Stanford

Introduction to Computational Quantum Systems

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Overview

Equations of motion

A quantum system of N-interacting particles is governed by

1. **wavefunction** $|\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)\rangle$ (zero-temperature):

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle, \quad \int |\psi|^2 d\mathbf{r} = 1 \qquad \text{(Schrödinger equation)}$$

with $|\psi\rangle$ we can compute expectation value $\langle\psi|\hat{O}|\psi\rangle$ such as energy $E = \langle\psi|\hat{H}|\psi\rangle$. Formally $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$. If $\hat{H}$ is time-independent $\longrightarrow \hat{H}|\psi\rangle = E|\psi\rangle$.

2. **density matrix** $\hat{\rho}(\mathbf{r}'_1, \ldots, \mathbf{r}'_N; \mathbf{r}_1, \ldots, \mathbf{r}_N; t)$ (finite-temperature):

$$i\frac{\partial}{\partial t}\hat{\rho} = [\hat{H}, \hat{\rho}], \quad \hat{\rho} \text{ is PSD}, \quad \mathrm{Tr}(\hat{\rho}) = 1 \qquad \text{(Von Neumann equation)},$$

with $\hat{\rho}$ we can compute expectation value $\mathrm{Tr}(\hat{\rho}\hat{O})$ such as energy $E = \mathrm{Tr}(\hat{\rho}\hat{H})$.

Second quantization

Usually, $|\psi\rangle$ need to be

- Symmetric over $\forall\ (\mathbf{r_i}, \mathbf{r_j})$ (Bosons)
- Anti-symmetric over $\forall\ (\mathbf{r_i}, \mathbf{r_j})$ (Fermions)

Introducing Slater basis sets $\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N}} \sum_P (\pm)^P \phi_1(x_{P(1)}) \phi_2(x_{P(2)}) \cdots \phi_N(x_{P(N)})$, where $\{\phi_i\} \in L_2(\mathbb{R}^3)$ and $\int |\phi_i|^2 d\mathbf{r} = 1$.

Denote $\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) := |\phi_1, \ldots, \phi_N\rangle \equiv |n_{\phi_1}, n_{\phi_2}, \ldots\rangle := \hat{c}^\dagger_{\phi_1} \hat{c}^\dagger_{\phi_2} \cdots \hat{c}^\dagger_{\phi_N} |\varnothing\rangle$

$\hat{c}^\dagger_{\phi_i}$ and $\hat{c}_{\phi_i}$ satisfy

- Commutation relation (Bosons)
- Anti-commutation relation (Fermions)

With this notation, we can also denote $\hat{H}$. In general:

$$\hat{H} = T_{ij} \hat{c}^\dagger_i \hat{c}_j + V_{ijkl} \hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_l \hat{c}_k + \cdots$$

$\cdots$ includes higher order interactions and those between different particles

Quantum field theory and path integral

QFT is essentially quantum mechanics with **infinite degrees of freedom**!

- Real-time path integral (one-particle example)
  - $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$
  - Time evolution operator: $\hat{U} = e^{-i\hat{H}t} = \left[e^{-i\hat{H}\Delta t}\right]^N$
  - $\langle q_\mathrm{f}|\hat{U}|q_\mathrm{i}\rangle = \langle q_\mathrm{f}|e^{-i\hat{T}\Delta t}e^{-i\hat{V}\Delta t} \wedge e^{-i\hat{T}\Delta t}e^{-i\hat{V}\Delta t} \wedge \cdots \wedge e^{-i\hat{T}\Delta t}e^{-i\hat{V}\Delta t}|q_\mathrm{i}\rangle = \int_{q(0)=q_\mathrm{i}}^{q(t)=q_\mathrm{f}} Dq\, e^{i\int_0^t dt' L(q,\dot{q})}$, where $L = T - V$
- Imaginary-time path integral (one-particle example)
  - Density matrix $\langle q_\mathrm{f}|\hat{\rho}|q_\mathrm{i}\rangle = \langle q_\mathrm{f}|e^{-\beta\hat{H}}|q_\mathrm{i}\rangle = \int_{q(0)=q_\mathrm{i}}^{q(\beta)=q_\mathrm{f}} Dq\, e^{-\int_0^\beta d\tau H(q,\dot{q})}$, where $H = T + V$
- The extreme path of the action gives classical mechanics!

Perturbation theory

How can QFT help us compute?

Define $\hat{\rho}_0 = e^{-\beta \hat{T}}$. Then $\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) = \mathrm{Tr}(\hat{\rho}_0) \frac{\mathrm{Tr}(T\hat{\rho}_0 \hat{O} e^{-\int_0^\beta d\tau \hat{V}})}{\mathrm{Tr}(\hat{\rho}_0)} = Z_0 \langle \hat{O} e^{-\int_0^\beta d\tau \hat{V}} \rangle_0$

- From Wick theorem, the above integral can be simplified to a series of Feynman diagrams, which can be further evaluated by $G_0 = \langle \hat{c}_i^\dagger \hat{c}_j \rangle_0$ (analytical expression exists).
- Approximations are ususally made when choosing specific Feynman diagrams for suitable physical applications.

Many-body Green's function methods

1. Main target: one-particle Green's function $G_{ij} = -i \langle T[c_i c_j^\dagger] \rangle$ and self-energy $\Sigma = G_0^{-1} - G^{-1}$. From G we can extract particle density, density matrix, and charge excitation energies. From Σ we can extract quasiparticle energies and quasiparticle lifetime.
2. Both many-body perturbation theory (MBPT) and dynamical mean-field theory (DMFT) belong to many-body Green's function methods.
   1. DMFT: local Feynman diagrams for strong-coupling systems
   2. MBPT: Feynman diagrams from perturbative expansions for weak-coupling systems

Many-body perturbation theory[1]

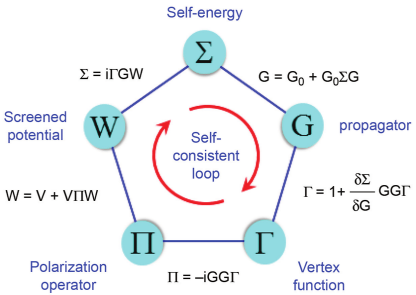


Figure 1: Hedin's pentagon.

1. Σ, $\Pi(P)$, W, Γ are introduced renormalized quantities from perturbation expansion.
2. $W \longrightarrow$ screened Coulomb interaction, $G \longrightarrow$ one particle Green's function
3. $G_0^{-1} = G^{-1} + \Sigma$ and $v^{-1} = W^{-1} + P$ are Dyson equations.
4. If $\Gamma \approx 1 \longrightarrow$ random phase approximation
5. $\Sigma \approx iGW \longrightarrow$ the GW approximation
6. Second order: Bethe-Salpeter equation

[1] Richard M Martin, Lucia Reining, and David M Ceperley. *Interacting electrons*. Cambridge University Press, 2016.

Dynamical mean-field theory[2]

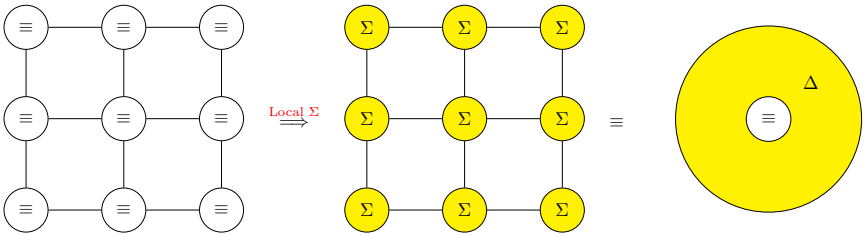


Figure 2: Graphic illustration of dynamical mean-field theory.

1. Assume self-energy Σ is local in space (exact in infinite dimensions).
2. Hybridization function Δ represents the interaction between the site and the environment.

[2] Richard M Martin, Lucia Reining, and David M Ceperley. *Interacting electrons*. Cambridge University Press, 2016.

Variational methods

Low-lying (ground-state) wavefunction and energy from $H\psi = E\psi$ can be obtained from minimization problem: $E = \min_{|\psi\rangle} \langle\psi|\hat{H}|\psi\rangle - E\left(\langle\psi|\psi\rangle - 1\right)$

- Variational Monte Carlo: $\langle\hat{H}\rangle = \frac{\langle\psi(a)|\hat{H}|\psi(a)\rangle}{\langle\psi(a)|\psi(a)\rangle} = \int \left(\frac{|\psi(a)|^2}{\int |\psi(a)|^2}\right) \frac{\hat{H}|\psi(a)\rangle}{\psi(a)}$
- Power method: $|\psi\rangle \propto \lim_{\beta\to\infty} e^{-\beta\hat{H}} |\psi_0\rangle$ and $\langle\hat{O}\rangle = \frac{\langle\psi_0|\hat{O}|\psi\rangle}{\langle\psi_0|\psi\rangle}$
  - Projector Quantum Monte Carlo, Auxiliary-field Quantum Monte Carlo etc
- Trucated Galerkin space: post-Hartree-Fock methods
- Density-matrix renormalization group (based on tensor-network ansatz)

Tensor-train representation

$$\psi(i_1, i_2, \ldots, i_d) \approx \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \cdots G_d(\alpha_{d-1}, i_d)$$

$$H(i_1, i_1', i_2, i_2', \ldots, i_8, i_8') \approx \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} G_1(i_1, i_1', \alpha_1) G_2(\alpha_1, i_2, i_2', \alpha_2) \cdots G_d(\alpha_{d-1}, i_d, i_d')$$

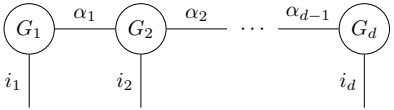


Figure 3: Tensor diagram for tensor-train/matrix product state (TT/MPS).

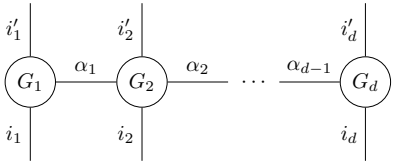


Figure 4: Tensor diagram for matrix product operator (MPO).

Tree tensor network

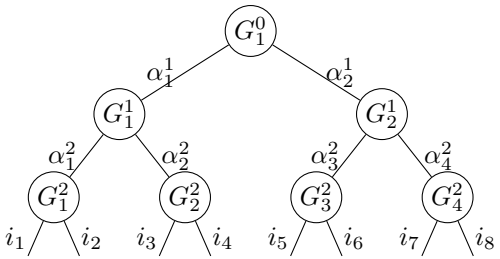


Figure 5: Tensor diagram for a 3-level binary tree tensor network (TTN).

$$\psi(i_1, i_2, \ldots, i_8) \approx \sum_{\alpha_1^1 \alpha_2^1 = 1}^{r_1} \sum_{\alpha_1^2 \alpha_2^2 \alpha_3^2 \alpha_4^2 = 1}^{r_2} G_1^0(\alpha_1^1, \alpha_2^1)$$
$$G_1^1(\alpha_1^1, \alpha_1^2, \alpha_2^2) G_2^1(\alpha_2^1, \alpha_3^2, \alpha_4^2)$$
$$G_1^2(\alpha_1^2, i_1, i_2) G_2^2(\alpha_2^2, i_3, i_4) G_3^2(\alpha_3^2, i_5, i_6) G_4^2(\alpha_4^2, i_7, i_8)$$

Density-matrix renormalization group

$$E = \min_{|\psi\rangle} \langle\psi|\hat{H}|\psi\rangle - E\left(\langle\psi|\psi\rangle - 1\right)$$

Express $\hat{H}$ as a MPO and use an MPS ansatz for $|\psi\rangle$:

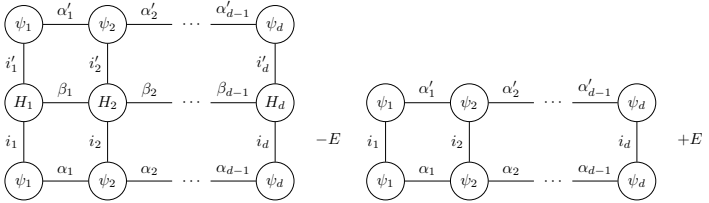
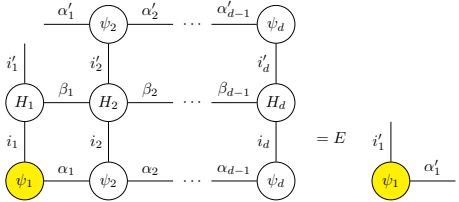


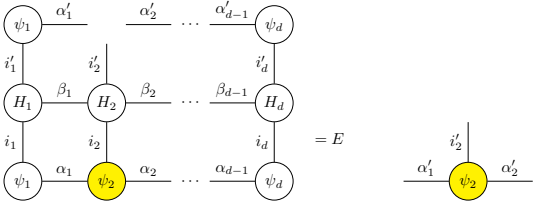
Figure 6: Graphic illustration of density-matrix renormalization group.

Density-matrix renormalization group

DMRG step 1:



DMRG step 2:



1. DMRG uses tensor network as ansatz.
2. DMRG is least squares method for local tensor cores rather than full space.
3. DMRG is ideally linearly scaled in number of cores.

Full and selected configuration interaction

- Full configuration interaction (exact diagonalization)

$$H_{\text{el}} = \begin{pmatrix} \langle \Phi_0 | \hat{H} | \Phi_0 \rangle & \langle \Phi_0 | \hat{H} | \Phi_a^r \rangle & \cdots \\ \langle \Phi_0 | \hat{H} | \Phi_a^r \rangle & \langle \Phi_a^r | \hat{H} | \Phi_a^r \rangle & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \xrightarrow{\text{Diagonalization}} \Psi$$

- Selected configuration interaction
  Limit the space of Ψ to low order, such as

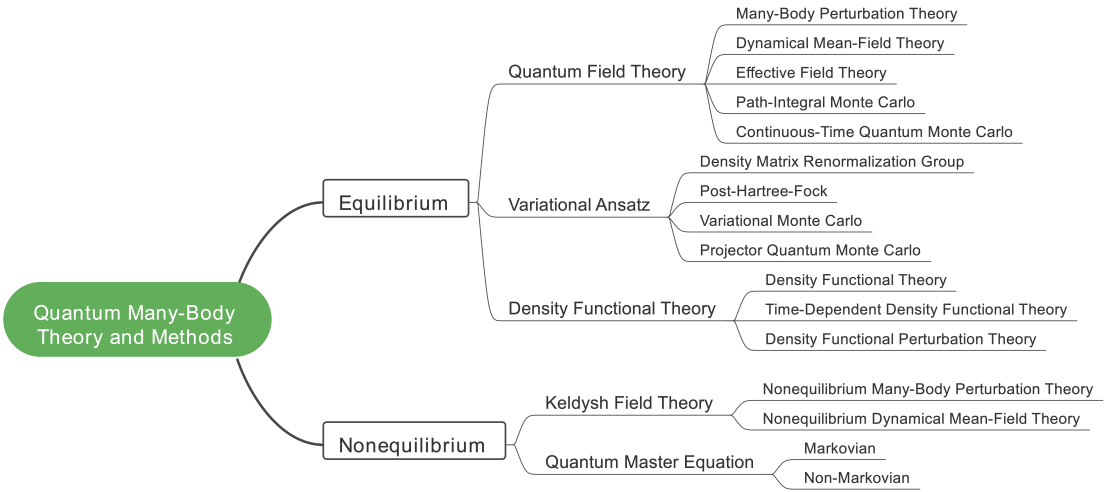
$$\Psi \approx c_0 \Phi_0 + \sum_{ra} c_a^r \Phi_a^r$$

$$H_{\text{el}} \approx \begin{pmatrix} \langle \Phi_0 | \hat{H} | \Phi_0 \rangle & \langle \Phi_0 | \hat{H} | \Phi_a^r \rangle \\ \langle \Phi_0 | \hat{H} | \Phi_a^r \rangle & \langle \Phi_a^r | \hat{H} | \Phi_a^r \rangle \end{pmatrix} \xrightarrow{\text{Diagonalization}} \Psi$$

Quantum Monte Carlo

- Variational Monte Carlo
  $E(\alpha) = \frac{\langle\Psi(\alpha)|\hat{H}|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle} = \int \left(\frac{|\Psi(\alpha)|^2}{\int |\Psi(\alpha)|^2} \right) \frac{\hat{H}|\Psi(\alpha)\rangle}{\Psi(\alpha)}$
  $E_{\text{min}} = \min_\alpha E(\alpha)$
- Projector Monte Carlo
  $|\Psi\rangle \propto \lim_{\beta\to\infty} e^{-\beta\hat{H}} |\Phi\rangle \longrightarrow |\Psi^{n+1}\rangle = e^{-\Delta\tau H} |\Psi^n\rangle$
  $E_{\text{min}} = \lim_{n\to\infty} \frac{\langle\Phi|\hat{H}|\Psi\rangle}{\langle\Phi|\Psi\rangle}$
- Path integral Monte Carlo
  Sample over the path integral

Summary of computational methods for quantum physics



Overview

Quantum many-body systems

As noted previously, the key quantity of a quantum system is wavefunction $|\psi\rangle$ (zero-temperature) or density matrix $\hat{\rho}$ (finite-temperature).

If $|\psi\rangle$ and $\hat{\rho}$ can not be solved by separation of variables $\longrightarrow$ strong correlations beyond mean-field theory (MFT)! Examples of MFT include Hartree-Fock, Kohn-Sham density functional theory, the *GW* method, Weiss mean-field theory etc.

Interpretation of strong correlations

Statistics perspective: correlation between two operators.

$$\langle \hat{A}(\mathbf{r})\hat{B}(\mathbf{r}')\rangle \begin{cases} \approx \langle \hat{A}(\mathbf{r})\rangle \langle \hat{B}(\mathbf{r}')\rangle : \text{MFT works} \\ \neq \langle \hat{A}(\mathbf{r})\rangle \langle \hat{B}(\mathbf{r}')\rangle : \text{MFT fails!} \end{cases}$$

Note $\langle \hat{O}\rangle := \begin{cases} \langle\psi|\hat{O}|\psi\rangle : \text{zero-temperature} \\ \frac{\mathrm{Tr}(\hat{O}e^{-\beta\hat{H}})}{\mathrm{Tr}(e^{-\beta\hat{H}})} : \text{finite-temperature} \end{cases}$

Wavefunction perspective: expansion of the exact wavefunction as an infinite series.

$$|\psi\rangle = c_0|\phi_0\rangle + \sum_{ra} c_a^r |\phi_a^r\rangle + \sum_{\substack{a<b \\ r<s}} c_{ab}^{rs} |\phi_{ab}^{rs}\rangle + \cdots$$

$$c_0 \begin{cases} \approx 1 : \text{MFT works} \\ \ll 1 : \text{MFT fails!} \end{cases}$$

Representative strongly correlated systems

Transverse-field Ising model: quantum phase transitions.

Figure 7: 1D spin chain.

$$\hat{H}_{\text{1D-TFI}} = g\sum_{i=1}^{d}\hat{\sigma}_x^i + J(\sum_{i=1}^{d-1}\hat{\sigma}_z^i\hat{\sigma}_z^{i+1} + \hat{\sigma}_z^d\hat{\sigma}_z^1).$$

Note $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are Pauli matrices.

$$|\frac{J}{g}| = \begin{cases} > 1\text{: ordered phase} \\ = 1\text{: quantum critical point} \longrightarrow \text{strong correlations!} \\ < 1\text{: disordered phase} \end{cases}$$

Representative strongly correlated systems

Fermi-Hubbard model (FHM): electron interactions in transition metal oxides.

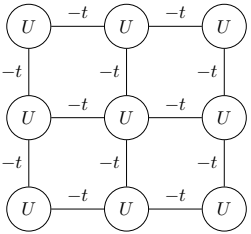


Figure 8: A schematic Fermi-Hubbard model.

$$\hat{H}_{\text{FHM}} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \hat{a}^{\dagger}_{i,\sigma} \hat{a}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

$$\frac{t}{U} = \begin{cases} \longrightarrow +\infty\text{: free electrons} \\ \longrightarrow 0\text{: Mott insulator} \longrightarrow \text{strong correlations!} \end{cases}$$

Representative strongly correlated systems

Spin defects and strongly-correlated states: emerging candidates for spin qubits in quantum information science.

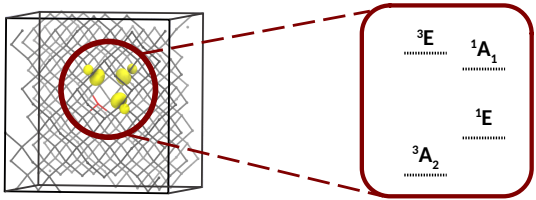


Figure 9: Structure and spectrum of negatively charged nitrogen-vacancy center (NV^-) in diamond.

First-principles predictions of strongly correlated singlet-states are challenging!

Resources

- Dissertation and talk from Prof. Michael Lindsey at Berkeley[3]
- An introductory book by Prof. Lin Lin at Berkeley and Prof. Jianfeng Lu at Duke[4]
- A self-contained book of quantum many-body theory[5]

[3] **Lindsey**.

[4] **lin2019mathematical**.

[5] **stefanucci2013nonequilibrium**.