Time-dependent Variational Methods for Many-Body Quantum Systems

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Workshop on Quantum Simulation and Quantum Devices

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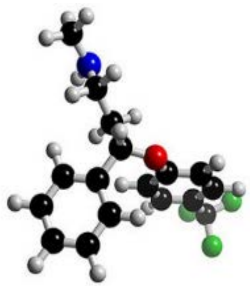
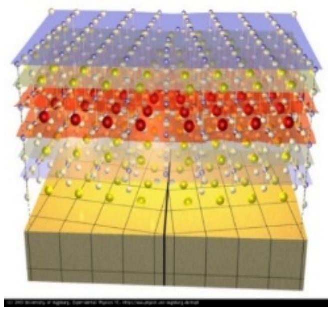
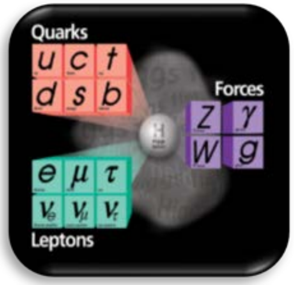
QUANTUM MANY-BODY PROBLEMS







Hard to describe

QUANTUM MANY-BODY PROBLEMS

Many methods:

- Exact diagonalization
- Mean-field
- Hartree-Fock
- BCS
- Gutzwiller
- Bogoliubov-de Gennes
- Dynamical mean-field
- Density Functional
- Coupled-cluster
- Tensor networks

QUANTUM MANY-BODY PROBLEMS

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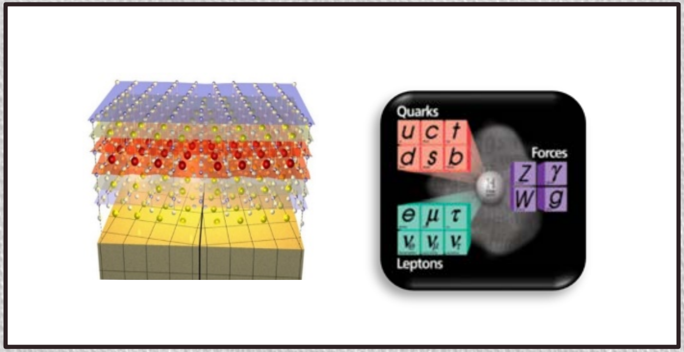
- Many are based on a variational principle
- Most of them are for thermal equilibrium

OUTLINE



- Time-dependent variational methods:
  - Non-Gaussian states
- Differential geometry:
  - Kähler manifolds
  - Imaginary time
- Benchmarks and applications
- Finite temperature

VARIATIONAL METHODS

VARIATIONAL METHODS
Ground State

- Hamiltonian: $H = \sum_n h_n$

- Variational principle: Ground state (T=0)

$$E_0 = \min_{\Psi} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

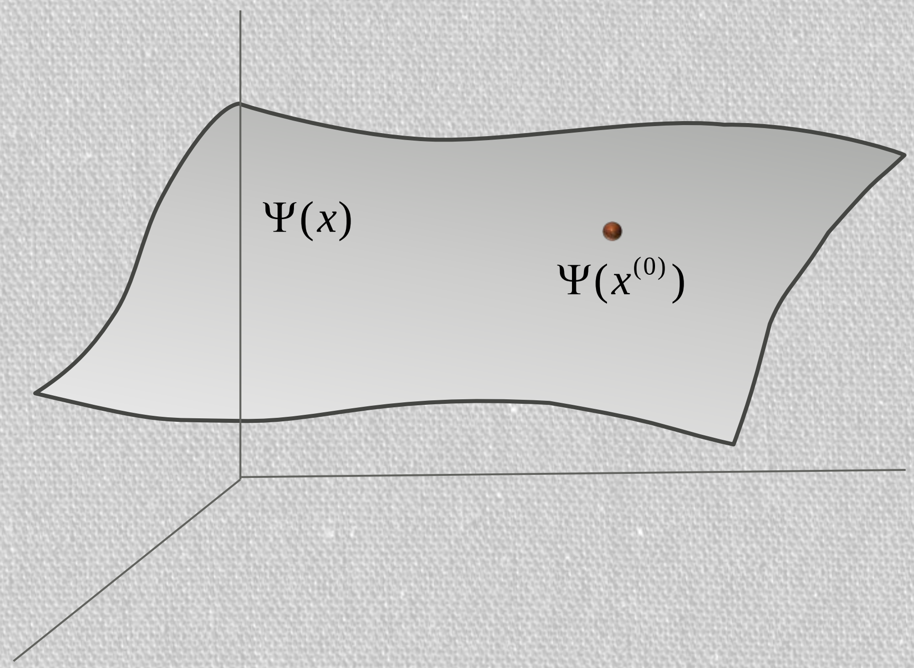
- Variational states: $|\Psi(x_1, \ldots, x_p)\rangle$ where $x_\mu \in \mathbb{R}$

$$E_0 \leq \min_{x} \frac{\langle \Psi(x) | H | \Psi(x) \rangle}{\langle \Psi(x) | \Psi(x) \rangle}$$

$\longrightarrow x^{(0)} \longrightarrow \langle O \rangle_0$

VARIATIONAL METHODS
Ground State

- Variational Manifold:



VARIATIONAL METHODS
Dynamics

- Action: $S = \int_0^t dt\ L(t)$

  Lagrangian: $L(t) = \frac{i}{2}\left[\langle \Psi \mid \partial_t \Psi \rangle - \langle \partial_t \Psi \mid \Psi \rangle\right] - \langle \Psi \mid H \mid \Psi \rangle$

- Variational principle:

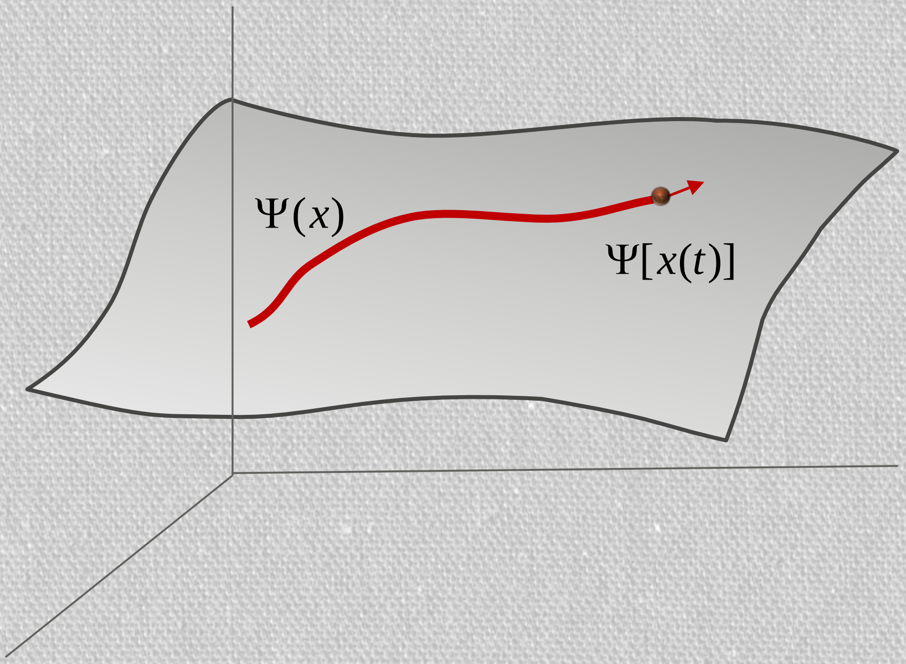
  $\partial S = 0$ $\longrightarrow$ (Euler-Lagrange) $i\partial_t \mid \Psi \rangle = H \mid \Psi \rangle$

- Variational states: $\mid \Psi(x_1, \ldots, x_p) \rangle$ where $x_\mu(t) \in \mathbb{R}$

  $\tilde{\partial} S = 0$ $\longrightarrow$ (Euler-Lagrange) $\dot{x}_\mu(t) = f_\mu(x)$

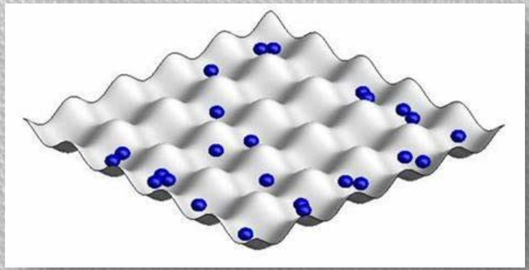
VARIATIONAL METHODS
Dynamics

- Variational Manifold:



VARIATIONAL METHODS
Example: Bose-Einstein Condensate

- Bose Hubbard model:



$$H = -t \sum_{\langle n,m \rangle} b_n^\dagger b_m + \frac{U}{2} \sum_n b_n^\dagger b_n^\dagger b_n b_n + \sum_n \mu_n b_n^\dagger b_n$$

- Variational states:

$$|\Psi(x_n, p_n)\rangle = e^{i\sum_n (x_n + ip_n) b_n^\dagger} |\Omega\rangle$$

It is convenient to define $\varphi_n = x_n + ip_n$

- Ground state: Gross-Pitaevskii equation
- Dynamics: Time-dependent Gross-Pitaevskii equation

QUANTUM MANY-BODY SYSTEMS

- Variational families:
  - Tensor Network States
  - Laughlin States
  - Gutzwiller Ansatz
  - Coherent States
  - Hartree-Fock States
  - BCS States

QUANTUM MANY-BODY SYSTEMS

- Variational families:
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(Coherent States, Hartree-Fock States, BCS States } Gaussian States)

QUANTUM MANY-BODY SYSTEMS
Gaussian States

- Bosons: $|\Psi\rangle = e^{i\sum_n \varphi_n b_n^\dagger} e^{i\sum_{n.m} \xi_{n,m} b_n^\dagger b_m^\dagger} |\Omega\rangle$
  - Displacement: Δ_n
  - Covariant matrix: $\Gamma_{n,m}$
- Fermions: $|\Psi\rangle = e^{i\sum_{n.m} \xi_{n,m} a_n^\dagger a_m^\dagger} |\Omega\rangle$
  - Covariant matrix: $\gamma_{n,m}$

\+ Describe many phenomena: BEC, BCS, etc

Easy to compute (Wick‘s theorem)

− Only weakly interacting (Wick‘s theorem)

No correlations between bosons and fermions

QUANTUM MANY-BODY SYSTEMS

Non-Gaussian States

Shi, Demler, JIC, Ann. Phys. (2018)

- States: $|\Psi\rangle \propto U|\Phi\rangle$

arbitrary Gaussian of fermions and/or bosons

non-Gaussian
such that we can compute
expectation values efficiently

$$E = \langle \Phi_G | U^\dagger H U | \Phi_G \rangle$$

- Example: $U = e^{-i\sum c_{x,y} n_x n_y} e^{-i\sum \lambda_{x,y} n_x (b_y + b_y^\dagger)} \ldots$

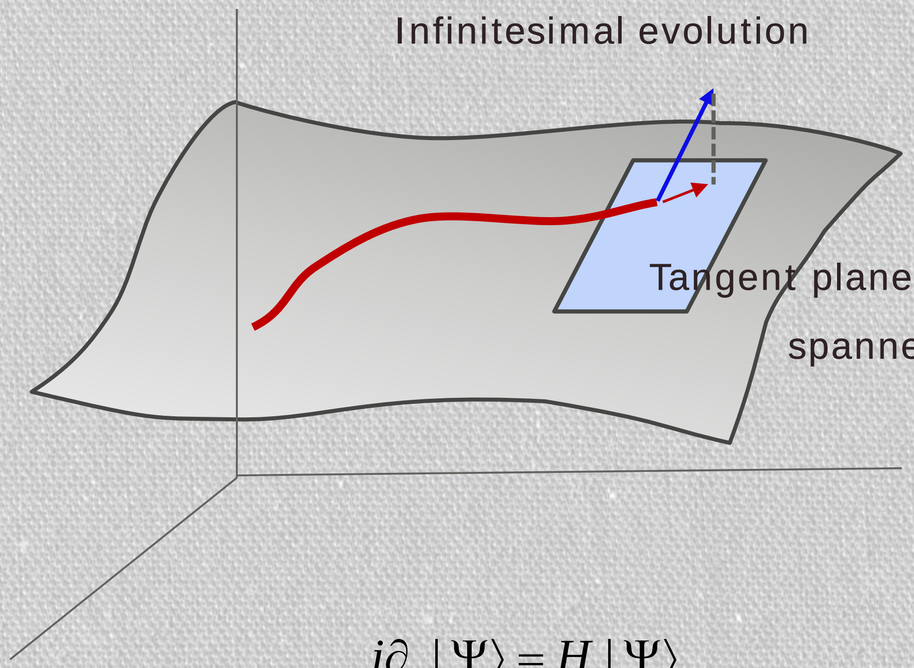
Parameters must be real

+
Include Gaussian states
Easy to compute
Describe correlations (beyond Wick's theorem)
Describe fermion-boson correlations

INTERPRETATION: DIFFERENTIAL GEOMETRY

DYNAMICS
Differential geometry

- Variational Manifold: $|\Psi(x^{\mu})\rangle$



$$i\partial_t |\Psi\rangle = H |\Psi\rangle$$

project onto the tangent plance

$$i\sum_{\mu} \dot{x}^{\mu} |v_{\mu}\rangle \qquad \mathbb{P}H |\Psi\rangle$$

DYNAMICS
Differential geometry

- Schrödinger Equation:

$$i\partial_t |\Psi\rangle = i\,\dot{x}^\mu |v_\mu\rangle = \mathbb{P} H |\Psi\rangle$$

spanned by $\partial_{x_n} |\Psi\rangle = |v_n\rangle$

- Projection: $i\,\dot{x}^\mu \langle v_\nu | v_\mu \rangle = \langle v_\nu | H | \Psi \rangle$
  - Real part: $\dot{x}^\mu(t) = f^\mu(x)$
  - Imaginary part: $\dot{x}^\mu(t) = g^\mu(x)$

Are not compatible in general

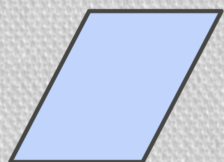
Tangent plane has to be considered as a real Hilbert space

$|v_\mu\rangle$ and $i|v_\mu\rangle$ are linearly independent

The projection has to be performed accordingly

DYNAMICS
Differential geometry

Tangent plane



$\partial_{x_n} |\Psi\rangle = |v_n\rangle$

$$\langle v_\mu | v_\nu \rangle = g_{\mu,\nu} + i\omega_{\mu,\nu}$$

Symplectic form: antisymmetric

Metric: symmetric, positive

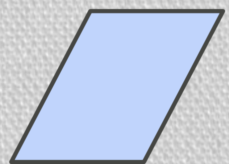
- Equations: 2 options:

(i) $\mathbb{P}\,(i\partial_t - H)|\Psi\rangle = 0 \;\Longrightarrow\; \dot{x}^\mu = -\Omega^{\mu,\nu}\partial_\nu E(x)$

(ii) $\mathbb{P}\,(\partial_t + iH)|\Psi\rangle = 0 \;\Longrightarrow\; \dot{x}^\mu = G^{\mu,\nu}\eta_\nu(x)$

DYNAMICS
Differential geometry

Tangent plane



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Only (i) coincides with the ones derived from the action

$\tilde{\partial} S = 0 \Longrightarrow$ Euler-Lagrange Eq. $\dot{x}^\mu = f^\mu(x)$

Energy is conserved: $d_t E = 0$

DYNAMICS
Differential geometry

- Evolution equations:

$$\dot{x}^{\mu} = -\Omega^{\mu,\nu}\partial_{\nu}E(x) \qquad \dot{x}^{\mu} = G^{\mu,\nu}\eta_{\nu}(x)$$

$$\langle v_{\mu} | v_{\nu}\rangle = g_{\mu,\nu} + i\omega_{\mu,\nu}$$

- Kähler mainfold: $i|v_{\mu}\rangle$ is in the tangent plane

$$i|v_{\mu}\rangle = \sum_{\nu} J_{\mu,\nu}|v_{\nu}\rangle \Rightarrow J^{2} = -\mathbb{I}$$

$$\Rightarrow J = -g\Omega \qquad \eta = J\partial E$$

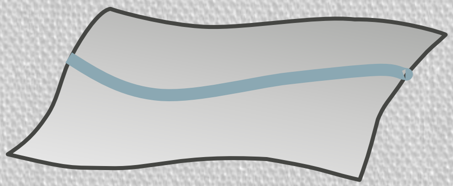
  - Real and imaginary parts of the equations are compatible

- Non-Kähler mainfold: $J^{2} \neq -\mathbb{I}$
  - Kählerization
  - Semi-Kählerization: ω is invertible

DYNAMICS
Other Quantities

- Conserved quantities: $[A, H] = 0$
  - Conserved if $A|\Psi\rangle \in \boldsymbol{T}$
  - Restrict the variational family

    (Lagrange Multipliers)



- Spectral functions:

$$A(q,\omega) = \int dt \ \langle \Psi_0 | a_q e^{-i(H-\omega)t} a_q^{+} | \Psi_0 \rangle$$

- Excitations:
  - Project onto the tangent plane: $h = \mathbb{P} H \mathbb{P}$
  - Linearize the equations of motion:

$$\dot{x}^{\mu} = -\Omega^{\mu,\nu} \partial_{\nu} E \approx -\Omega^{\mu,\nu} \, \partial_{\nu,\eta} E \Big|_{x^{(0)}} x^{\eta} = K_{\mu,\eta} x^{\eta}$$

DYNAMICS
Imaginary time

- Variational principle:

$$S = \int dt \, \langle \Psi | \partial_\tau - H | \Psi \rangle$$

normalization

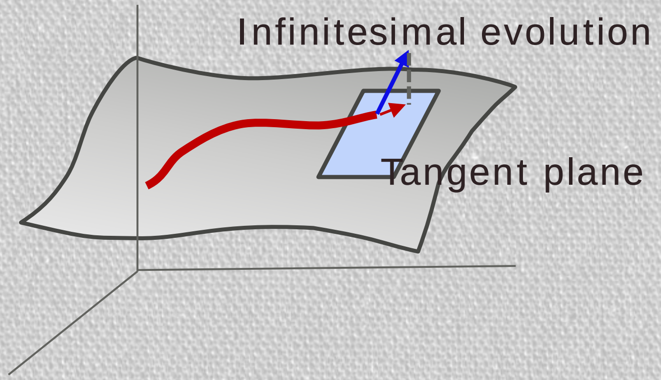
non-hermitian

DYNAMICS
Imaginary time

- Imaginary time evolution:

$$\partial_\tau |\Psi\rangle = -(H - \langle H\rangle)|\Psi\rangle$$

converges to the ground state

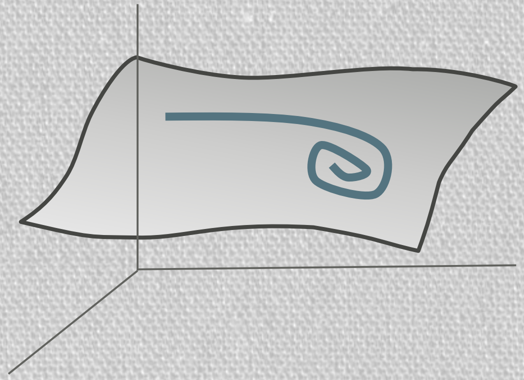


- Projection onto the tangent plane:

$$\mathbb{P}\,(\partial_\tau + H - \langle H\rangle)|\Psi(x)\rangle = 0$$

$$\dot{x}^\mu = -G^{\mu,\nu}\partial_\nu E(x)$$

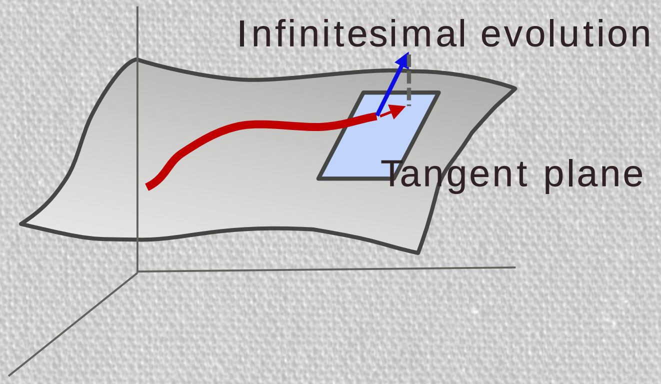
It ensures that the energy decreases with time



SUMMARY

$$|v_\mu\rangle = \partial_\mu |\Psi\rangle$$ tangent plane

$$\langle v_\mu | v_\nu\rangle = g_{\mu,\nu} + i\omega_{\mu,\nu}$$



- Real-time evolution:

$$\dot{x}^\mu = -\Omega^{\mu,\nu}\partial_\nu E(x)$$

  - ω invertible
  - Conserves energy
  - Other quantities
  - Kähler: more consistent

- Imaginary time:

$$\dot{x}^\mu = -G^{\mu,\nu}\partial_\nu E(x)$$

  - Energy decreases monotonically
  - Other quantities

APPLICATIONS

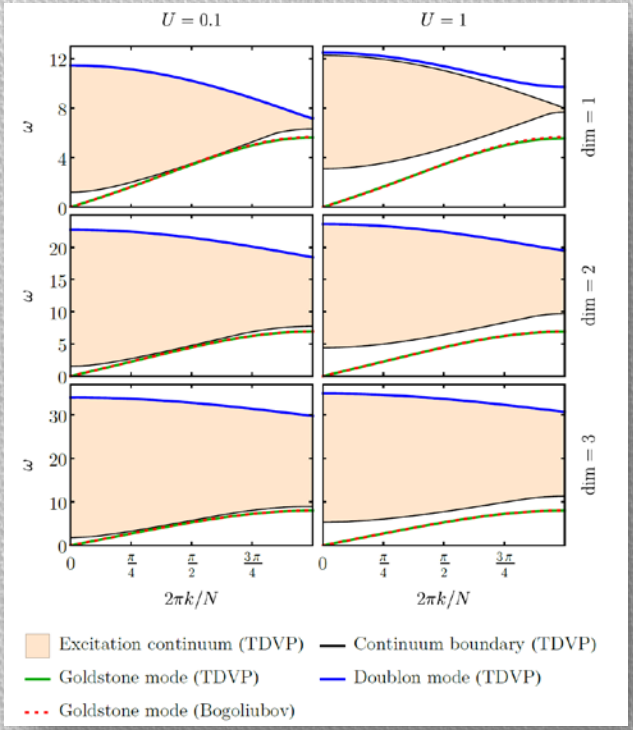
APPLICATIONS: Bose-Hubbard model

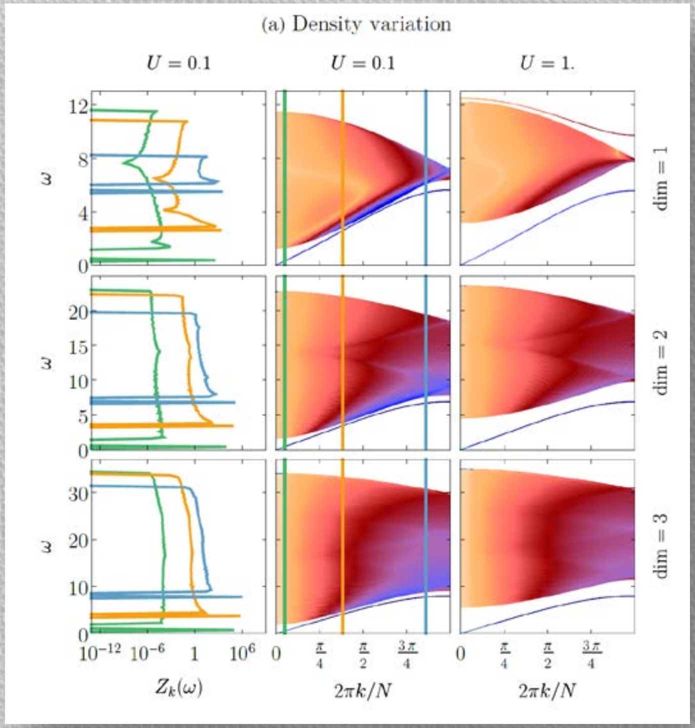
Guaita, Hackl, Shi, Hubig, Demler, JIC, PRB (2019)

- Model:

$$H = -t \sum_{\langle n,m \rangle} b_n^\dagger b_m + \frac{U}{2} \sum_n b_n^\dagger b_n^\dagger b_n b_n - \mu \sum_n b_n^\dagger b_n$$

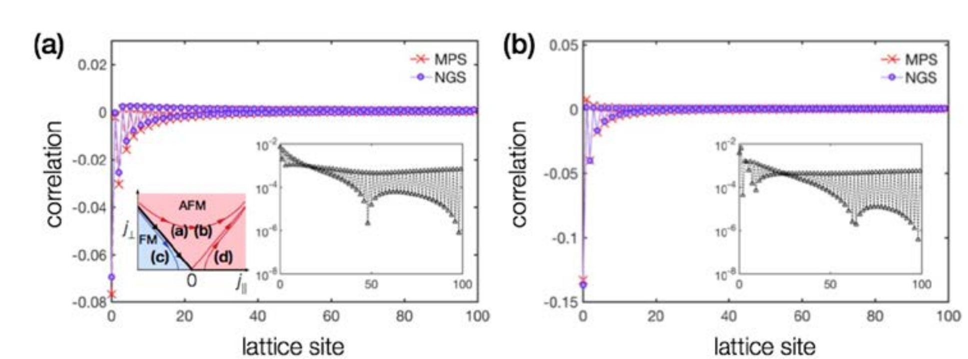
- Variational states: Full Gaussian family (not only displacements)





APPLICATIONS: Benchmark

1D: Spin-boson and Kondo problems Ashida, Shi, Bañuls, JIC, Demler, PRB (2018)

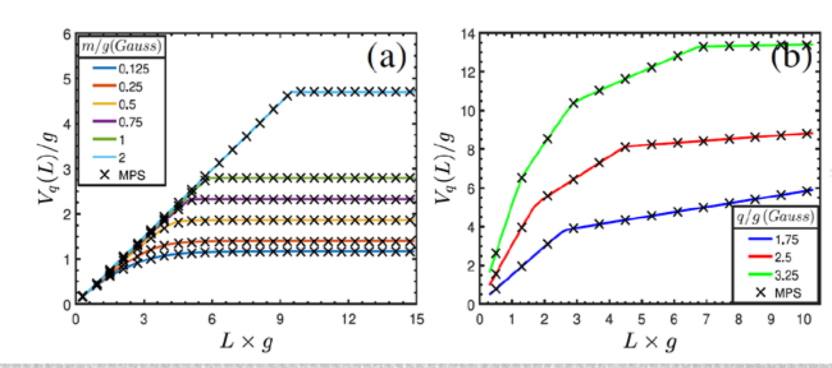


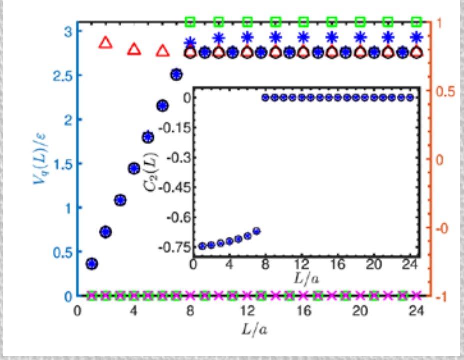
1D: Polarons in the SSH and Holstein models

2D: SC and CDW phases in Holstein model

Shi, Demler, JIC, Ann. Phys. (2018)

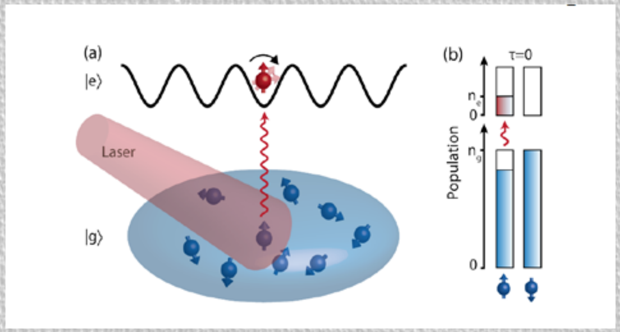
1D: LGT with U(1) and SU(2) Gauge groups Sala, Shi, Kühn, Bañuls, Demler, JIC, PRD (2018)





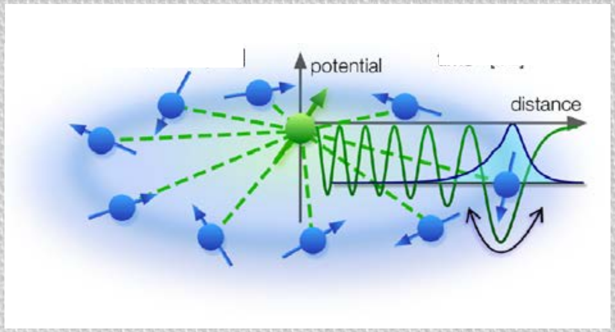
APPLICATIONS:
Bose-Hubbard model

Anisotropic Kondo with cold atoms



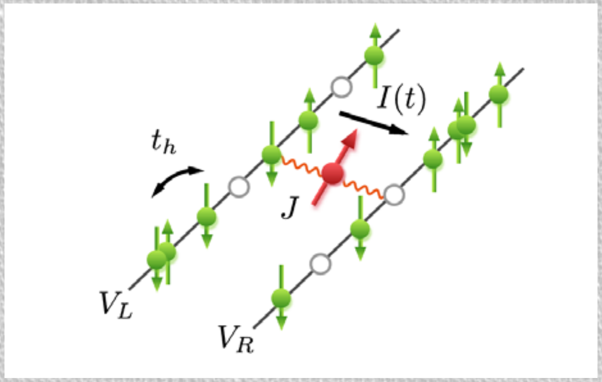
Kanász, Ashida, Shi, Moca, Ikeda, Fölling, JIC, Zaránd, Demler, PRB (2018)

Central Rydberg problem



Ashida, Shi, Schmidt, Sadeghpour, JIC, Demler, PRL (2019)

Anisotropic 2-lead Kondo



Ashida, Shi, Bañuls, JIC, Demler, PRL (2018)

FINITE TEMPERATURE

Shi, JIC, Demler, arXiv:soon

VARIATIONAL METHODS
Finite temperature

- Hamiltonian: $H = \sum_n h_n$

- Gibbs state: $\rho_T = \frac{e^{-H/T}}{Z}$

- Purification: $|\Psi_T\rangle \prec \left(e^{-H/2T} \otimes \mathbb{I}\right)|\Phi\rangle$

with $|\Phi\rangle = \sum_n |n,n\rangle$

$$\rho_T = \mathrm{tr}_a\left[|\Psi_T\rangle\langle\Psi_T|\right]$$

VARIATIONAL METHODS
Finite temperature

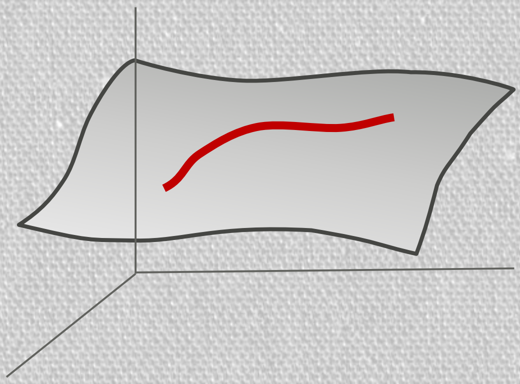
- Imaginary time evolution: $\partial_\tau |\Psi_p\rangle = (H \otimes \mathbb{I} - \langle H \rangle)|\Psi_p\rangle$

$$|\Psi_p(0)\rangle = |\Phi\rangle \Rightarrow |\Psi_p(1/2T)\rangle = |\Psi_T\rangle$$

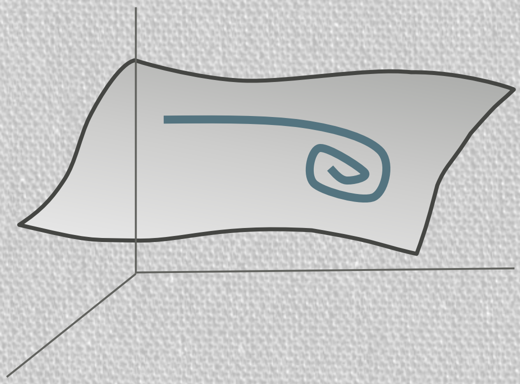
Errors accumulate

- Compare T=0

Finite T



T=0



VARIATIONAL METHODS
Finite temperature

- Variational Principle:

$$F_T = \min_{\rho} \mathrm{Tr}\left[F_T(\rho)\rho\right]$$

where $F_T(\rho) = H - T\log(\rho)$

- Evolution Equation:

$$\partial_\tau |\Psi_p\rangle = (F_T \otimes \mathbb{I} - \langle F_T\rangle)|\Psi_p\rangle$$

  - It is non-linear
  - Converges to the (purification of the) Gibbs state
  - It is a fixed point

VARIATIONAL METHODS
Finite temperature

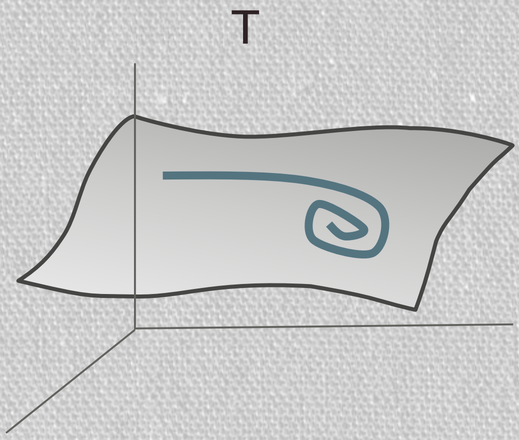
- Variational Principle: Non-Gaussian states

$$\partial_\tau |\Psi_p(x)\rangle = \mathbb{P}(F_T \otimes \mathbb{I} - \langle F_T \rangle) |\Psi_p(x)\rangle$$

⬇

$$\dot{x}^\mu = f^\mu(x)$$

The free energy decreases monotonically



VARIATIONAL METHODS
Finite temperature

$$\dot{x}^{\mu} = f_{\mu}(x)$$

- Conservation laws
- Real time evolution
- Excitation spectrum
- Spectral functions

VARIATIONAL METHODS
Benchmark

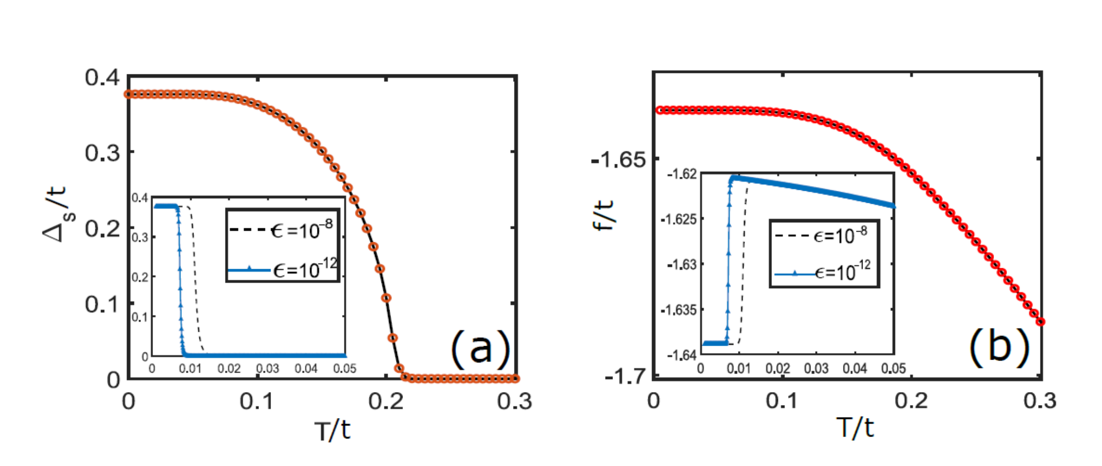
2D BCS model:

$$H = -t \sum_{\langle n,m \rangle,\sigma} c^{\dagger}_{n,\sigma} c_{m,\sigma} + U \sum_{n} c^{\dagger}_{n,\uparrow} c_{n,\uparrow} c^{\dagger}_{n,\downarrow} c_{n,\downarrow}$$

Gaussian state: $|\Phi_G\rangle$

Comparison: Mean field, imaginary time evolution, Gaussian

$U/t = 2$ $50x50$ lattice half-filling



VARIATIONAL METHODS
Results

2D Holstein model:

$$H = -t \sum_{\langle n,m \rangle,\sigma} c^{\dagger}_{n,\sigma} c_{m,\sigma} + \omega_b \sum_n b^{\dagger}_n b_n + g \sum_{n,\sigma} x_{n,\sigma} c^{\dagger}_{n,\sigma} c_{n,\sigma}$$

Reduces to the BCS model for g small

Non-Gaussian state:

$$|\Psi_p(x)\rangle \prec \left(U \otimes \mathbb{I}\right) |\Phi_G\rangle$$

Lang-Firsov: $$U(\lambda_{n.m}) = e^{i \sum_{n,m,\sigma} \lambda_{n,m} p_m c^{\dagger}_{n,\sigma} c_{n,\sigma}}$$

Two cases:

- Translationally invariant (period 2)
- General

VARIATIONAL METHODS
Results

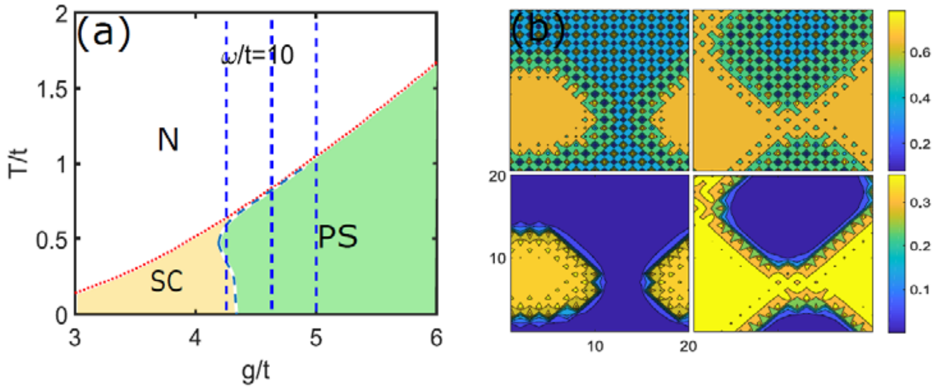
2D Holstein model: $\omega_b / t = 10$

$50x50$ lattice

$20x20$ lattice

$g / t = 5, T / t = 0.2$

$\nu = 0.6$ $\nu = 0.56$



SUMMARY

- Time-dependent variational principle
- Non-Gaussian states
    - Include many phenomena (Gaussian)
    - Can describe more complex correlations
- Differential geometry
    - Kähler manifolds
    - Imaginary-time evolution
- Finite temperature variational principle

Good complement to other methods, eg, tensor networks

Outlook: open systems, other variational families, other problems