

1-Body Problem

Discretizing Hamiltonian (finite-difference method)

Time-Independent Schrödinger Eq.

- . Factorization along coordinate axis
- . Potential with spherical symmetry
- . Finite difference methods

Time-Dependent Schr \ddot{o} dinger Eq.

- . Spectral
- . Direct numerical integration
 - . Forward Euler
 - . Exact Quantum Evolution
 - . Implicit (Backward-Forward)

Many Body Problem

Quantum Spin Models

- . Hamilton Matrix
- . Transverse-field Ising Model (TFIM)

Finding Ground States

- . Power Method
- . Lanczos Method

Quantum Dynamics

- . Taylor Expansion

Trotter-Suzuki Decomp.

- . Time Evl. of TFIM

Indistinguishable Particles Fermions & Bosons

Fock Space

- . Fermions
- . Spinful fermions
- . Bosons

Creation-Accihilation Operator

- . Fermionic operator
- Bosonic operator

- . Tight-binding model
- . Bose-Hubbard Model
- . T-V model

Exact Diagonalizations

- . Bosons
- . Fermions

1) The electronic structure problem

$$\hat{H} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_{r_i}^2 + V_{\text{ext}}(\vec{r}_i) \right) + \sum_{i < j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

Bohr-Oppenheimer Approximation

$$V_{\text{ext}}(\vec{r}) = -e \sum_{i=1}^N \frac{z_i}{|\vec{r} - \vec{r}_i|}$$

Notation for one-body and two-body

$$V_1(r) = -\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{ext}}(r)$$

$$V_2(r, r') = \frac{e^2}{|\vec{r} - \vec{r}'|}$$

Electronic Structure of Molecules & Atoms

2) Hamiltonian in second quantization

$$t_{ij} = \int d\vec{r} \phi_i^*(\vec{r}) \hat{a}_i(\vec{r}) \hat{b}_j(\vec{r}) \rightarrow \text{orbital wavefunctions}$$

$$V_{ijkl} = \int d\vec{r} \int d\vec{r}' \phi_i^*(\vec{r}) \phi_j^*(\vec{r}') \hat{a}_l^\dagger(\vec{r}, \vec{r}') \hat{a}_k(\vec{r}) \phi_l(\vec{r}')$$

$$\hat{H} = \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \frac{1}{2} \sum_{ijkl\sigma\sigma'} V_{ijkl} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}^\dagger \hat{c}_{k\sigma'} \hat{c}_{l\sigma'}$$

3) Basis Functions

STOC (Slater Type)

GTOC (Gauss Type)

4) Hartree-Fock Method

4.1) Spinless case

• N particle wf as a Slater determinant

$$\cdot E = \langle \Phi | H | \Phi \rangle \rightarrow |\Phi\rangle = |a_1^+ \dots a_N^+ \rangle$$

$$\begin{array}{c} \diagup \quad \diagdown \\ H_1 \quad H_2 \\ (\text{one-body}) \quad (\text{two-body}) \\ \text{term} \quad t_{ij} \end{array}$$

$$\cdot E = \sum_{\alpha} t_{\alpha\alpha} + \frac{1}{2} \sum_{\alpha\beta} (V_{\alpha\beta\alpha\beta} - V_{\alpha\beta\beta\alpha})$$

$$\star E_H = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta\alpha\beta} = \frac{1}{2} \int d\vec{r} d\vec{r}' \rho(\vec{r}) \underbrace{\frac{e^2}{|\vec{r} - \vec{r}'|}}_{\text{electrostatic interaction}} \rho(\vec{r}')$$

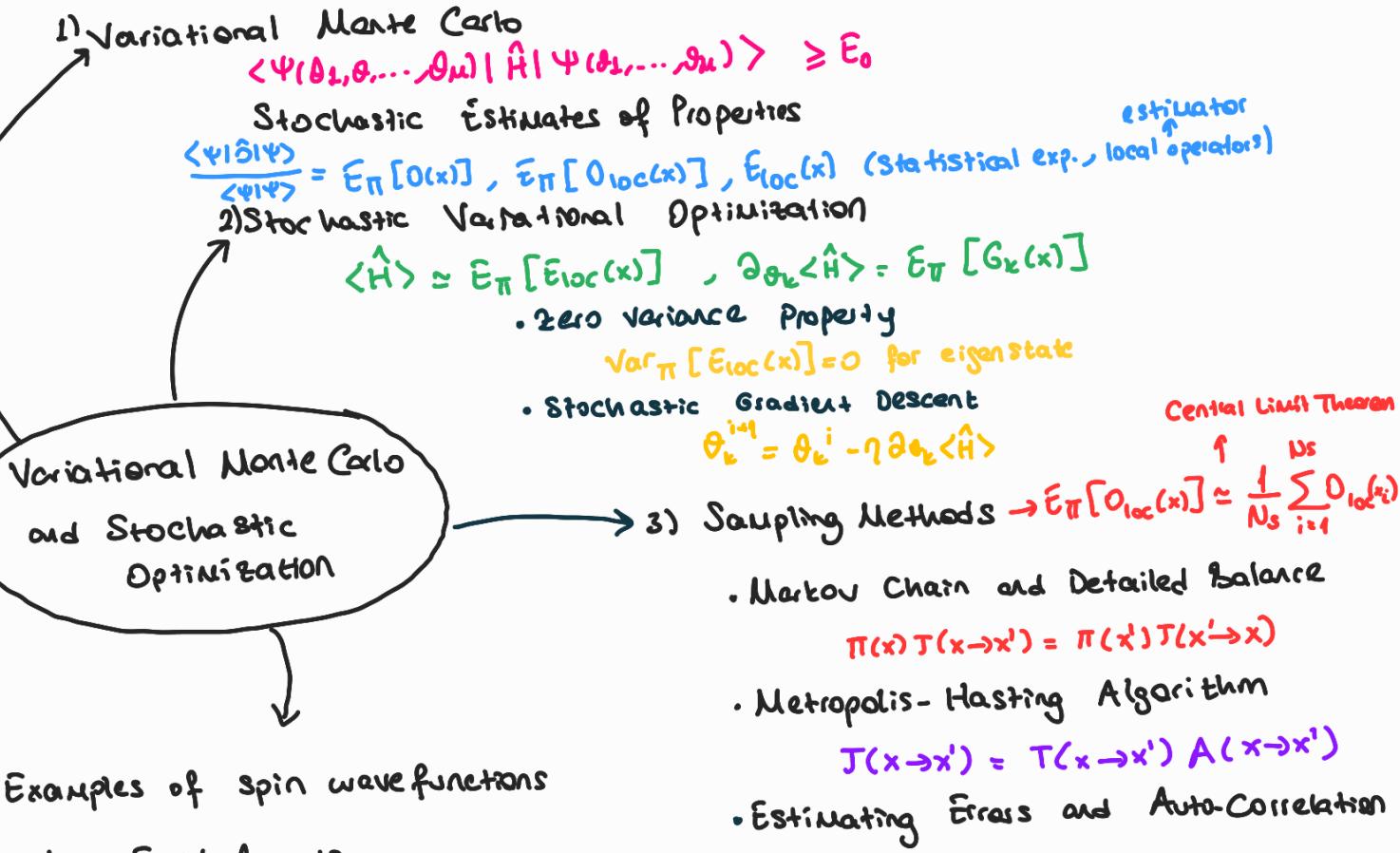
direct (Hartree) term

Density Functional Theory

Electron Density

Variational principle for the density

Kohn-Sham Scheme



4) Examples of spin wavefunctions

. Mean-Field Ansatz

$$\langle s_1, s_2, \dots, s_N | \Psi \rangle = \prod_{i=1}^N \Phi_i(s_i), \quad \varphi_i(s) = \frac{\Phi_i(s)^2}{\Phi_i(s)^2 + \Phi_i(\downarrow)^2}, \quad M=2N \text{ var. parameters}$$

. Jastrow Ansatz

$$\langle s_1, s_2, \dots, s_N | \Psi \rangle = \exp \left[\sum_i J_i^{(1)} s_i + \sum_{i < j} J_{ij}^{(2)} (s_i, s_j) + \dots + \frac{1}{p!} \sum_{i_1, i_2, \dots, i_p} J_{i_1, i_2, \dots, i_p}^{(p)} (s_{i_1}, s_{i_2}, \dots, s_{i_p}) \right] \rightarrow \text{Use MCNC (markovchain monte carlo)}$$

1) Artificial Neural Networks : the Machine

$$a_j^{(l)} = \phi^{(l)}(z_j^{(l)})$$

$$z_j^{(l)} = \sum_i W_{ij}^{(l)} a_i^{(l-1)} + b_j^{(l)}$$

2) Supervised Learning

$$\text{Loss Func } L(\theta) = \frac{1}{N_s} \sum_{i=1}^{N_s} [f(x_i; \theta) - y_i]^2$$

Machine Learning Methods for Many-Body Quantum Systems

3) Neural-Network Quantum States

$$\langle s | \Psi(\theta) \rangle = F(s_1, s_2, \dots, s_N; \theta)$$

$$\text{Loss function } \mathcal{L}(\theta) = \frac{\langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle}{\langle \Psi(\theta) | \Psi(\theta) \rangle}$$

4) Taking Gradients

4.1) Back propagation algorithm

$$\text{Goal} = \frac{\partial F(x, \theta)}{\partial \theta_k} \quad \Delta_j^{(0)} = \sum_k \Delta_k^{(0)} W_{jk}^{(0)} \phi'(z_j^{(0)})$$

$$\Delta_j^{(k)} = \frac{\partial F}{\partial z_j^{(k)}}$$

$$\Delta_j^{(0)} = \frac{\partial F}{\partial z_j^{(0)}} = \phi'(z_j^{(0)})$$

sensitivity
 ↓ Forward Pass $a_j^{(1)}, a_j^{(2)}, \dots, a_j^{(D)}$
 $z_j^{(1)}, z_j^{(2)}, \dots, z_j^{(D)}$ → $F(x)$

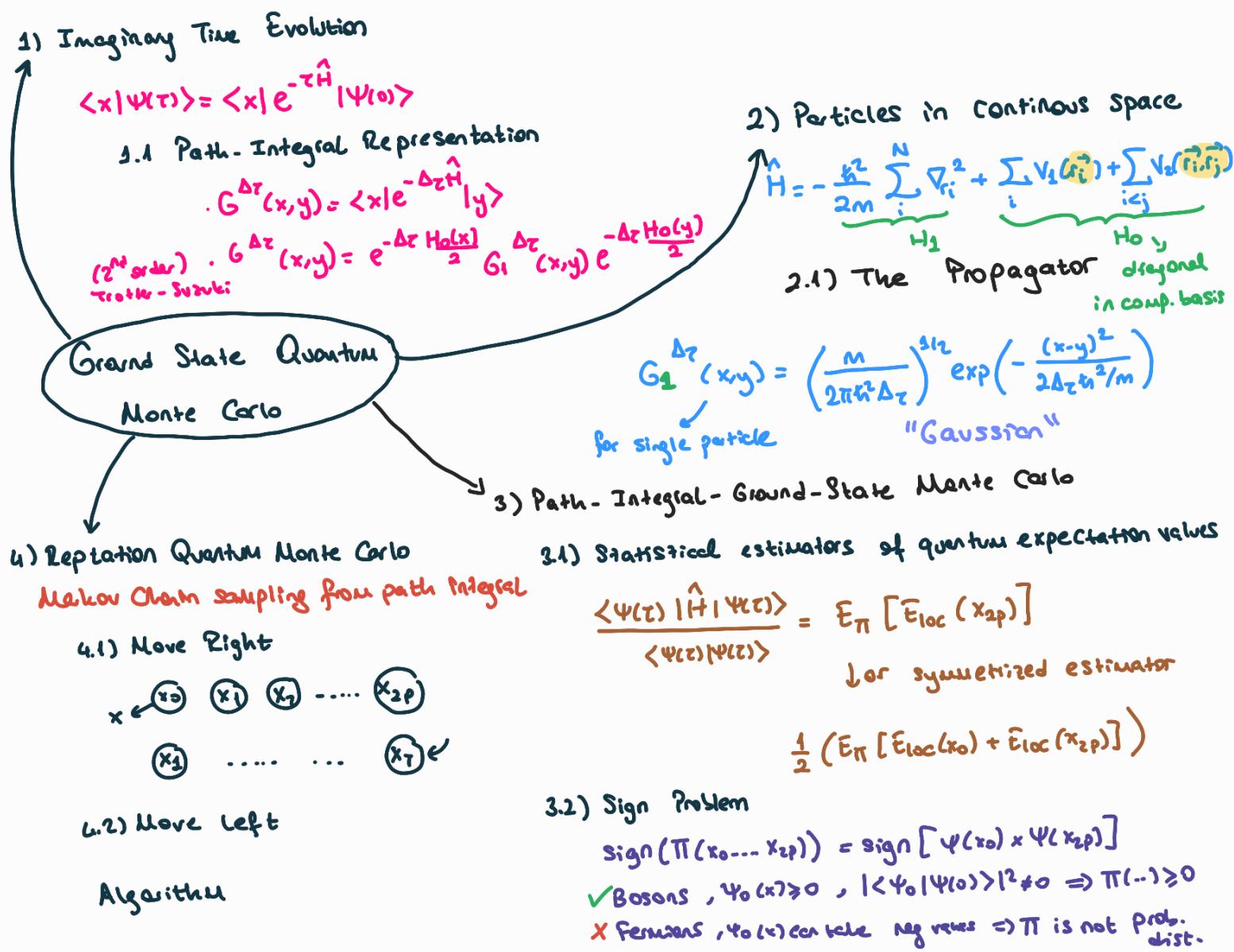
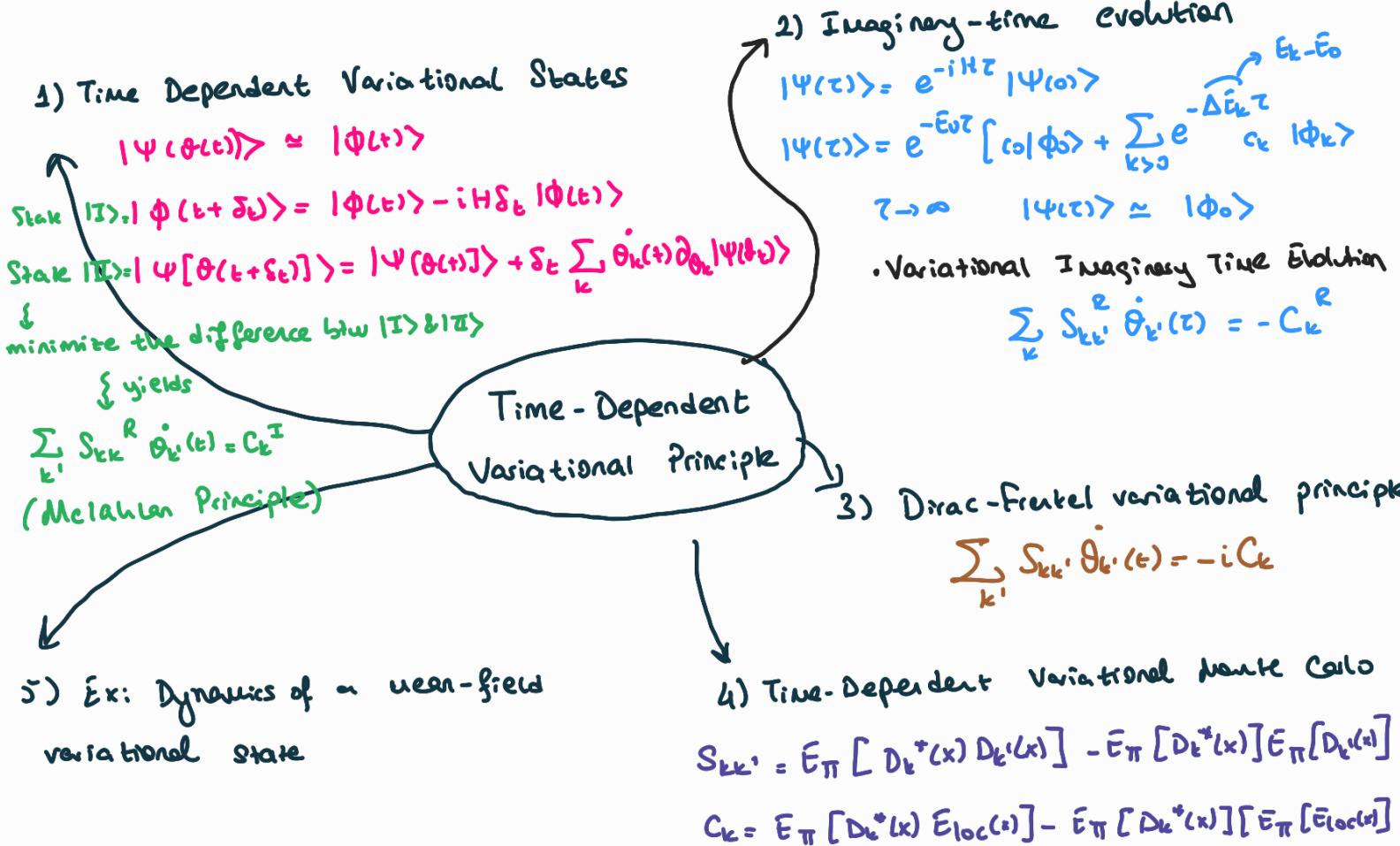
4.2) Computing gradients of the energy

$$\frac{\partial E(\theta)}{\partial \theta_k} = \mathcal{E}_\pi[G_k(x)]$$

$$\frac{1}{N_s} \sum_i (\hat{E}_{loc}(x_i) - E_\pi(\hat{E}_{loc}(x_i))) \frac{\partial}{\partial \theta_k} \hat{F}_k(x^{(i)}; \theta)$$

2) Backward Pass

$$\Delta_j^{(0)} \rightarrow \Delta_j^{(D-1)} \rightarrow \dots \Delta_j^{(1)}$$



1) Thermal Density Matrix

$$\langle \hat{O} \rangle = \frac{\text{Tr}(\hat{O} e^{-\beta \hat{H}})}{Z}$$

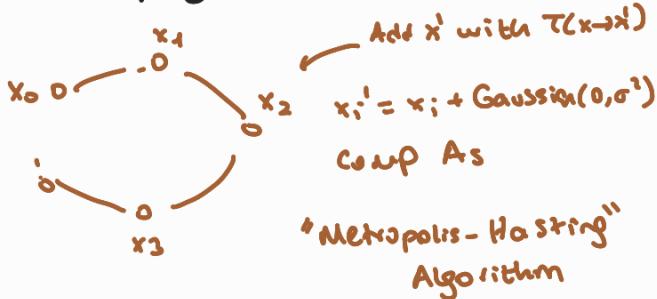
partition function $Z = \text{Tr}(e^{\beta(-\hat{H})})$

$$p^\beta(x, y) = \langle x | e^{\beta(-\hat{H})} | y \rangle = G^\beta(x, y)$$

$$Z = \sum_x p^\beta(x, x)$$

Finite Temperature
Quantum Monte Carlo

2.2) Sampling Paths



3.1) Path-Integral Representation

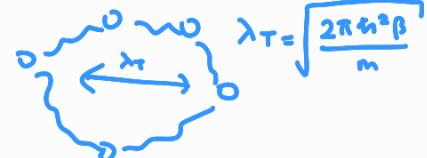
$$Z = \sum_{x_0} p^\beta(x_0, x_p) = \sum_{x_0=x_p=0} \prod_{i=0}^{p-1} G_i^\beta(x_i, x_{i+1}) e^{-\beta H_0(x_i)} \delta(x_p = x_0)$$

$$\langle O \rangle = \frac{1}{Z} \sum_{i=0}^p E_\pi [O(x_i)]$$

since periodic boundary

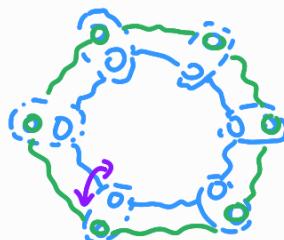
2) Continuous-Space Particles

$$\hat{H} = \sum_i T_i + \hat{V}(x)$$



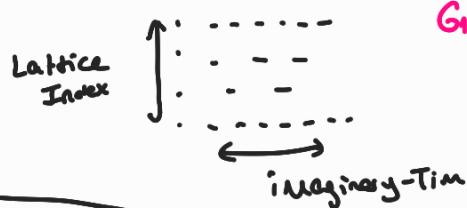
2.1) Bose Symmetry

$$p_B^\beta(x_1, x_2) = \frac{1}{N!} \sum_p p^\beta(x_p, P(x_p))$$



particle exchanges yield
single larger ring

1) Transverse-Field Ising Model



Path Int. Repr.

$$G_i^\beta(x, y) = \prod_{j=1}^N g_i^\beta(\sigma_j^z(x), \sigma_j^z(y))$$

Relation to 2D Classical Ising Model

Path Integral Monte-Carlo
for Lattice Models

Variational Quantum Algorithms