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left\langle \frac{\partial\hat{H}}{\partial t} \right\rangle = 0$$

TD Schrodinger equation

$$\partial_t \left|\Psi(t)\right\rangle = -i\hat{H}\left|\Psi(t)\right\rangle$$

Why do we care about the energy?

$$E[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle$$

Ehrenfest theorem

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \left\langle \frac{\partial\hat{\mathcal{O}}(t)}{\partial t} \right\rangle - i\left\langle [\hat{\mathcal{O}}(t), \hat{H}] \right\rangle$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left\langle \frac{\partial\hat{H}}{\partial t} \right\rangle = 0$$

TD Schrodinger equation

$$\partial_t |\Psi(t)\rangle = -i\hat{H}|\Psi(t)\rangle$$

$$\langle\Psi_m|\hat{H}|\Psi_n\rangle = \delta_{mn}E_n$$

Conserved quantum number

- Observable → Can be measured
- Does not change in time

Observable of Hamiltonian

- Determines dynamics/conserved observables
- The observation does not (de-)excite the system

Why do we care about the energy?

$$E[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle$$

Ehrenfest theorem

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \left\langle \frac{\partial \hat{\mathcal{O}}(t)}{\partial t} \right\rangle - i \left\langle [\hat{\mathcal{O}}(t), \hat{H}] \right\rangle$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left\langle \frac{\partial \hat{H}}{\partial t} \right\rangle = 0$$

TD Schrodinger equation

$$\partial_t \left| \Psi(t) \right\rangle = -i\hat{H} \left| \Psi(t) \right\rangle$$

$$\langle \Psi_m | \hat{H} | \Psi_n \rangle = \delta_{mn} E_n$$

Thermal equilibrium

$$\rho = \sum_n e^{-\beta E_n} \left| \Psi_n \rangle\langle \Psi_n \right|$$

Conserved quantum number

- Observable $\rightarrow$ Can be measured
- Does not change in time

Observable of Hamiltonian

- Determines dynamics/conserved observables
- The observation does not (de-)excite the system

Thermodynamically

- Energy flows: High $\rightarrow$ Low
- 0K system $\rightarrow$ Ground state

Quasi-energy $\equiv$ Energy?

Original Floquet formulation

- First order periodic equation → Floquet

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$\left[\hat{H}(t) - i\partial_t\right] |\Psi(t)\rangle = 0$$

Original Floquet formulation

- First order periodic equation → Floquet
- Derived to satisfy Schrodinger equation

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$\left[\hat{H}(t) - i\partial_t\right] |\Psi(t)\rangle = 0$$

Floquet decomposition

$$\hat{U}(t) = \hat{P}(t) e^{-i\hat{G}t}$$

$$\hat{P}(t+T) = \hat{P}(t)$$

$$\hat{G} = \sum_n \epsilon_n |\Phi_n(0)\rangle\langle\Phi_n(0)|$$

$$\hat{P}(t) |\Phi(0)\rangle = |\Phi(t)\rangle$$

Original Floquet formulation

- First order periodic equation → Floquet
- Derived to satisfy Schrodinger equation

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$[\hat{H}(t) - i\partial_t] |\Psi(t)\rangle = 0$$

Floquet Schrodinger equation

$$[\hat{H}(t) - i\partial_t] |\Phi_n(t)\rangle = \epsilon_n |\Phi_n(t)\rangle$$

Original Floquet formulation

- First order periodic equation $\rightarrow$ Floquet
- Derived to satisfy Schrodinger equation

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$[\hat{H}(t) - i\partial_t] \left|\Psi(t)\right\rangle = 0$$

Floquet Schrodinger equation

$$\hat{H}^F \left|\Phi_n(t)\right\rangle = \epsilon_n \left|\Phi_n(t)\right\rangle$$

$$\begin{pmatrix} \Phi_n \text{ :Floquet eigenstate} \\ \epsilon_n \text{ :Quasi-energy} \end{pmatrix}$$

Original Floquet formulation

- First order periodic equation → Floquet
- Derived to satisfy Schrodinger equation
- Analogous to Bloch states

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$[\hat{H}(t) - i\partial_t] |\Psi(t)\rangle = 0$$

Floquet Schrodinger equation

$$\hat{H}^F |\Phi_n(t)\rangle = \epsilon_n |\Phi_n(t)\rangle$$

Physical Floquet state

$$|\Psi_n(t)\rangle = e^{-i\epsilon_n t} |\Phi_n(t)\rangle$$

$$\begin{pmatrix} \Phi_n \text{ :Floquet eigenstate} \\ \epsilon_n \text{ :Quasi-energy} \end{pmatrix}$$

Original Floquet formulation

- First order periodic equation $\rightarrow$ Floquet
- Derived to satisfy Schrodinger equation
- Analogous to Bloch states
  (Crystal momentum)

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$\left[\hat{H}(t) - i\partial_t\right] |\Psi(t)\rangle = 0$$

Floquet Schrodinger equation

$$\hat{H}^F |\Phi_n(t)\rangle = \epsilon_n |\Phi_n(t)\rangle$$

Physical Floquet state

$$|\Psi_n(t)\rangle = e^{-i\epsilon_n t} |\Phi_n(t)\rangle$$

$$\begin{pmatrix} \Phi_n \text{ :Floquet eigenstate} \\ \epsilon_n \text{ :Quasi-energy} \end{pmatrix}$$

Original Floquet formulation

- First order periodic equation $\rightarrow$ Floquet
- Derived to satisfy Schrodinger equation
- Analogous to Bloch states (Crystal momentum)
- Quasi-energy is not an observable
- No energy equivalent
- No ordering of the states

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$\left[\hat{H}(t) - i\partial_t\right] |\Psi(t)\rangle = 0$$

Floquet Schrodinger equation

$$\hat{H}^F |\Phi_n(t)\rangle = \epsilon_n |\Phi_n(t)\rangle$$

Physical Floquet state

$$|\Psi_n(t)\rangle = e^{-i\epsilon_n t} |\Phi_n(t)\rangle$$

$$\mathcal{O}(t) = \langle\Psi(t)|\hat{\mathcal{O}}|\Psi(t)\rangle \neq \langle\Phi(t)|\hat{\mathcal{O}}|\Phi(t)\rangle$$

$$\begin{pmatrix} \Phi_n & \text{:Floquet eigenstate} \\ \epsilon_n & \text{:Quasi-energy} \end{pmatrix}$$

Original Floquet formulation

- First order periodic equation $\rightarrow$ Floquet
- Derived to satisfy Schrodinger equation
- Analogous to Bloch states (Crystal momentum)
- Quasi-energy is not an observable
- No energy equivalent
- No ordering of the states
- ! Only propagation information

Periodic Hamiltonian

$$\hat{H}(t+T) = \hat{H}(t)$$

TD Schroedinger eq

$$[\hat{H}(t) - i\partial_t] |\Psi(t)\rangle = 0$$

Floquet Schrodinger equation

$$\hat{H}^F |\Phi_n(t)\rangle = \epsilon_n |\Phi_n(t)\rangle$$

Physical Floquet state

$$|\Psi_n(t)\rangle = e^{-i\epsilon_n t} |\Phi_n(t)\rangle$$

$$\mathcal{O}(t) = \langle\Psi(t)|\hat{\mathcal{O}}|\Psi(t)\rangle \neq \langle\Phi(t)|\hat{\mathcal{O}}|\Phi(t)\rangle$$

$$\begin{pmatrix} \Phi_n \text{ :Floquet eigenstate} \\ \epsilon_n \text{ :Quasi-energy} \end{pmatrix}$$

Role of quasi-energy

	Energy	Quasi-energy
Observable	Yes	No
Ordering	Yes	No
Oscillation freq.	Yes	Yes
Commuting operators	Static/conserved	Time-periodic
Thermodynamics	Fully determined	Allowed transitions
Ground state	$0K$ state	Not exist

We need another quantum number!

A new Floquet picture

A new Floquet picture

Fundamental symmetry

$$[\hat{H}(t), \hat{T}] = 0$$

- From fundamental symmetry[6]

$$(\hat{T}\hat{O}(t) = \hat{O}(t+T)\hat{T})$$

[6] Le, C. M. et al. (2022) *Physical Review A*, **105**, 052213; Le, C. M. (2021) *University of Tokyo*, PhD thesis .

A new Floquet picture

- From fundamental symmetry[6]
- Derived by Bloch analogy

Fundamental symmetry

$$[\hat{H}(t), \hat{T}] = 0$$

Effective commutation

$$[\hat{H}^F, \hat{\bar{H}}_n] = 0$$

Floquet eigenstates

$$\begin{cases} \hat{H}^F \left|\Phi_{na}\right\rangle = \epsilon_n \left|\Phi_{na}\right\rangle \\ \hat{\bar{H}}_n \left|\Phi_{na}\right\rangle = \bar{E}_{na} \left|\Phi_{na}\right\rangle \end{cases}$$

$$(\hat{T}\hat{O}(t) = \hat{O}(t+T)\hat{T})$$

[6] Le, C. M. et al. (2022) *Physical Review A*, **105**, 052213; Le, C. M. (2021) *University of Tokyo*, PhD thesis .

A new Floquet picture

- From fundamental symmetry[6]
- Derived by Bloch analogy

Fundamental symmetry

$$[\hat{H}(t), \hat{T}] = 0$$

Bloch symmetry

$$[\hat{H}, \hat{\vec{\mathbf{R}}}] = 0$$

Bloch eigenstates

$$\begin{cases} \hat{\vec{\mathbf{k}}} u_{\vec{\mathbf{k}}n} = \vec{\mathbf{k}} u_{\vec{\mathbf{k}}n} \\ \hat{H}_{\vec{\mathbf{k}}} u_{\vec{\mathbf{k}}n} = E_{\vec{\mathbf{k}}n} u_{\vec{\mathbf{k}}n} \end{cases}$$

$$\begin{pmatrix} \hat{T}\hat{O}(t) = \hat{O}(t+T)\hat{T} \\ \hat{\vec{\mathbf{R}}}\hat{O}(\vec{\mathbf{r}}) = \hat{O}(\vec{\mathbf{r}}+\vec{\mathbf{R}})\hat{\vec{\mathbf{R}}} \end{pmatrix}$$

[6] Le, C. M. et al. (2022) *Physical Review A*, **105**, 052213; Le, C. M. (2021) *University of Tokyo*, PhD thesis .

A new Floquet picture

- From fundamental symmetry[6]
- Derived by Bloch analogy
- Complete eigenstate picture

Fundamental symmetry

$$[\hat{H}(t), \hat{T}] = 0$$

Effective commutation

$$[\hat{H}^F, \hat{\bar{H}}_n] = 0$$

Floquet eigenstates

$$\begin{cases} \hat{H}^F |\Phi_{na}\rangle = \epsilon_n |\Phi_{na}\rangle \\ \hat{\bar{H}}_n |\Phi_{na}\rangle = \bar{E}_{na} |\Phi_{na}\rangle \end{cases}$$

Average energy

$$\begin{aligned} \bar{E}_{na} &= \langle\Phi_{na}|\hat{\bar{H}}_n|\Phi_{na}\rangle \\ &= \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_{-\mathcal{T}}^{\mathcal{T}} \langle\Psi_{na}|\hat{H}(t)|\Psi_{na}\rangle \, \mathrm{d}t \end{aligned}$$

$$(\hat{T}\hat{O}(t) = \hat{O}(t+T)\hat{T})$$

[6] Le, C. M. et al. (2022) *Physical Review A*, **105**, 052213; Le, C. M. (2021) *University of Tokyo*, PhD thesis .

A new Floquet picture

- From fundamental symmetry[6]
- Derived by Bloch analogy
- Complete eigenstate picture
- Observable (energy equivalent)
- Ordering quantum number
- Lower-bounded

Fundamental symmetry

$$[\hat{H}(t), \hat{T}] = 0$$

Effective commutation

$$[\hat{H}^F, \hat{\bar{H}}_n] = 0$$

Floquet eigenstates

$$\begin{cases} \hat{H}^F \left|\Phi_{na}\right\rangle = \epsilon_n \left|\Phi_{na}\right\rangle \\ \hat{\bar{H}}_n \left|\Phi_{na}\right\rangle = \bar{E}_{na} \left|\Phi_{na}\right\rangle \end{cases}$$

Average energy

$$\bar{E}_{na} = \langle\Phi_{na}|\hat{\bar{H}}_n|\Phi_{na}\rangle = \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_{-\mathcal{T}}^{\mathcal{T}} \langle\Psi_{na}|\hat{H}(t)|\Psi_{na}\rangle \, \mathrm{d}t$$

$$(\hat{T}\hat{O}(t) = \hat{O}(t+T)\hat{T})$$

[6] Le, C. M. et al. (2022) *Physical Review A*, **105**, 052213; Le, C. M. (2021) *University of Tokyo*, PhD thesis .

Role of average energy

	Energy	Quasi-energy	Average energy
Observable	Yes	No	Yes
Ordering	Yes	No	Yes
Oscillation freq.	Yes	Yes	No
Commuting operators	Static/conserved	Time-periodic	
Thermodynamics	Fully determined	Allowed transitions	Overall transition
Ground state	$0K$ state	$\approx 0K$ state?	

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix}$$

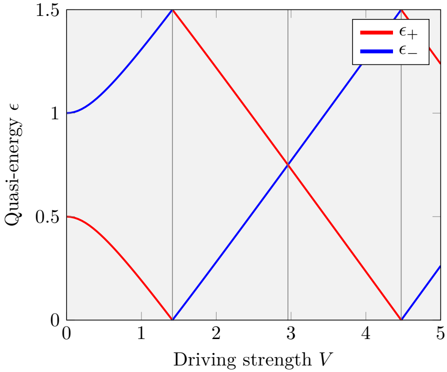

Figure: Original quasi-energy picture

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix}$$

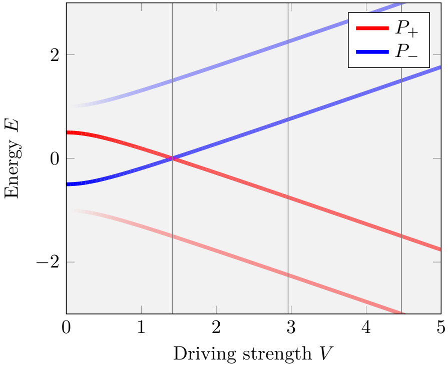

Figure: Energy spectra

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix}$$

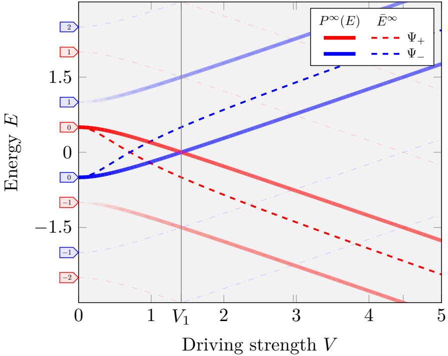

Figure: Average energy

Example: Particle in a box

$$\hat{H}(t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + v_1 \sin\left(\frac{\pi x}{2a}\right)\cos(\omega t)$$

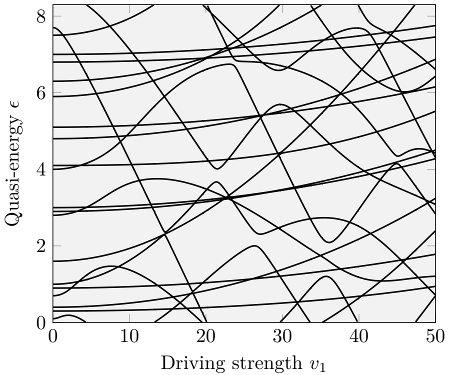

Figure: Original quasi-energy picture

Example: Particle in a box

$$\hat{H}(t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + v_1 \sin\left(\frac{\pi x}{2a}\right)\cos(\omega t)$$

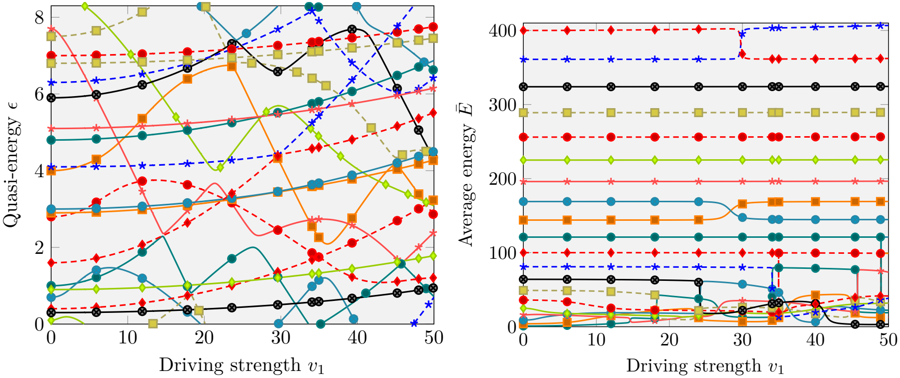

Figure: Quasi-energy + Average energy

Example: Particle in a box

$$\hat{H}(t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + v_1 \sin\left(\frac{\pi x}{2a}\right)\cos(\omega t)$$

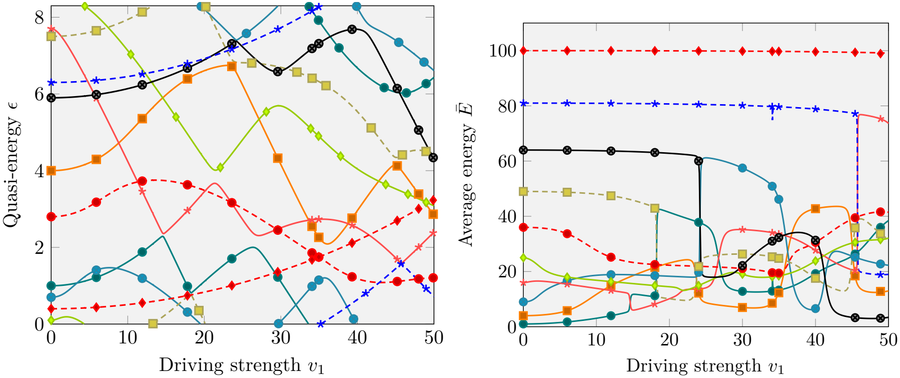

Figure: Lowest energy eigenstates

Contents

Static open quantum system

Open quantum system

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}_{SB}$$

- System coupled to thermal bath

Static open quantum system

- System coupled to thermal bath
- Depends on the master equation
- Simplest form: Lindbladian

Open quantum system

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_m \left[-\Gamma_{nm} \rho_n + \Gamma_{mn} \rho_m \right]$$

$$\left(\rho(t) = \sum_n \rho_n(t) \left| \Psi_n(0) \right\rangle\!\left\langle \Psi_n(0) \right| \right)$$

Static open quantum system

Open quantum system

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}_{SB}$$

- System coupled to thermal bath
- Depends on the master equation
- Simplest form: Lindbladian
  - Weak coupling
  - Markov approx., etc.

Lindladian master equation

$$\partial_t \rho_n(t) = 2\sum_m \left[-\Gamma_{nm}\rho_n + \Gamma_{mn}\rho_m\right]$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \left|\Psi_n(0)\right\rangle\!\left\langle\Psi_n(0)\right| \\ \\ \\ \end{pmatrix}$$

Static open quantum system

- System coupled to thermal bath
- Depends on the master equation
- Simplest form: Lindbladian
  - Weak coupling
  - Markov approx., etc.

Open quantum system

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_m \left[-\Gamma_{nm}\rho_n + \Gamma_{mn}\rho_m \right]$$

Dissipation strength

$$\Gamma_{mn} = V_{mn}^2 \pi \nu(|\omega_{mn}|) N_B(-\omega_{mn})$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \, |\Psi_n(0)\rangle\langle\Psi_n(0)| \\ \omega_{mn} = E_n - E_m \\ V_{mn} = \langle \Psi_m | \hat{V}_{SB} | \Psi_n \rangle \end{pmatrix}$$

Static open quantum system

- System coupled to thermal bath
- Depends on the master equation
- Simplest form: Lindbladian
  - Weak coupling
  - Markov approx., etc.
- Focus on the steady state
- Ignore coherence, Lamb shift, etc.

Open quantum system

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2\sum_m \left[-\Gamma_{nm}\rho_n + \Gamma_{mn}\rho_m\right]$$

Dissipation strength

$$\Gamma_{mn} = V_{mn}^2 \pi\nu(|\omega_{mn}|) N_B(-\omega_{mn})$$

Steady state

$$\partial_t \rho_n(t) = 0$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \left|\Psi_n(0)\right\rangle\!\left\langle\Psi_n(0)\right| \\ \omega_{mn} = E_n - E_m \\ V_{mn} = \langle\Psi_m|\hat{V}_{SB}|\Psi_n\rangle \end{pmatrix}$$

Floquet open quantum system

Floquet Open quantum system

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_{m,k} \left[-\Gamma_{nm}^{(k)} \rho_n + \Gamma_{mn}^{(k)} \rho_m \right]$$

Dissipation strength

$$\Gamma_{mn}^{(k)} = \left| V_{mn}^{(k)} \right|^2 \pi \nu(|\omega_{mnk}|) N_B(-\omega_{mnk})$$

Steady state

$$\partial_t \rho_n(t) = 0$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \left|\Phi_n(0)\right\rangle\!\left\langle\Phi_n(0)\right| \\ \omega_{mnk} = \epsilon_n - \epsilon_m + k\omega \\ V_{mn}^{(k)} = \sum_l \left\langle \Phi_m^{(l)} \middle| \hat{V}_{SB} \middle| \Psi_n^{(k+l)} \right\rangle \end{pmatrix}$$

Floquet open quantum system

- Solved like the static system

Floquet Open quantum system

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_{m,k} \left[-\Gamma^{(k)}_{nm} \rho_n + \Gamma^{(k)}_{mn} \rho_m \right]$$

Dissipation strength

$$\Gamma^{(k)}_{mn} = \left| V^{(k)}_{mn} \right|^2 \pi \nu(|\omega_{mnk}|) N_B(-\omega_{mnk})$$

Steady state

$$\partial_t \rho_n(t) = 0$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \left|\Phi_n(0)\right\rangle\!\left\langle\Phi_n(0)\right| \\ \omega_{mnk} = \epsilon_n - \epsilon_m + k\omega \\ V^{(k)}_{mn} = \sum_l \left\langle \Phi^{(l)}_m \middle| \hat{V}_{SB} \middle| \Psi^{(k+l)}_n \right\rangle \end{pmatrix}$$

Floquet open quantum system

Floquet Open quantum system

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_{m,k} \left[-\Gamma^{(k)}_{nm} \rho_n + \Gamma^{(k)}_{mn} \rho_m \right]$$

Dissipation strength

$$\Gamma^{(k)}_{mn} = \left| V^{(k)}_{mn} \right|^2 \pi \nu(|\omega_{mnk}|) N_B(-\omega_{mnk})$$

Steady state

$$\partial_t \rho_n(t) = 0$$

$$\begin{pmatrix} \rho(t) = \sum_n \rho_n(t) \left|\Phi_n(0)\right\rangle\!\left\langle\Phi_n(0)\right| \\ \omega_{mnk} = \epsilon_n - \epsilon_m + k\omega \\ V^{(k)}_{mn} = \sum_l \left\langle \Phi^{(l)}_m \middle| \hat{V}_{SB} \middle| \Psi^{(k+l)}_n \right\rangle \end{pmatrix}$$

- Solved like the static system
- Multiple dissipation channels

Floquet open quantum system

- Solved like the static system
- Multiple dissipation channels

→ No longer thermal distribution

→ SS depends on bath coupling

Floquet Open quantum system

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{V}_{SB}$$

Lindladian master equation

$$\partial_t \rho_n(t) = 2 \sum_{m,k} \left[-\Gamma^{(k)}_{nm} \rho_n + \Gamma^{(k)}_{mn} \rho_m \right]$$

Dissipation strength

$$\Gamma^{(k)}_{mn} = \left| V^{(k)}_{mn} \right|^2 \pi \nu(|\omega_{mnk}|) N_B(-\omega_{mnk})$$

Steady state

$$\partial_t \rho_n(t) = 0$$

$$\left(\begin{array}{c} \rho(t) = \sum_n \rho_n(t) \left|\Phi_n(0)\right\rangle\!\left\langle\Phi_n(0)\right| \\ \omega_{mnk} = \epsilon_n - \epsilon_m + k\omega \\ V^{(k)}_{mn} = \sum_l \left\langle \Phi^{(l)}_m \middle| \hat{V}_{SB} \middle| \Psi^{(k+l)}_n \right\rangle \end{array} \right)$$

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix} + V_{SB}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}(b+b^\dagger) + \omega_B b^\dagger b$$

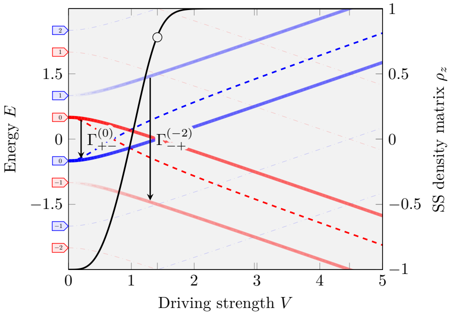

Figure: Steady state $\rho_{SS} = \frac{1+\rho_z}{2}|\Phi_+\rangle\langle\Phi_+| + \frac{1-\rho_z}{2}|\Phi_-\rangle\langle\Phi_-|$

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix} + V_{SB}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}(b + b^\dagger) + \omega_B b^\dagger b$$

Notice

- $\exists$ non-overlapping states
- Steady state $\approx$ Ground state

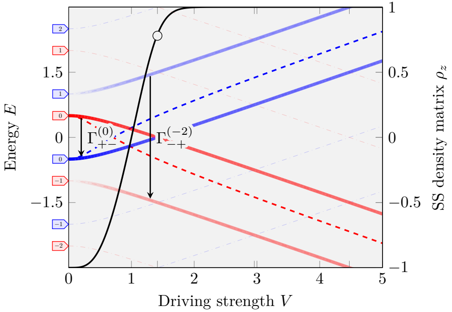

Figure: Steady state $\rho_{SS} = \frac{1+\rho_z}{2}\left|\Phi_+\right\rangle\!\left\langle\Phi_+\right| + \frac{1-\rho_z}{2}\left|\Phi_-\right\rangle\!\left\langle\Phi_-\right|$

Role of Floquet ground states

Energy spectra

$$\left|\Phi_n^{(k)}\right\rangle = \sqrt{P_n^{(k)}}\left|\tilde{\Phi}_n^{(k)}\right\rangle$$

- Separate the amplitude of the energy spectra

$$\begin{pmatrix} \left|\Phi_n(t)\right\rangle = \sum_k e^{-ik\omega t}\left|\Phi_n^{(k)}\right\rangle \\ \left\langle\tilde{\Phi}_n^{(k)}\middle|\tilde{\Phi}_n^{(k)}\right\rangle = 1 \end{pmatrix}$$

Role of Floquet ground states

Energy spectra

$$\left|\Phi_n^{(k)}\right\rangle = \sqrt{P_n^{(k)}}\left|\tilde{\Phi}_n^{(k)}\right\rangle$$

$$\Gamma_{mn}^{(k)} \propto \left|V_{mn}^{(k)}\right|^2 \propto \sum_l P_m^{(l)} P_n^{(k+l)}$$

- Separate the amplitude of the energy spectra
- Dissipation is proportional to spectra

$$\begin{pmatrix} \left|\Phi_n(t)\right\rangle = \sum_k e^{-ik\omega t}\left|\Phi_n^{(k)}\right\rangle \\ \left\langle \tilde{\Phi}_n^{(k)} \middle| \tilde{\Phi}_n^{(k)} \right\rangle = 1 \end{pmatrix}$$

Role of Floquet ground states

- Separate the amplitude of the energy spectra
- Dissipation is proportional to spectra
- Define: spectra overlap measure

Energy spectra

$$\left|\Phi_n^{(k)}\right\rangle = \sqrt{P_n^{(k)}}\left|\tilde{\Phi}_n^{(k)}\right\rangle$$

$$\Gamma_{mn}^{(k)} \propto \left|V_{mn}^{(k)}\right|^2 \propto \sum_l P_m^{(l)} P_n^{(k+l)}$$

Spectra overlap measure

$$S_{mn} \approx \max_k \left\{ \sum_l P_m^{(l)} P_n^{(k+l)} \Big|_{\bar{E}_n > \bar{E}_m}^{\epsilon_n + k\omega < \epsilon_m} \right\}$$

$$\begin{pmatrix} \left|\Phi_n(t)\right\rangle = \sum_k e^{-ik\omega t}\left|\Phi_n^{(k)}\right\rangle \\ \left\langle \tilde{\Phi}_n^{(k)} \middle| \tilde{\Phi}_n^{(k)} \right\rangle = 1 \end{pmatrix}$$

Role of Floquet ground states

- Separate the amplitude of the energy spectra
- Dissipation is proportional to spectra
- Define: spectra overlap measure
- If weakly overlapping states:
  - Dissipation: high AE → low AE
  - Steady state: AE ground state

Energy spectra

$$\left|\Phi_n^{(k)}\right\rangle = \sqrt{P_n^{(k)}}\left|\tilde{\Phi}_n^{(k)}\right\rangle$$

$$\Gamma_{mn}^{(k)} \propto \left|V_{mn}^{(k)}\right|^2 \propto \sum_l P_m^{(l)} P_n^{(k+l)}$$

Spectra overlap measure

$$S_{mn} \approx \max_k \left\{ \sum_l P_m^{(l)} P_n^{(k+l)} \Big|_{\substack{\epsilon_n + k\omega < \epsilon_m \\ \bar{E}_n > \bar{E}_m}} \right\}$$

Approx. master equation

$$\bar{E}_n > \bar{E}_m \rightarrow \begin{cases} \partial_t \rho_n = -\Gamma_{nm}\rho_n + \mathcal{O}(S_{mn}) \\ \partial_t \rho_m = -\mathcal{O}(S_{mn}) + \Gamma_{nm}\rho_m \end{cases}$$

$$\begin{pmatrix} \left|\Phi_n(t)\right\rangle = \sum_k e^{-ik\omega t}\left|\Phi_n^{(k)}\right\rangle \\ \left\langle \tilde{\Phi}_n^{(k)} \middle| \tilde{\Phi}_n^{(k)} \right\rangle = 1 \end{pmatrix}$$

Example: Two-level system

$$\hat{H}(t) = \begin{bmatrix} \frac{\omega_0}{2} & \frac{V}{2}e^{-i\omega t} \\ \frac{V}{2}e^{i\omega t} & -\frac{\omega_0}{2} \end{bmatrix} + V_{SB}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}(b + b^\dagger) + \omega_B b^\dagger b$$

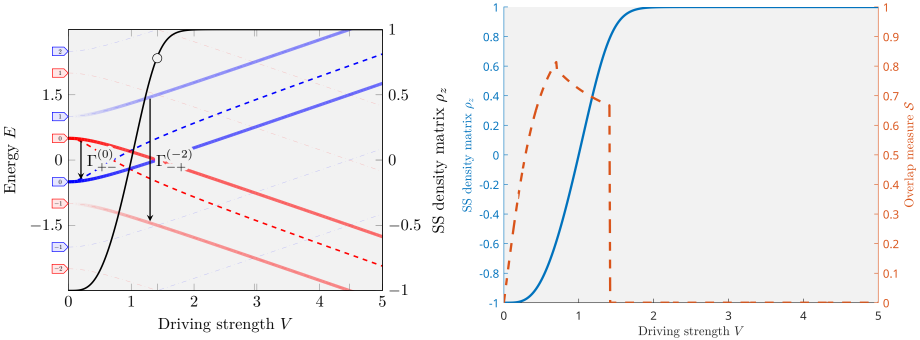

Figure: Steady state and spectra overlap

Floquet Hartree-Fock:

- Possible because of Ritz variation
- Similar derivation to static HF

Hartree-Fock ansatz

$$\Phi_0(\vec{\mathbf{r}}_1\vec{\mathbf{r}}_2\ldots t) \approx \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(\vec{\mathbf{r}}_1 t) & \phi_2(\vec{\mathbf{r}}_1 t) & \ldots \\ \phi_1(\vec{\mathbf{r}}_2 t) & \phi_2(\vec{\mathbf{r}}_2 t) & \ldots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

Floquet Hartree-Fock:

- Possible because of Ritz variation
- Similar derivation to static HF
- **Ansatz:** Many-body Floquet ground state is close to a Slater determinant

Floquet Hartree-Fock:

- Possible because of Ritz variation
- Similar derivation to static HF
- **Ansatz:** Many-body Floquet ground state is close to a Slater determinant
- Constrained minimization problem:
  - **Constraints:** Orthonormal orbitals, Many-body quasi-energy eigenstate

Hartree-Fock ansatz

$$\Phi_0(\vec{\mathbf{r}}_1\vec{\mathbf{r}}_2\ldots t) \approx \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\vec{\mathbf{r}}_1 t) & \phi_2(\vec{\mathbf{r}}_1 t) & \ldots \\ \phi_1(\vec{\mathbf{r}}_2 t) & \phi_2(\vec{\mathbf{r}}_2 t) & \ldots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

HF self-consistency

$$\left[\hat{F}(t) - i\partial_t\right] |\phi_i(t)\rangle = \varepsilon_i |\phi_i(t)\rangle$$

$$\left(\hat{F}[\phi] |\phi_i\rangle = \hat{h} |\phi_i\rangle + \sum \langle\phi_j|\hat{V}_{ee}|\phi_j\phi_i\rangle \right)$$

Floquet Hartree-Fock:

- Possible because of Ritz variation
- Similar derivation to static HF
- **Ansatz:** Many-body Floquet ground state is close to a Slater determinant
- Constrained minimization problem:
  - **Constraints:** Orthonormal orbitals, Many-body quasi-energy eigenstate
  - **Objective:** Many-body average energy

Hartree-Fock ansatz

$$\Phi_0(\vec{\mathbf{r}}_1\vec{\mathbf{r}}_2\dots t) \approx \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(\vec{\mathbf{r}}_1 t) & \phi_2(\vec{\mathbf{r}}_1 t) & \dots \\ \phi_1(\vec{\mathbf{r}}_2 t) & \phi_2(\vec{\mathbf{r}}_2 t) & \dots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

HF self-consistency

$$[\hat{F}(t) - i\partial_t]\,|\phi_i(t)\rangle = \varepsilon_i\,|\phi_i(t)\rangle$$

HF minimization

$$\bar{E}_0 = \min_{\{\phi\}}\Big\{\bar{\mathcal{E}}[\phi] + \sum_{ij}\lambda_j\,\langle\varphi_j|\hat{F} - i\partial_t - \varepsilon_i|\phi_i\rangle + \sum_{ij}\mu_{ij}\Big(\langle\phi_j|\phi_i\rangle - \delta_{ij}\Big)\Big\}$$

$$\begin{pmatrix} \hat{F}[\phi]\,|\phi_i\rangle = \hat{h}\,|\phi_i\rangle + \sum\langle\phi_j|\hat{V}_{ee}|\phi_j\phi_i\rangle \\ \bar{\mathcal{E}}[\phi] = \sum\langle\phi_i|\hat{h}|\phi_i\rangle + \frac{1}{2}\langle\phi_i\phi_j|\hat{V}_{ee}|\phi_i\phi_j\rangle \end{pmatrix}$$

Example: Hubbard dimer

$$\hat{H}(t) = \frac{v(t)}{2}(\hat{n}_1 - \hat{n}_2) - t(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$$

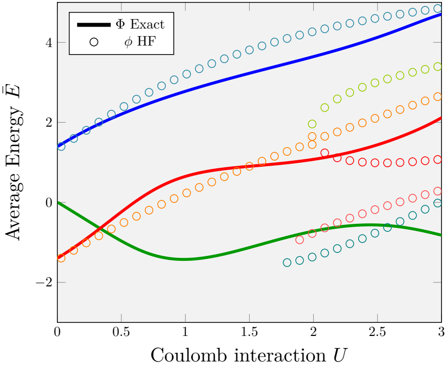

Figure: Average energy

Example: Hubbard dimer

$$\hat{H}(t) = \frac{v(t)}{2}(\hat{n}_1 - \hat{n}_2) - t(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$$

$$|\Phi(0)\rangle = |\phi_{\uparrow\theta}(0)\phi_{\downarrow\theta}(0)\rangle$$

$$|\phi_\theta(0)\rangle = \begin{pmatrix}\cos\theta \\ \sin\theta\end{pmatrix}$$

NSCF: Static HF → Floquet

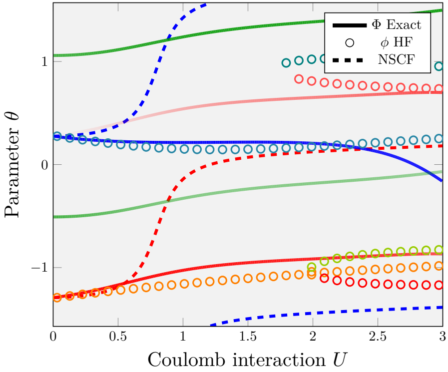

Figure: Initial state parameter

Advantages

- Self-consistent driving and MB interaction
- Guarantees time-periodicity (cf. TD-HF)
- Does not require accurate propagation

Disadvantages

- No neat single equation form (cf. static HF)
- No self-consistent loop approach
- Exist self-consistent artifact solutions that break the ansatz

Conclusion

New Floquet formalism

- Ordered states with lower bounded ground state
- Resolves adiabatic continuity
- Has Ritz variational principle and more

Ground state application

- It is the steady state if weakly overlapping spectra
- First principles methods can be adapted

Things to come

Open quantum system

- Apply to quasi-energy (near) degenerate states as well
- Finite temperature approximation
- General applicability

First principles methods

- Floquet Hartree-Fock for real systems
- Post Hartree-Fock methods
- Density Functional Theory