

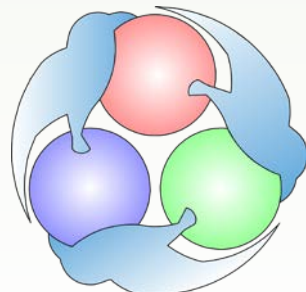
Benchmarking studies of collective quantum tunneling and density functionals

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W. Deng, G. Chen, G. Ding, S. Wang, J. Peng, and HZL, arxiv:2604.01906

S. Wang, S. Degen, and HZL, in preparation

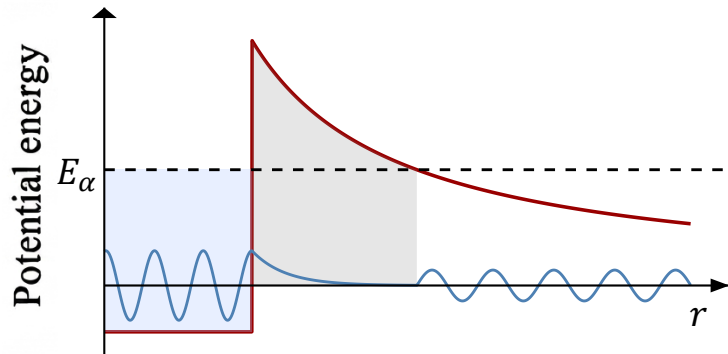
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 - ✓ The two-well model and exact solution
 - ✓ Real-time mean-field approach and the self-trapping effect
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- Benchmarking studies of density functionals
 - ✓ DFT with functional renormalization group approach
 - ✓ Quantum thermodynamics in the single-site Bose-Hubbard model
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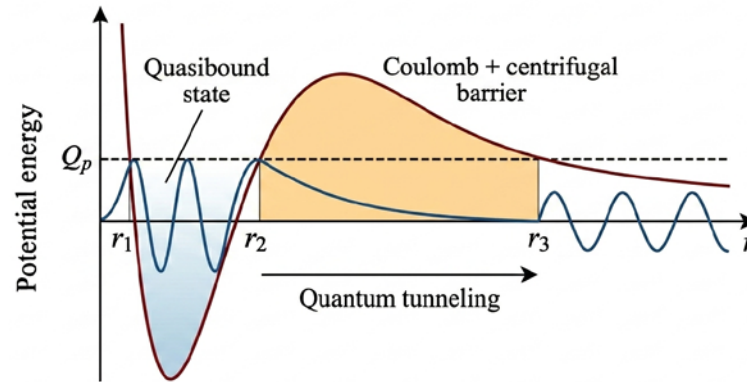
Quantum tunneling

□ One of the fundamental problems in physics *A. B. Balantekin and N. Takigawa, RMP 70, 77 (1998)*

✓ Alpha decay

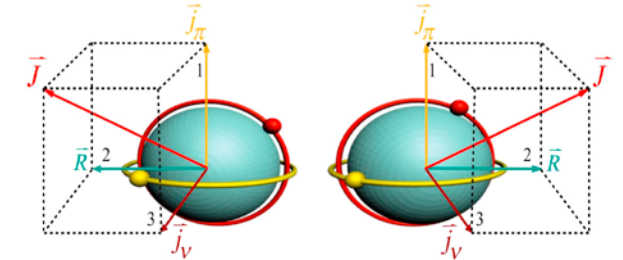


✓ Proton radioactivity



✓ Nuclear chirality

JPG 37, 064025 (2010)



✓ Macroscopic quantum tunneling

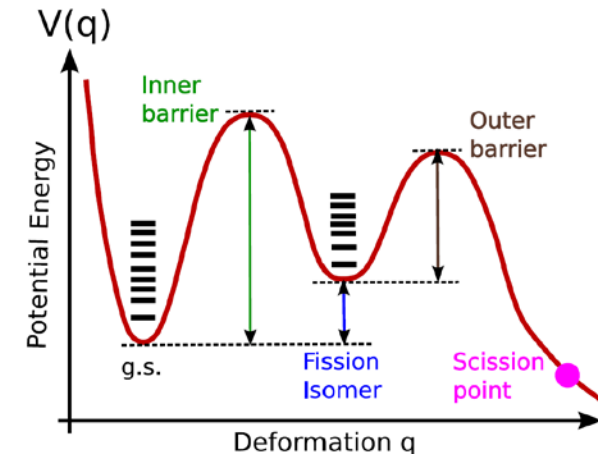


Ill. Niklas Elmehed © Nobel Prize Outreach
John Clarke
Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach
Michel H. Devoret
Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach
John M. Martinis
Prize share: 1/3

✓ Nuclear fission *PPNP 125, 103963 (2022)*

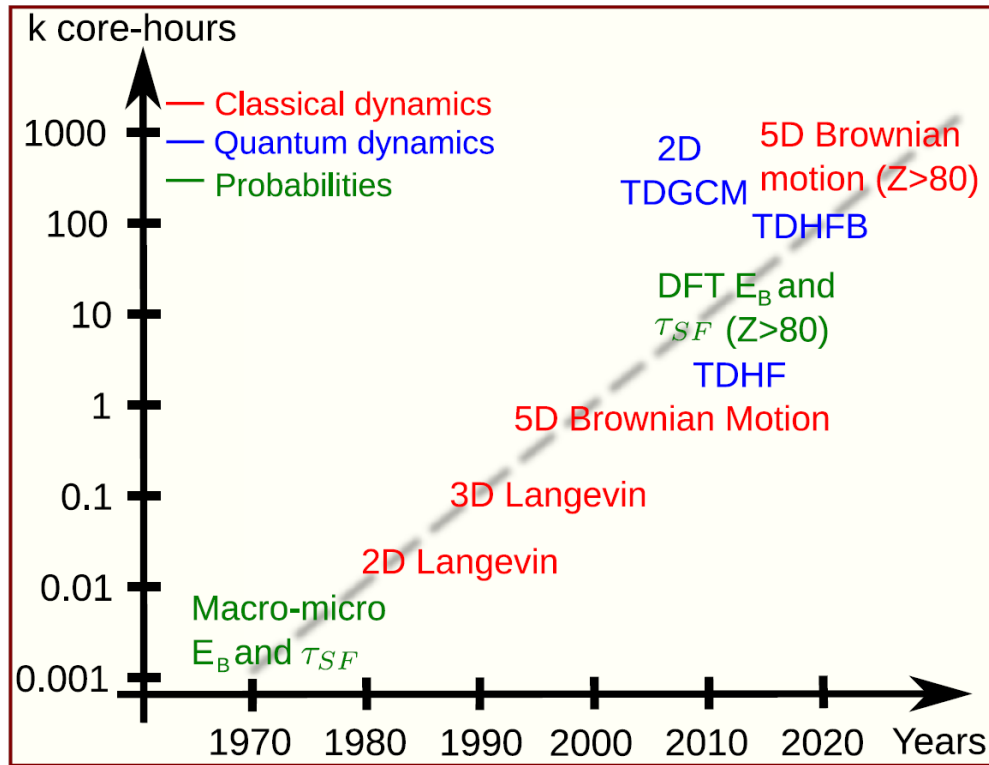


Theoretical methods for nuclear fission

- Liquid drop model *J. R. Nix, Nucl. Phys. A 130, 241 (1969)*
- Semi-empirical approaches *K-H Schmidt et al, Nucl. Data Sheets 131, 107 (2016)*
- Stochastic approaches
 - ✓ Langevin equation *T. Ichikawa et al, J. Nucl. Radiochem. Sci. 3 67 (2002)*
Y. Aritomo, S. Chiba, Phys. Rev. C 88, 044614 (2013)
 - ✓ Brownian shape-motion model *J. Randrup, P. Möller, Phys. Rev. Lett. 106, 132503 (2011)*
P. Möller and C. Schmitt, Eur. Phys. J. A 53, 7 (2017)
- Macroscopic–microscopic approach
M. Brack et al, Rev. Mod. Phys. 44 (2), 320 (1972); P. Jachimowicz et al, At. Data Nucl. Data Tables 138,101393 (2021)
- Microscopic self-consistent approaches
 - ✓ Time-dependent generator coordinate method (TDGCM)
H. Goutte et al, Phys. Rev. C 71, 024316 (2005); M. Verriere, D. Regnier, Front. Phys. 8, 233 (2020)
 - ✓ Time-dependent density functional theory (TDDFT)
C. Simenel and A. S. Umar, Phys. Rev. C 89, 031601 (2014); M. Pancic et al, Front. Phys. 8, 351 (2020)

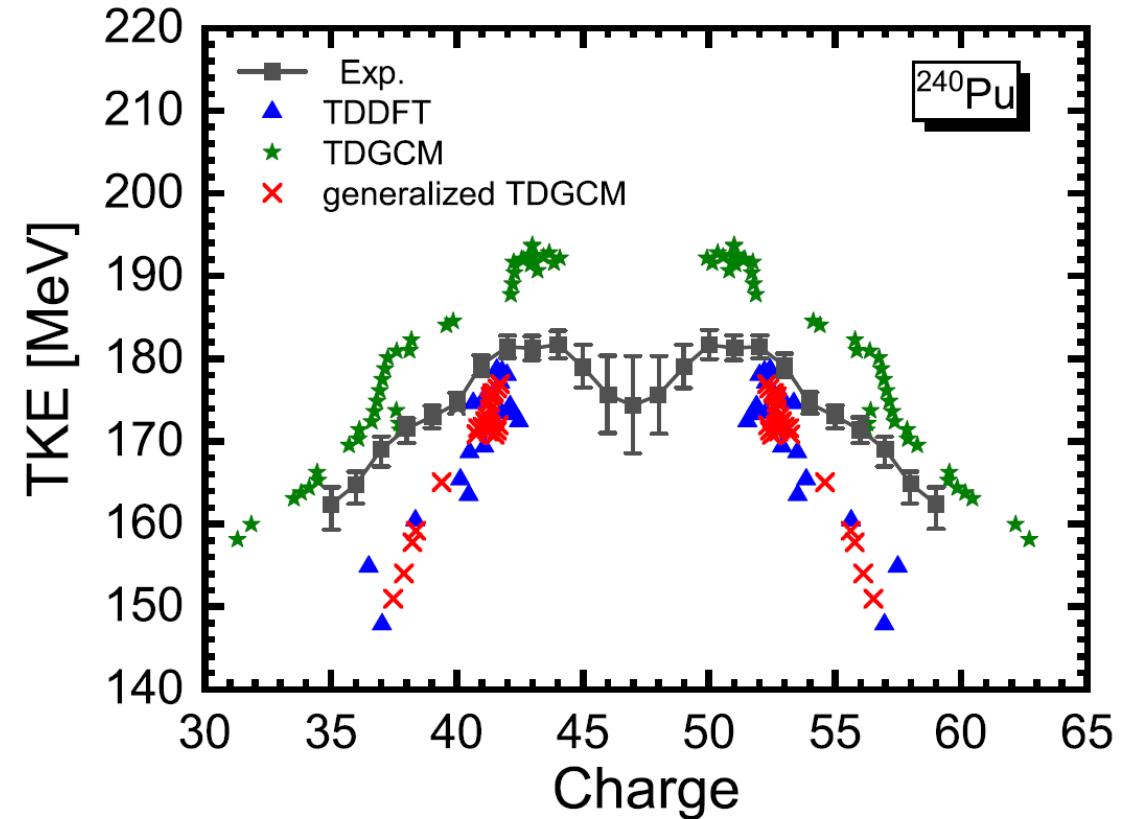
Comparison among methods

Approximate computational cost



N. Schunck and D. Regnier, Prog. Part. Nucl. Phys. 125, 103963 (2022)

Observables: total kinetic energies



B. Li et al, Phys. Rev. C 111, L051302 (2025)

→ **Benchmarking theoretical methods to exactly solvable models.**

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Two-well model

- System Hamiltonian of two distinguishable particles in two potential wells

$$\hat{H}(1,2) = \hat{h}_0(1) + \hat{h}_0(2) + \hat{v}(1,2)$$

- Eigenstates of the single-particle Hamiltonian

$$|\pm\rangle = \frac{1}{\sqrt{2}} (|L\rangle \pm |R\rangle)$$

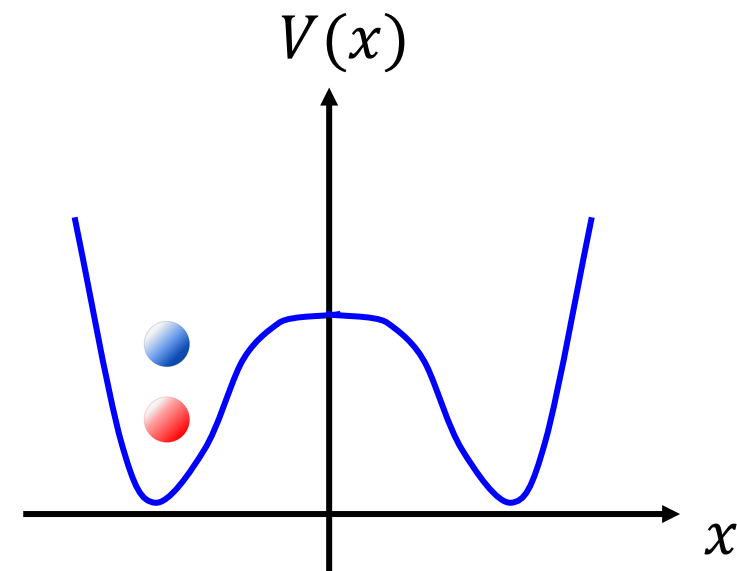
- Single-particle Hamiltonian

$$\hat{h}_0 = \alpha |-\rangle\langle-| = \frac{\alpha}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

- Two-body interaction

$$\hat{v}(1,2) = \mu (|LL\rangle\langle LL| + |RR\rangle\langle RR|)$$

- Initial state: $|LL\rangle$



Exact solution

- In the basis $\{|LL\rangle, |LR\rangle, |RL\rangle, |RR\rangle\}$, the Hamiltonian is

$$\hat{H} = \begin{pmatrix} \alpha + \mu & -\alpha/2 & -\alpha/2 & 0 \\ -\alpha/2 & \alpha & 0 & -\alpha/2 \\ -\alpha/2 & 0 & \alpha & -\alpha/2 \\ 0 & -\alpha/2 & -\alpha/2 & \alpha + \mu \end{pmatrix}$$

- State of the system at time t

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

- Left-well number operator and its expectation value \rightarrow **tunneling**

$$\hat{N}_L = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \langle \hat{N}_L \rangle = 1 + \frac{\beta - \mu}{2\beta} \cos\left(\frac{\beta + \mu}{2} t\right) + \frac{\beta + \mu}{2\beta} \cos\left(\frac{\beta - \mu}{2} t\right), \quad \beta = \sqrt{4\alpha^2 + \mu^2}$$

Real-time mean-field approach

- Hartree approximation: $\hat{H}(1,2) \approx \hat{h}_H(1) + \hat{h}_H(2)$

$$\hat{h}_H(i) = \hat{h}_0(i) + \langle \psi_j | \hat{v}(1,2) | \psi_j \rangle$$

$$|\psi(t)\rangle = L(t)|L\rangle + R(t)|R\rangle \quad \rightarrow \quad i \frac{d}{dt} |\psi(t)\rangle = \hat{h}_H(t) |\psi(t)\rangle$$

- Real-time mean-field equations of **collective coordinates**

$$\theta \equiv \arcsin(|L|^2 - |R|^2), \quad \phi \equiv \arg(R/L)$$

$$\dot{\theta} = -\sin \phi \quad \dot{\phi} = \tan \theta \cos \phi + \mu \sin \theta$$

- Average number of particles in the left well

$$\langle \hat{N}_L \rangle = 2|L|^2 = 1 + \sin \theta (t)$$

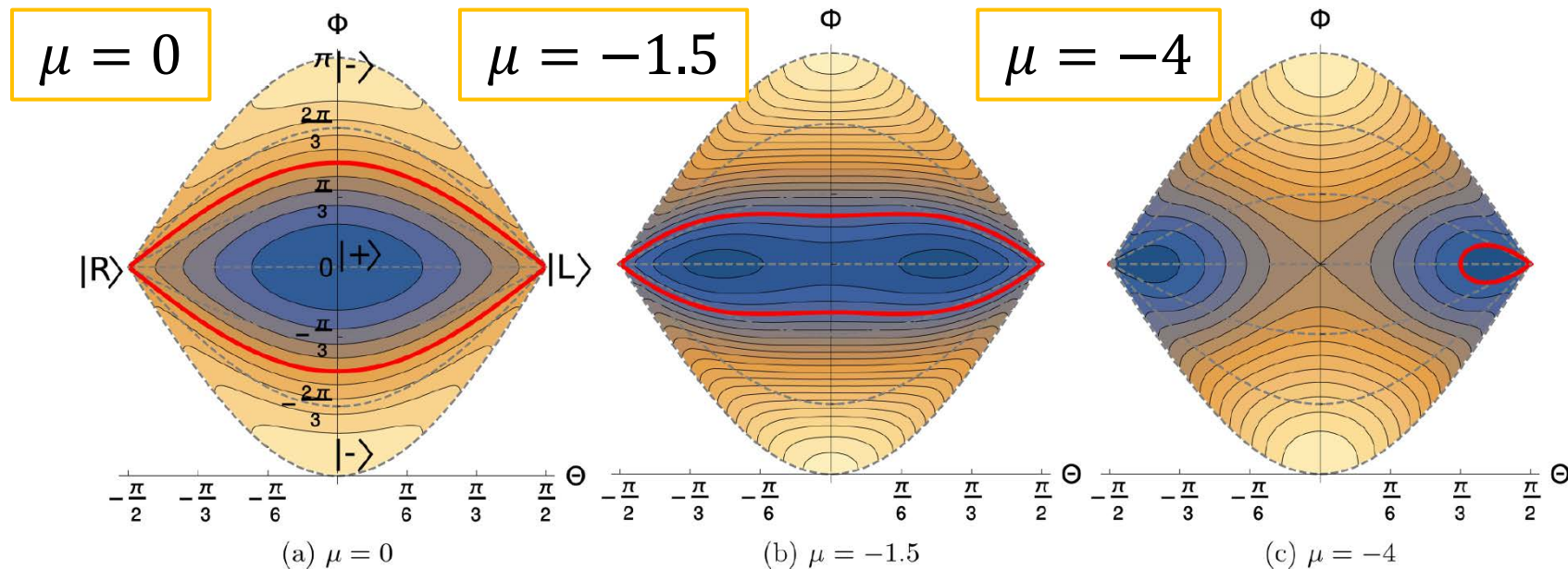
Self-trapping effect

- The total Hartree energy is conserved

$$E = 1 - \cos \theta \cos \phi + \frac{\mu}{2} [1 + \sin^2 \theta] \rightarrow dE/dt = 0$$

$$E(\theta = \pm\pi/2, \phi) = 1 + \mu = E(\theta = 0, \phi) = 1 + \frac{\mu}{2} - \cos \phi$$

- For $|\mu| > 2$, **self-trapping** effect occurs *P. McGlynn and C. Simenel, Phys. Rev. C, 102, 064614 (2020)*



Time-dependent generator coordinate method

- The generated state with generator coordinate θ

$$|\Phi(t)\rangle = \sum_{\theta} |\Psi(\theta)\rangle g(\theta, t)$$

$$\begin{aligned} |\Psi(\theta)\rangle &= |\psi_1(\theta)\rangle \otimes |\psi_2(\theta)\rangle \\ &= \frac{1 + \sin \theta}{2} |LL\rangle + \frac{\cos \theta}{2} |LR\rangle + \frac{\cos \theta}{2} |RL\rangle + \frac{1 - \sin \theta}{2} |RR\rangle \end{aligned}$$

- The time-dependent Griffin–Hill–Wheeler (GHW) equation

$$\sum_{\theta} \left(\mathcal{H}(\theta', \theta) - i\hbar \mathcal{N}(\theta', \theta) \frac{d}{dt} \right) g(\theta, t) = 0$$

- The expectation value of the left-well number operator

$$\langle \hat{N}_L \rangle = \sum_{\theta, \theta'} \left[\frac{(1 + \sin \theta)(1 + \sin \theta')}{2} + \frac{\cos \theta \cos \theta'}{2} \right] g^*(\theta, t) g(\theta', t)$$

Generator coordinates θ and ϕ

- The generated state with generator coordinates θ, ϕ

$$|\Phi(t)\rangle = \sum_{\theta, \phi} |\Psi(\theta, \phi)\rangle g(\theta, \phi, t)$$

$$|\Psi(\theta, \phi)\rangle = \frac{1+\sin \theta}{2} |LL\rangle + \frac{\cos \theta}{2} e^{i\phi} |LR\rangle + \frac{\cos \theta}{2} e^{i\phi} |RL\rangle + \frac{1-\sin \theta}{2} e^{2i\phi} |RR\rangle$$

- The expectation value

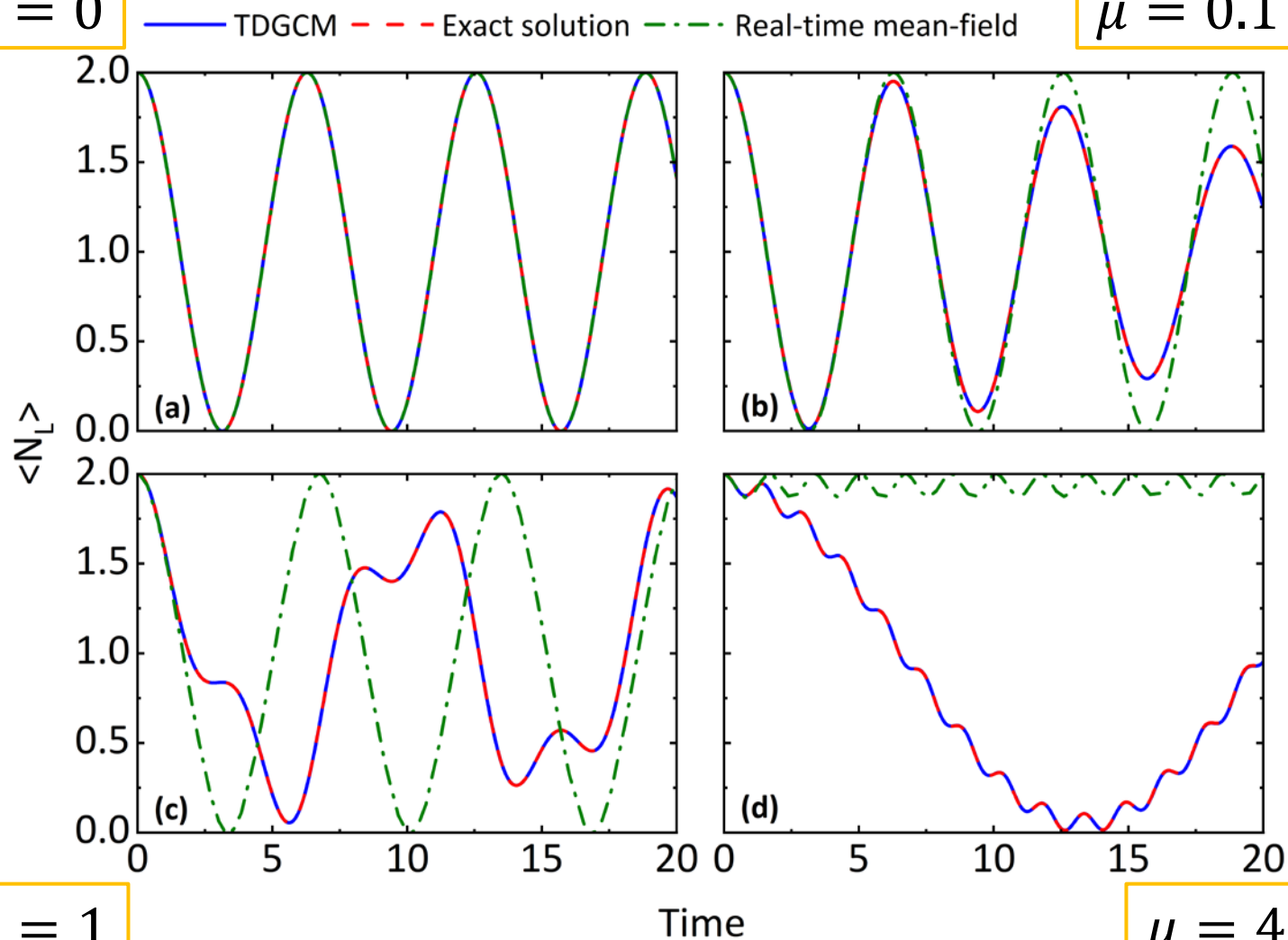
$$\langle \hat{N}_L \rangle = \sum_{\theta, \phi; \theta', \phi'} \left[\frac{(1+\sin \theta)(1+\sin \theta')}{2} + \frac{\cos \theta \cos \theta'}{2} e^{i(\phi' - \phi)} \right] g^*(\theta, \phi, t) g(\theta', \phi', t)$$

$\phi = 0$ reduce to the case that only θ is used as generate coordinates.

TDGCM with $(\theta_1, \theta_2, \theta_3, \dots, \theta_n)$

$\mu = 0$

$\mu = 0.1$



✓ $\theta_1 = \pi/2$ for initial condition

✓ $n \geq 3$ is needed

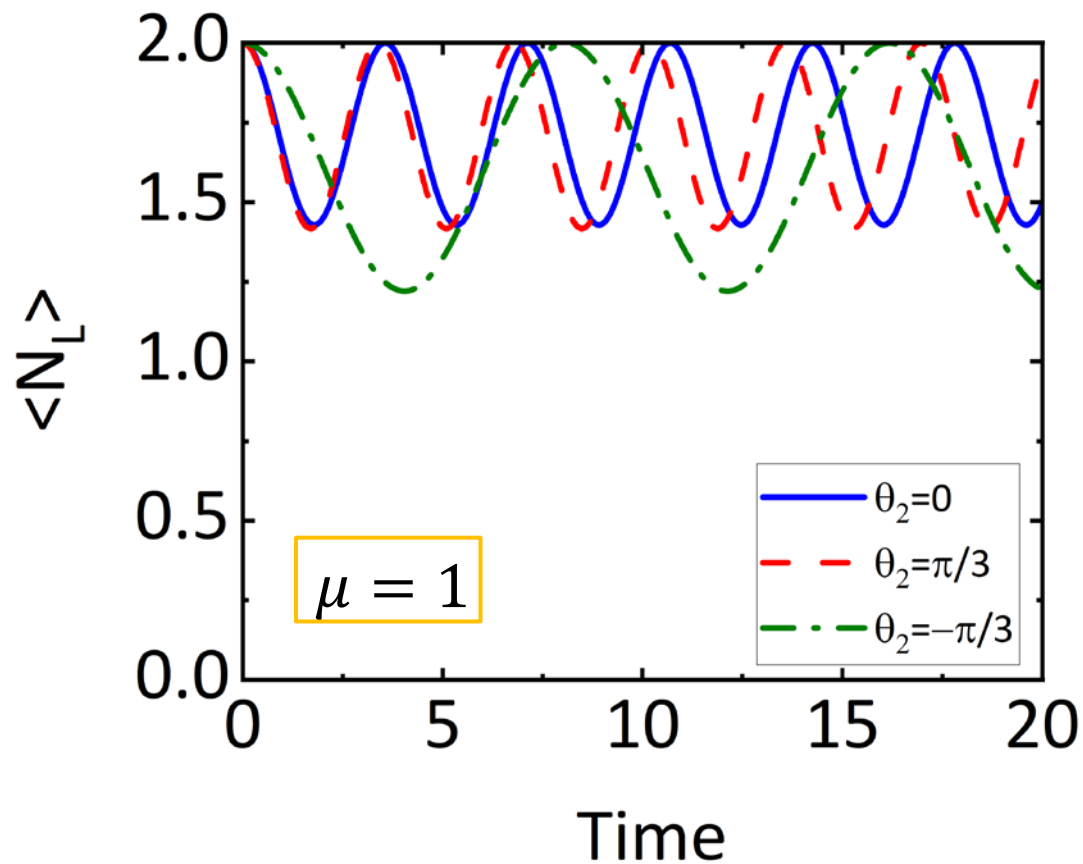
✓ Independent of the chosen θ

✓ No spurious self-trapping effect

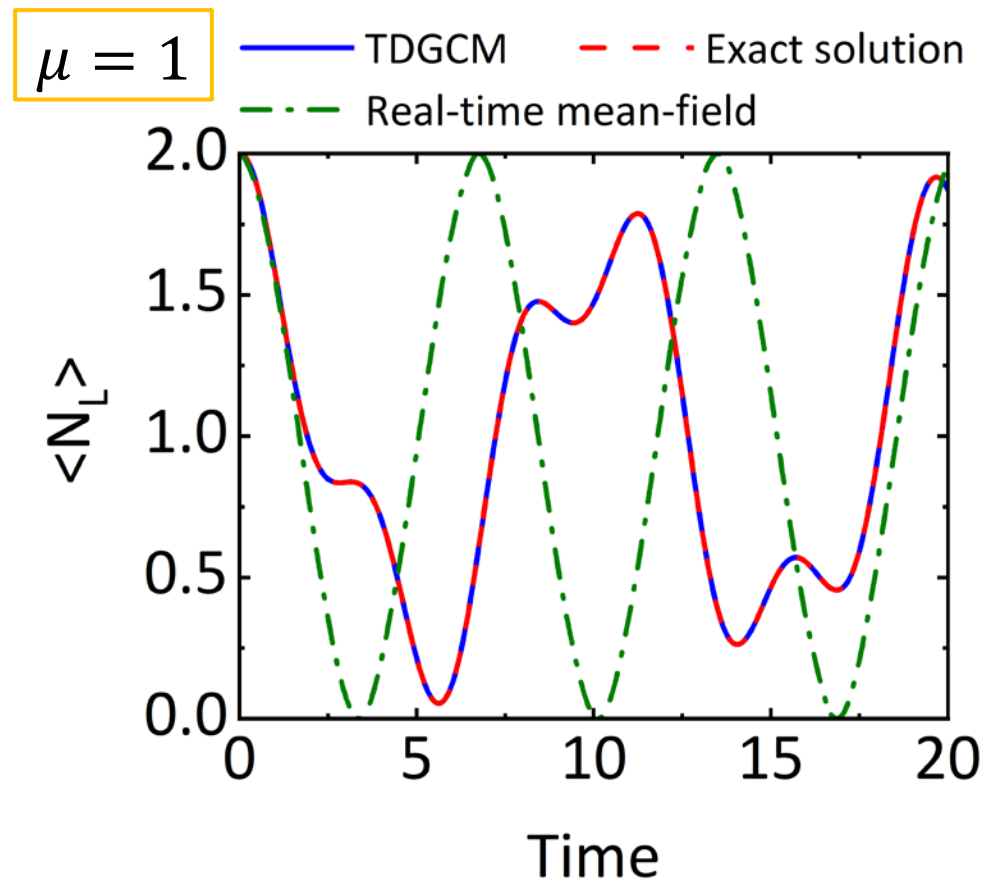
$\mu = 1$

$\mu = 4$

TDGCM with (θ_1, θ_2) and $(\theta_1, \theta_2, \phi_1, \phi_2)$



- ✓ $\theta_1 = \pi/2$, results are θ_2 -dependent
- ✓ no tunneling



- ✓ Two θ 's and two ϕ 's
- ✓ $\theta_1 = \pi/2$ and $\phi_1 = 0$

Expectation values of generator coordinate θ

$$\theta = \arcsin(|L|^2 - |R|^2), \quad \phi = \arg(R/L)$$

① Inversion method with mean-field approximation

$$\langle \theta \rangle = \arcsin(\langle \hat{N}_L(t) \rangle - 1)$$

$$\langle \hat{N}_L \rangle = \langle \Phi | \hat{N}_L | \Phi \rangle = 2|c_{LL}(t)|^2 + |c_{LR}(t)|^2 + |c_{RL}(t)|^2$$

$$\langle \theta \rangle = \arcsin(|c_{LL}(t)|^2 - |c_{RR}(t)|^2)$$

② Density matrix method

$$\rho = |\Phi(t)\rangle\langle\Phi(t)|$$

$$\langle \hat{N}_{1L} \rangle = \text{trace}(\rho \hat{N}_{1L}) \quad \langle \hat{N}_{1R} \rangle = \text{trace}(\rho \hat{N}_{1R})$$

$$\langle \theta \rangle = \arcsin(\langle \hat{N}_{1L} \rangle - \langle \hat{N}_{1R} \rangle) = \arcsin(|c_{LL}(t)|^2 - |c_{RR}(t)|^2)$$

Expectation values of generator coordinate θ

③ Reduced density matrix method

$$\rho(1) = \langle L_2 | \rho | L_2 \rangle + \langle R_2 | \rho | R_2 \rangle$$

$$\langle \theta \rangle = \arcsin(\rho(1)_{11} - \rho(1)_{22}) = \arcsin(|c_{LL}(t)|^2 - |c_{RR}(t)|^2)$$

→ ① ② ③ yield **identical outcomes**.

④ Probability-based weighted average

$$\sum_{\theta'} \mathcal{N}(\theta, \theta') u_k(\theta') = n_k u_k(\theta)$$

$$|k\rangle = \frac{1}{\sqrt{n_k}} \sum_{\theta} u_k(\theta) |\Psi(\theta)\rangle \quad (n_k \neq 0)$$

$$|g(\theta)|^2 = \left| \sum_{k, n_k \neq 0} g_k u_k(\theta) \right|^2$$

$$|\Phi(t)\rangle = \sum_{k, n_k \neq 0} g_k |k\rangle$$

$$\langle \hat{\theta} \rangle = \sum_{\theta} \theta |g(\theta)|^2$$

Expectation values of generator coordinate θ

⑤ Overlap-based weighted average

$$\langle \Psi(\theta) | \Phi(t) \rangle = \sum_{k, n_k \neq 0} g_k \frac{1}{\sqrt{n_k}} \sum_{\theta'} u_k(\theta') \langle \Psi(\theta) | \Psi(\theta') \rangle$$

$$\langle \hat{\theta} \rangle = \sum_{\theta} \theta |\langle \Psi(\theta) | \Phi(t) \rangle|^2$$

⑥ Eigenvalue-based weighted average

$$\langle \hat{\theta} \rangle = \sum_{\theta, \theta'} g^*(\theta, t) g(\theta', t) \langle \Psi(\theta) | \hat{\theta} | \Psi(\theta') \rangle = \sum_{\theta, \theta'} \theta' g^*(\theta, t) g(\theta', t) \mathcal{N}(\theta, \theta')$$

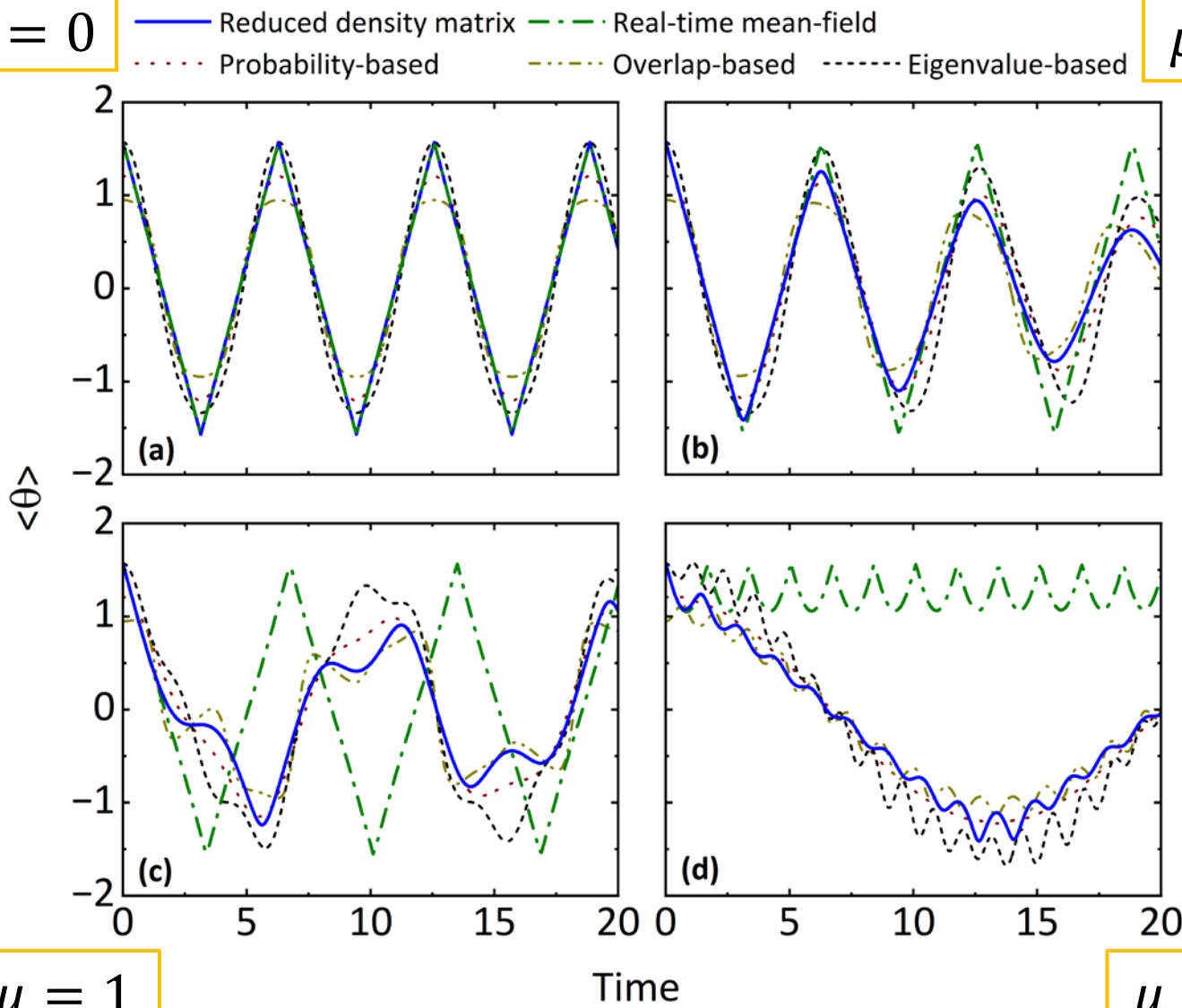
⑦ Real-time mean-field approach

$$\begin{aligned} \dot{\theta} &= -\sin \phi \\ \dot{\phi} &= \tan \theta \cos \phi + \mu \sin \theta \end{aligned}$$

Expectation values of generator coordinate θ

$\mu = 0$

$\mu = 0.1$



- ✓ Density-matrix-based approaches are most robust
- ✓ Weighted-average methods introduce method-dependent biases

$\mu = 1$

$\mu = 4$

Expectation values of generator coordinate ϕ

- ① Inversion method with mean-field approximation

$$\langle \phi \rangle = -\arcsin(\dot{\theta})$$

- ② Reduced density matrix method

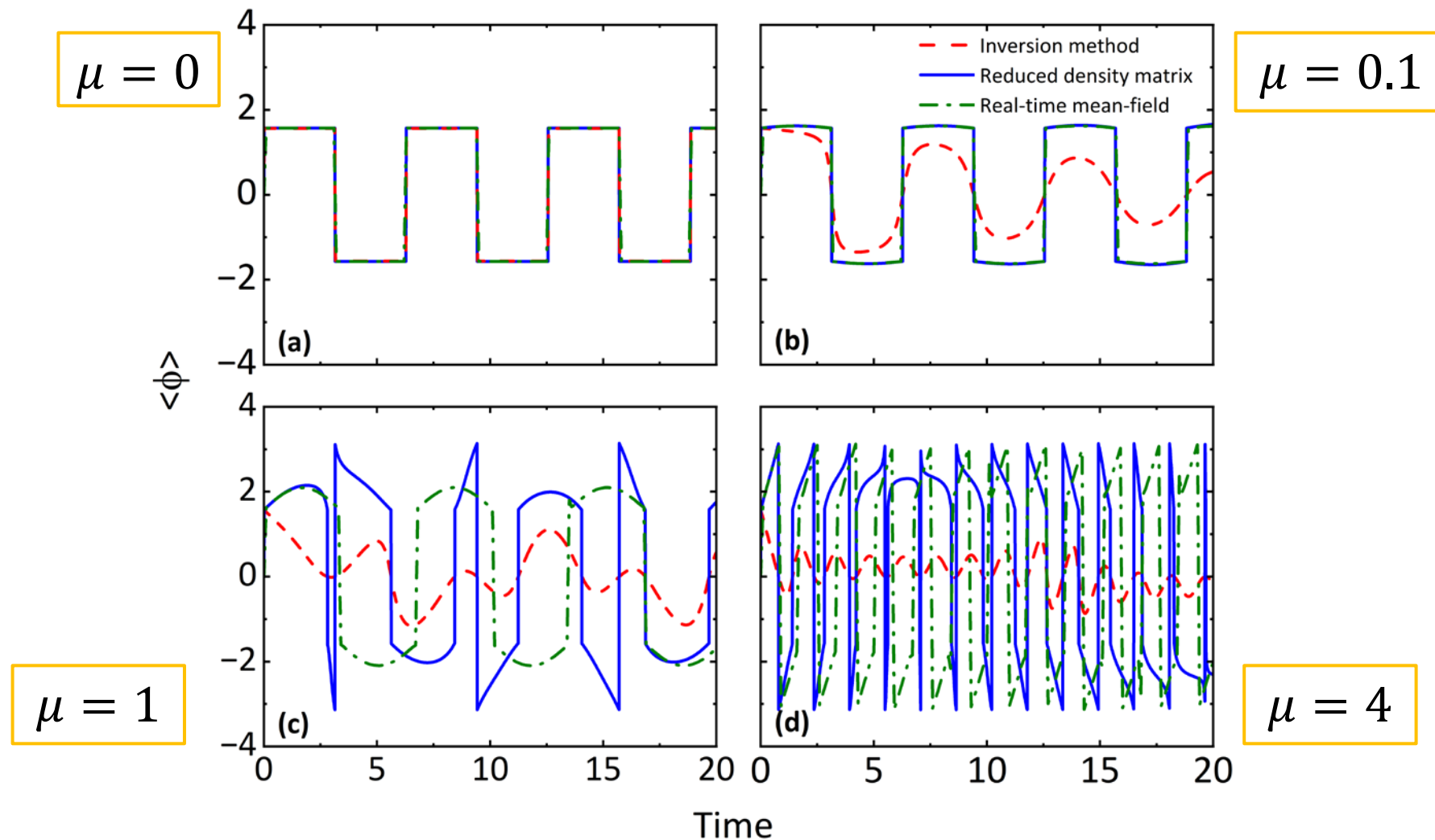
$$\langle \phi \rangle = \arg(R/L) = \arg(\rho(1)_{22}/\rho(1)_{12})$$

- ③ Real-time mean-field approach

$$\dot{\theta} = -\sin \phi \quad , \quad \dot{\phi} = \tan \theta \cos \phi + \mu \sin \theta$$

With $\phi = 0$, all weighted-average methods yield $\langle \phi \rangle = 0$.

Expectation values of generator coordinate ϕ



✓ Extracting phase information from a many-body state remains nontrivial

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A dream for new-generation DFT

quantum-field-theory
oriented DFT

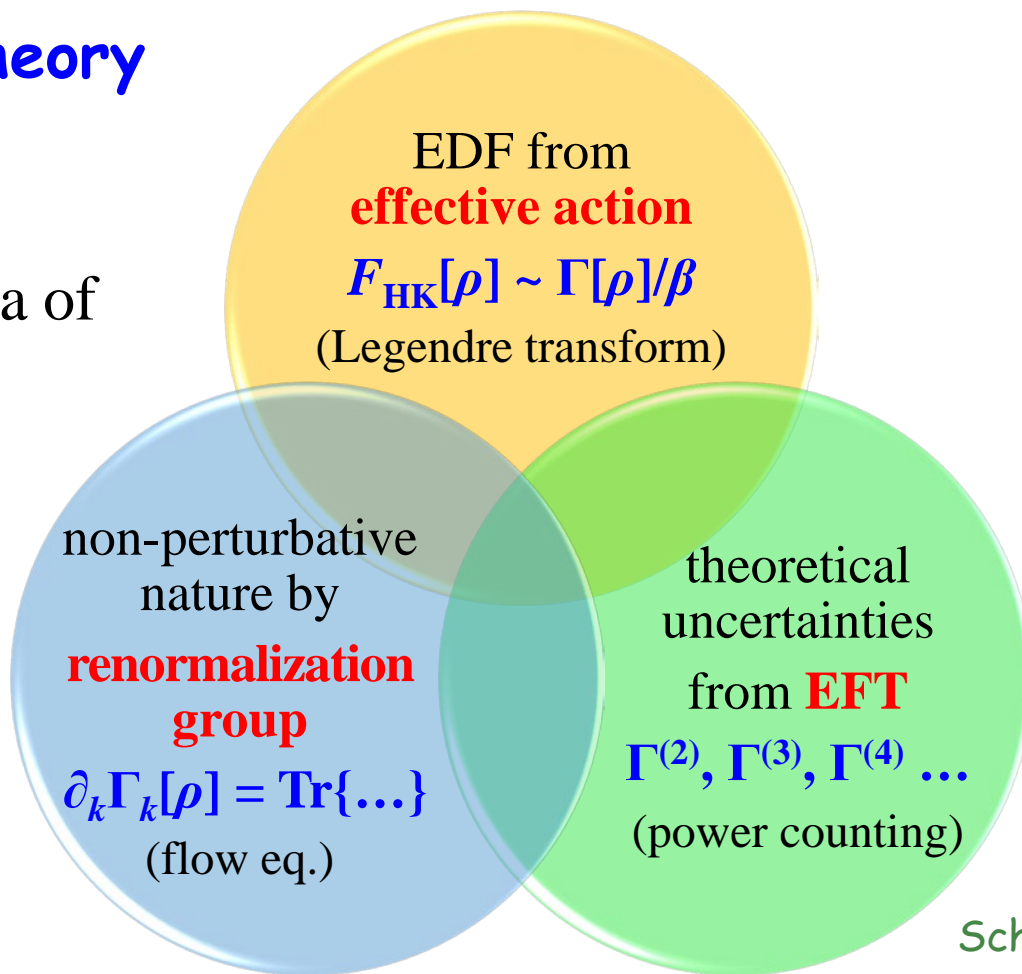
We proposed the idea of
Functional RG +
Kohn-Sham scheme

(KS-FRG)

HZL, Niu, Hatsuda,
PLB 779, 436 (2018)

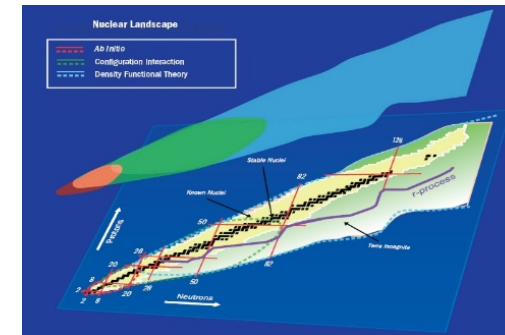


@ INPC2016, Australia



Interdisciplinary:
(lattice) QCD
hadron
cold atom
condensed matter
quantum chemistry

.....



<http://www.unedf.org/>

also cf.

Schwenk & Polonyi, arXiv:0403011 [nucl-th]
Kutzelnigg, JMS 768, 163 (2006)
Drut, Furnstahl, Platter, PPNP 64, 120 (2010)
Braun, JPG 39, 033001 (2012)
Metzner et al., RMP 84, 299 (2012)
Drews & Weise, PPNP 93, 69 (2017)

.....

DFT with functional-renormalization-group approach

□ DF defined as functional Legendre transformation R. Fukuda et al., Prog. Theo. Phys. 92, 4 (1994)

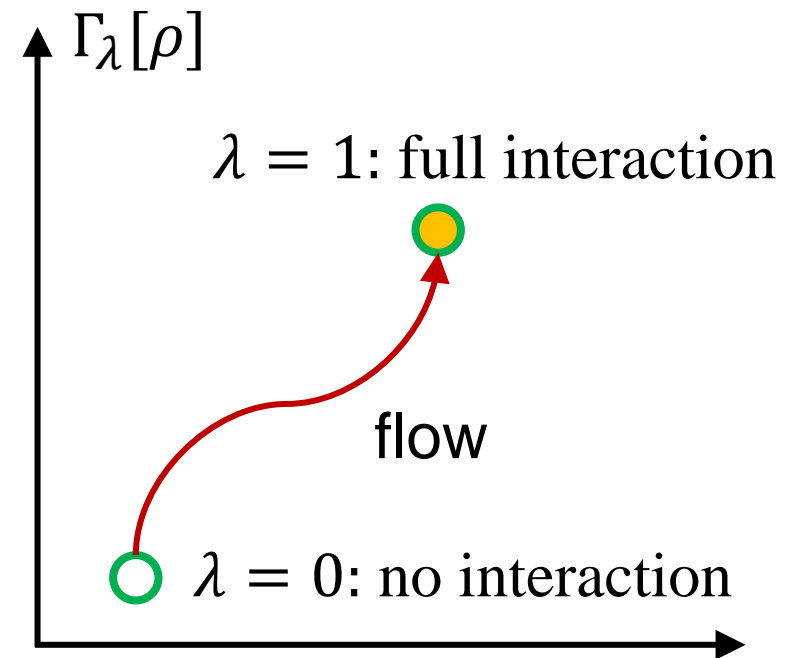
$$W[J] = \ln \mathcal{Z}[J] = \ln \int \mathcal{D}[\psi^*] \mathcal{D}[\psi] \exp \left\{ -S[\psi^*, \psi] + \int J \cdot \rho \right\}$$

$$\Gamma[\rho] = \sup_J \left(\int J \cdot \rho - W[J] \right)$$

$$E[\rho] = \lim_{\beta \rightarrow \infty} \frac{\Gamma[\rho]}{\beta}$$

□ Flow equation of effective action

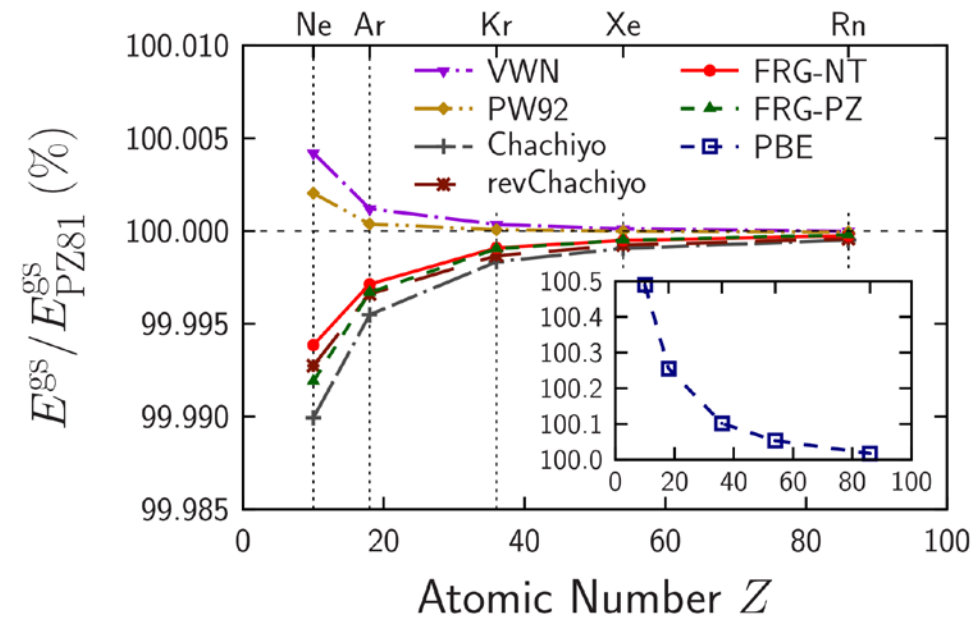
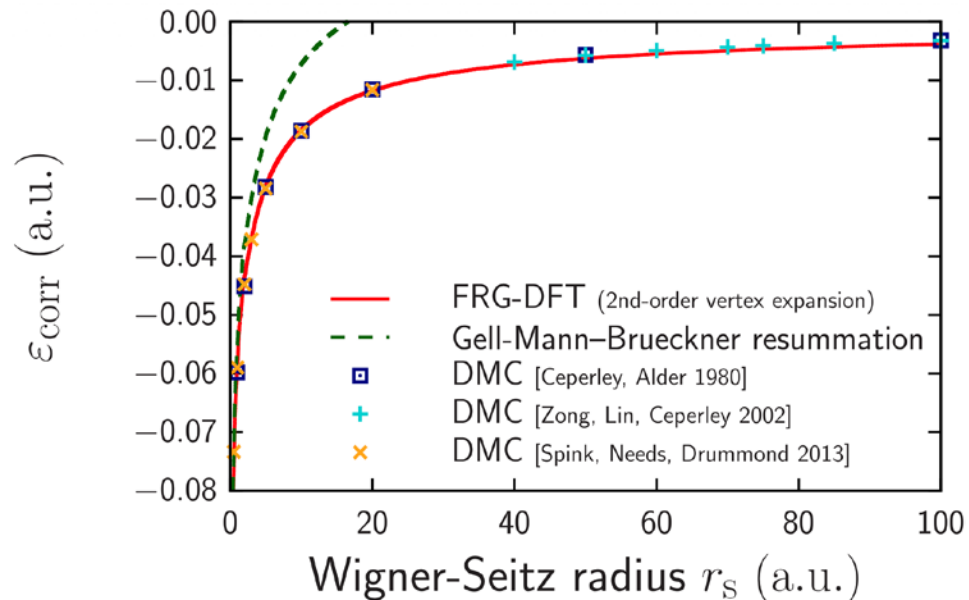
$$\Gamma_{\lambda=1}[\rho] = \Gamma_{\lambda=0}[\rho] + \int_0^1 d\lambda \partial_\lambda \Gamma_\lambda[\rho]$$



Effective action flow with λ

Status of FRG-DFT

- ✓ Conceptual advent *J. Polonyi and K. Sailer, PRB (2002), PRD (2005); A. Schwenk and J. Polonyi, arXiv (2004)*
- ✓ Toy model studies *J. Braun, JPG (2012); S. Kemler and J. Braun, JPG (2013); J.F. Rentrop+, JPA (2015)*
S. Kemler, M. Pospiech, and J. Braun, JPG (2017); T. Yokota, K. Yoshida, and T. Kunihiro, PRC (2019)
- ✓ Combination with Kohn-Sham scheme *H. Liang, Y. Niu, and T. Hatsuda, PLB (2018)*
- ✓ Application to electronic systems *T. Yokota and T. Naito, PRB (2019), PRR (2021), PRB (2022)*
T. Yokota, H. Kasuya, K. Yoshida et al., PTEP (2021)



Open questions of FRG-DFT

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{2} \int_0^\beta d\tau \int d\mathbf{x} d\mathbf{x}' V(\mathbf{x}, \mathbf{x}') \\ \times \left[\rho(\tau, \mathbf{x}) \rho(\tau, \mathbf{x}') - \delta(\mathbf{x} - \mathbf{x}') \rho(\tau, \mathbf{x}) + \left(\Gamma_\lambda^{(2)}[\rho] \right)^{-1}(\tau, \mathbf{x}; \tau, \mathbf{x}') \right]$$

- How to derive the **self-interaction correction term** in flow equations naturally?
- How to truncate the **hierarchy of flow equations** efficiently?
- How to evaluate the performance at **finite temperature**?
- ...

→ **Benchmarking FRG-DFT to exactly solvable models.**

Single-site Bose-Hubbard model

$$\hat{H}_0 = \frac{g}{2} \hat{a}^+ \hat{a}^+ \hat{a} \hat{a}$$

- Easy model with exact solution accessible in the Hamiltonian approach

$$\mathcal{Z}(\mu, T) = \text{Tr} e^{-\beta(\hat{H}_0 - \mu \hat{N})} = \sum_{N=0}^{\infty} \exp \left\{ -\beta \left[\frac{g}{2} N(N-1) - \mu N \right] \right\}$$

→ Free energy, chemical potential, particle number fluctuations, correlation functions, ...

- Subtleties emerge in coherent-state path integrals [L. Salasnich and C. Vianello, arXiv:2511.11547](#)

$$\mathcal{Z}(\mu, T) = \sum_{N=0}^{\infty} \exp \left\{ -\beta \left[\frac{g}{2} N^2 - \mu N \right] \right\} \quad (\text{incorrect})$$

→ Benchmarking FRG-DFT in the single-site Bose-Hubbard (SSBH) model

Exact flow equations of effective action

- Hamiltonian \hat{H} involving bosonic creation and annihilation operators

$$\hat{H} = \int d\mathbf{x} \hat{\phi}^\dagger(\mathbf{x}) h_0(\mathbf{x}) \hat{\phi}(\mathbf{x}) + \frac{1}{2} \int d\mathbf{x} d\mathbf{x}' V(\mathbf{x}, \mathbf{x}') \hat{\phi}^\dagger(\mathbf{x}) \hat{\phi}^\dagger(\mathbf{x}') \hat{\phi}(\mathbf{x}') \hat{\phi}(\mathbf{x})$$

- Exact flow equations identifies **self-interaction correction (SIC) term**

$$\begin{aligned} \partial_\lambda \Gamma_\lambda^{\text{naive}}[\rho] &= \frac{1}{2} \int_0^\beta d\tau \int d\mathbf{x} d\mathbf{x}' V(\mathbf{x}, \mathbf{x}') \\ &\quad \times [\rho(\tau, \mathbf{x}) \rho(\tau, \mathbf{x}') + (\Gamma_\lambda^{(2)}[\rho])^{-1}(\tau, \mathbf{x}; \tau, \mathbf{x}')] \end{aligned}$$

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\rho] &= \frac{1}{2} \int_0^\beta d\tau \int d\mathbf{x} d\mathbf{x}' V(\mathbf{x}, \mathbf{x}') \\ &\quad \times [\rho(\tau, \mathbf{x}) \rho(\tau, \mathbf{x}') - \delta(\mathbf{x} - \mathbf{x}') \rho(\tau, \mathbf{x}) + (\Gamma_\lambda^{(2)}[\rho])^{-1}(\tau, \mathbf{x}; \tau, \mathbf{x}')] \end{aligned}$$

For SSBH:

$$\partial_\lambda \Gamma_\lambda^{\text{SIC}}[N] = \frac{g}{2} \int_0^\beta d\tau \left\{ N(\tau)^2 - N(\tau) + \left[\Gamma_\lambda^{\text{SIC}(2)} \right]^{-1}(\tau, \tau) \right\}$$

Truncation scheme

$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)} \quad \partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \tilde{G}_\lambda^{(3)}$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2 - \frac{g}{2} \frac{1}{\beta} \tilde{G}_\lambda^{(4)} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \left(\tilde{G}_\lambda^{(3)} \right)^2$$

① Scheme I: Minimal closure

$$\tilde{G}_\lambda^{(3)} = \tilde{G}_\lambda^{(4)} = 0$$

② Scheme II: Frozen closure

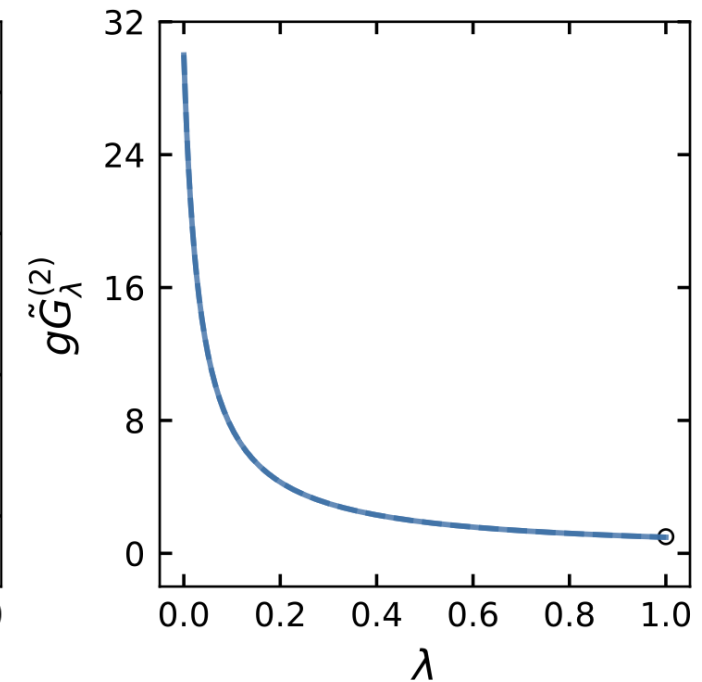
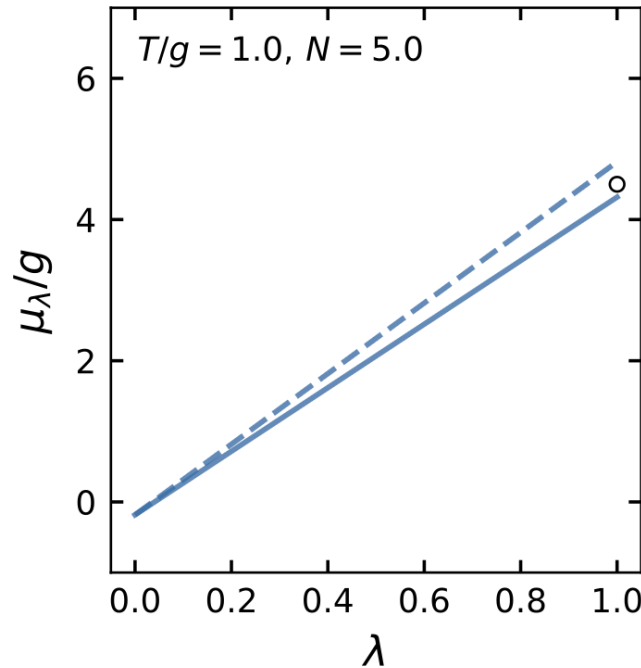
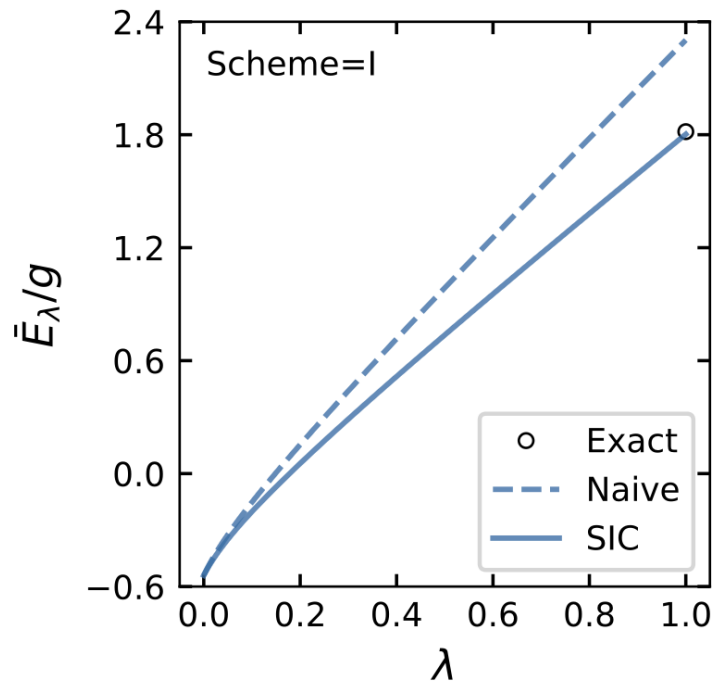
$$\tilde{G}_\lambda^{(3)} = \tilde{G}_{\lambda=0}^{(3)}; \quad \tilde{G}_\lambda^{(4)} = \tilde{G}_{\lambda=0}^{(4)}$$

③ Scheme III: Effective occupation closure

$$\tilde{G}_\lambda^{(3)} = \tilde{G}_{\lambda=0}^{(3)}(n_{\text{eff},\lambda}); \quad \tilde{G}_\lambda^{(4)} = \tilde{G}_{\lambda=0}^{(4)}(n_{\text{eff},\lambda})$$

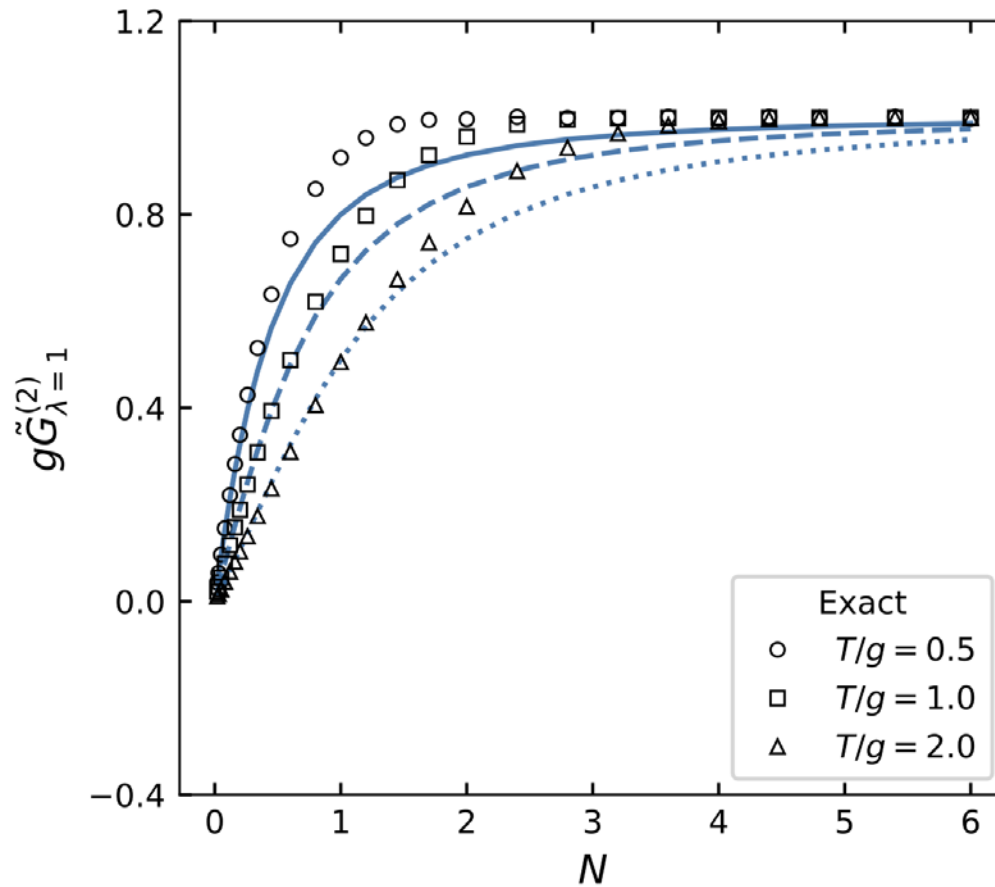
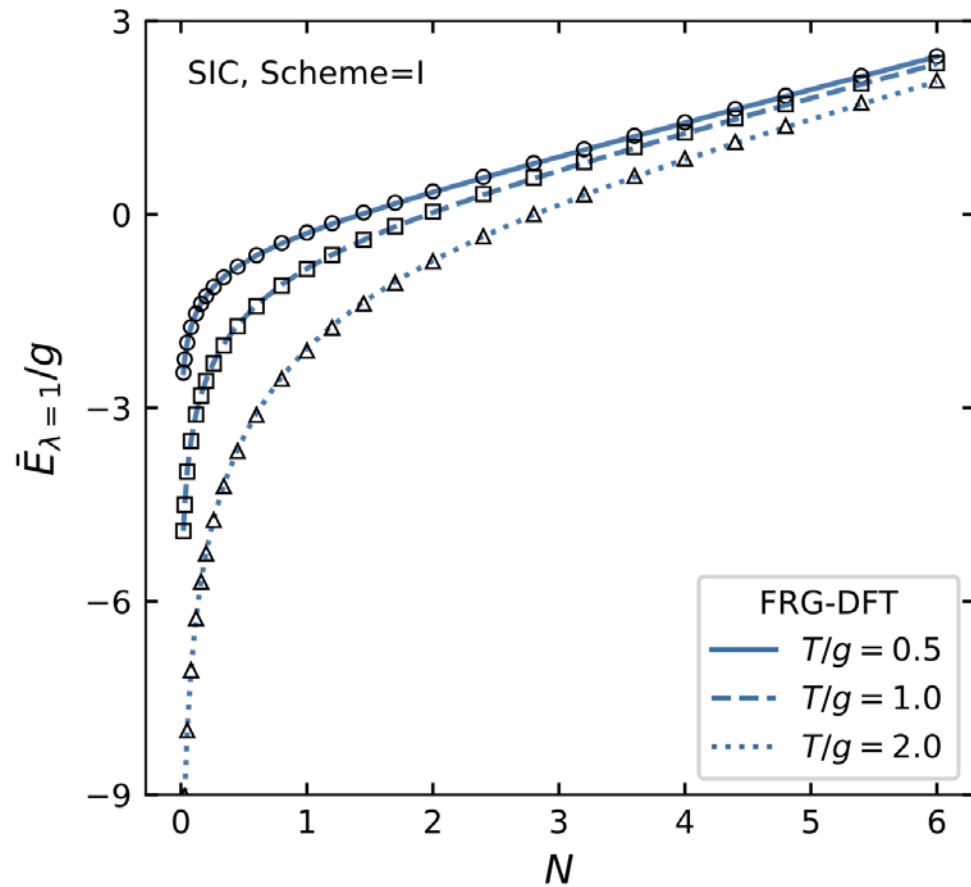
Solution with Scheme I: Minimal closure

$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)} \quad \partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} \quad \partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2$$



- ✓ The self-interaction correction term is necessary.
- ✓ The simplest truncation scheme has already good performance.

Solution with Scheme I: Minimal closure



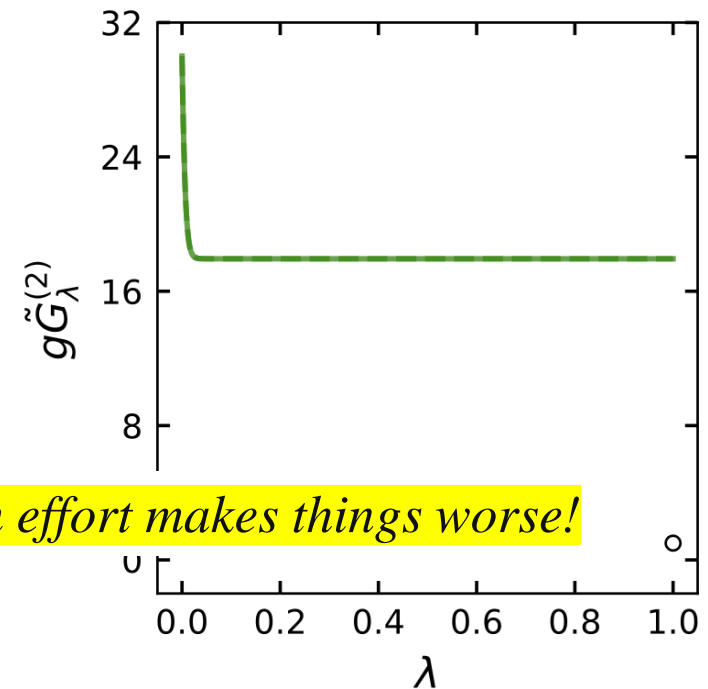
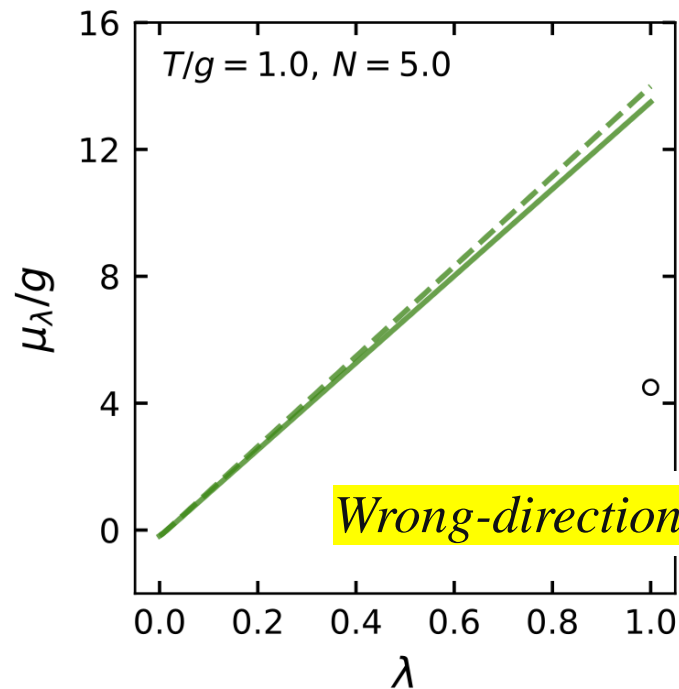
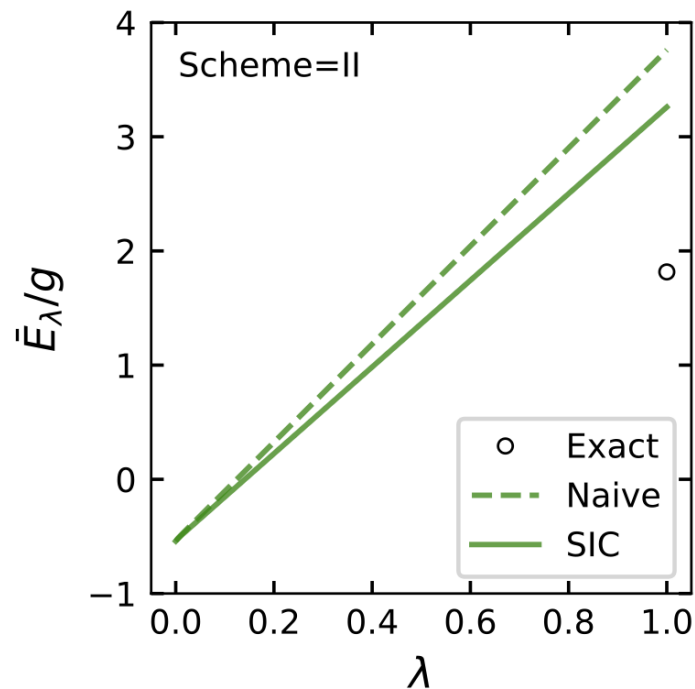
- ✓ Minimal closure works surprisingly good for energy.
- ✓ Two-density correlation function requires more information as input.

Solution with Scheme II: Frozen closure

$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)}$$

$$\partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \tilde{G}_{\lambda=0}^{(3)}$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2 - \frac{g}{2} \frac{1}{\beta} \tilde{G}_{\lambda=0}^{(4)} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \left(\tilde{G}_{\lambda=0}^{(3)} \right)^2$$

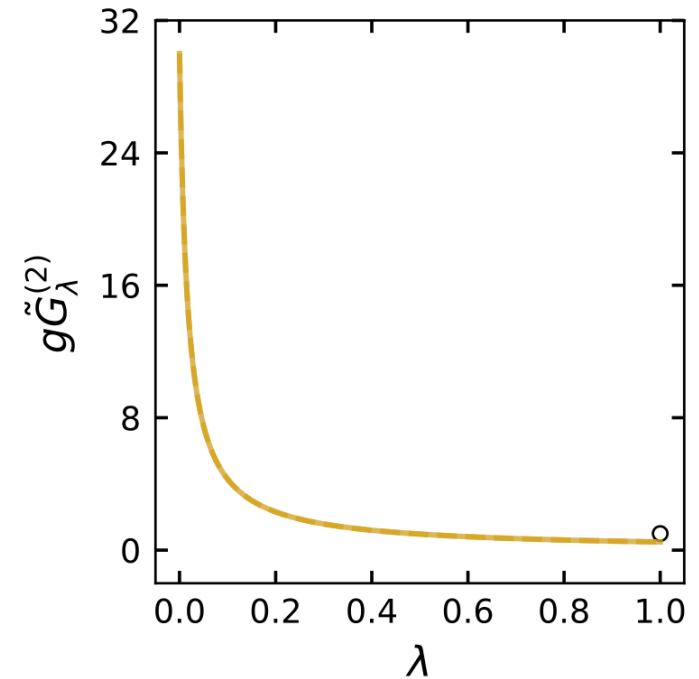
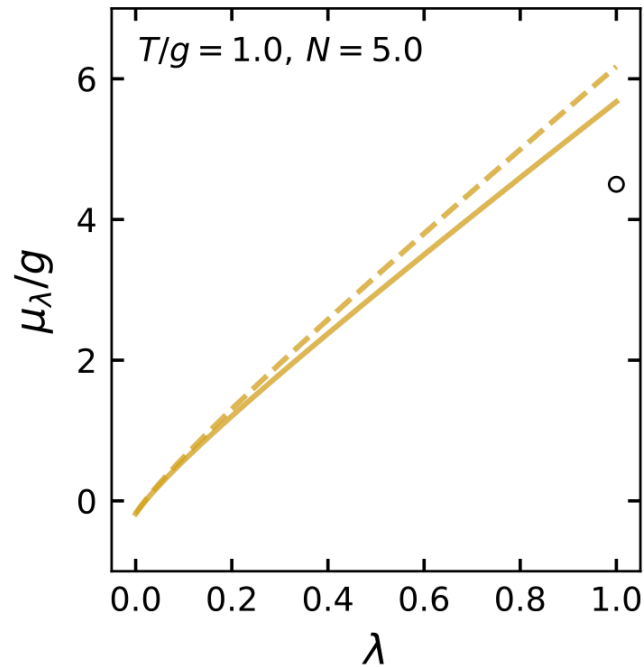
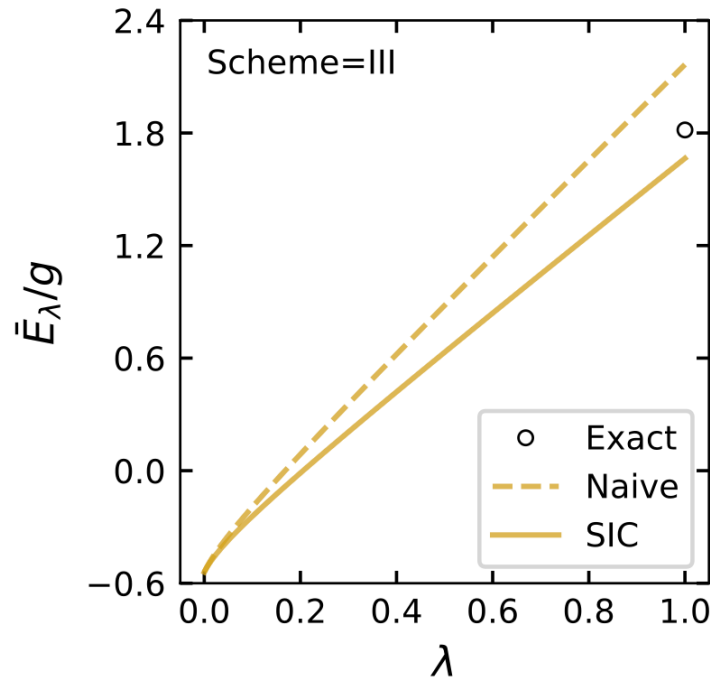


Wrong-direction effort makes things worse!

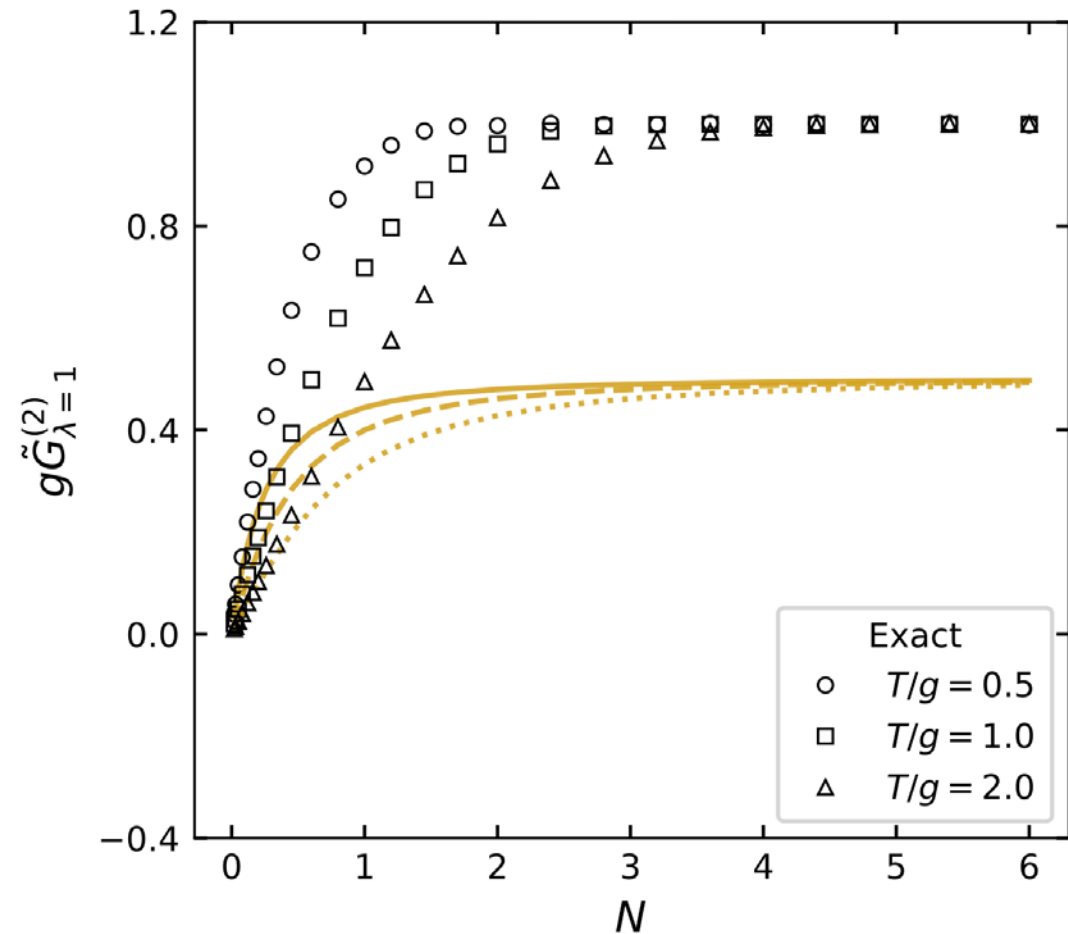
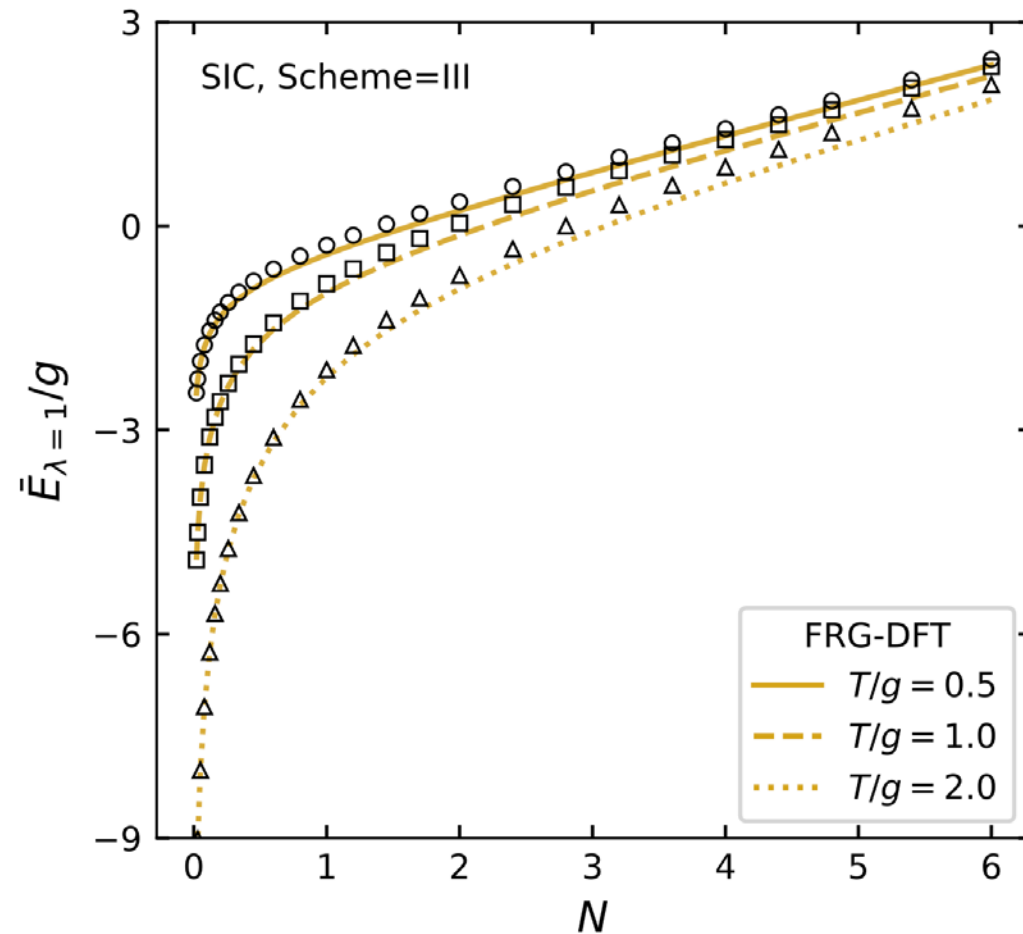
Solution with Scheme III: Effective occupation closure

$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)} \quad \partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \tilde{G}_{\lambda=0}^{(3)}(n_{\text{eff},\lambda})$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2 - \frac{g}{2} \frac{1}{\beta} \tilde{G}_{\lambda=0}^{(4)}(n_{\text{eff},\lambda}) + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \left(\tilde{G}_{\lambda=0}^{(3)}(n_{\text{eff},\lambda}) \right)^2$$



Solution with Scheme III: Effective occupation closure



✓ Effective occupation closure is still not good.

Scheme IV: Maximum entropy closure

- In scheme III:

$$\tilde{G}_\lambda^{(2)} \mapsto n_{\text{eff},\lambda} \mapsto \tilde{G}_\lambda^{(3)}, \tilde{G}_\lambda^{(4)}$$

We impose a free-theory-inspired ansatz for the distribution \rightarrow **bias**

- Scheme IV: reconstruct the distribution $p(N)$ with least bias by maximizing the Shannon entropy (**maximum entropy principle**)

$$S[p] \equiv - \sum_{N=0}^{\infty} p(N) \ln p(N)$$

E.g., if only normalization is known, maximizing $S[p]$ amounts to extremizing

$$\mathcal{L}[p] = - \sum_{i=1}^M p_i \ln p_i - \lambda \left(\sum_{i=1}^M p_i - 1 \right)$$

The results is $p_i = 1/M$. All probabilities are equal.

Scheme IV: Maximum entropy closure

- In flow equations, the Shannon entropy is maximized with fixed $\langle N \rangle, \text{Var}\langle N \rangle$

$$\begin{aligned} \mathcal{L}[p] = & - \sum_{N=0}^{\infty} p(N) \ln p(N) - \alpha \left(\sum_{N=0}^{\infty} p_N - 1 \right) \\ & - a \left(\sum_{N=0}^{\infty} N p_N - N_0 \right) - b \left(\sum_{N=0}^{\infty} N^2 p_N - N_0^2 - \frac{1}{\beta} \tilde{G}_\lambda^{(2)} \right) \end{aligned}$$

Parameters $a(\lambda), b(\lambda)$ in distribution $p_\lambda(N)$ are solved by $\langle N \rangle, \text{Var}\langle N \rangle$ constraints

$$p_\lambda(N) = \frac{1}{Z_\lambda(a, b)} \exp[-a(\lambda)N - b(\lambda)N^2]$$

$\tilde{G}_\lambda^{(3)}$ and $\tilde{G}_\lambda^{(4)}$ are mutually consistent and in consistent with $\tilde{G}_\lambda^{(2)}$ and $\langle N \rangle$.

$$\tilde{G}_\lambda^{(3)} = \beta^2 \langle (N - \langle N \rangle)^3 \rangle$$

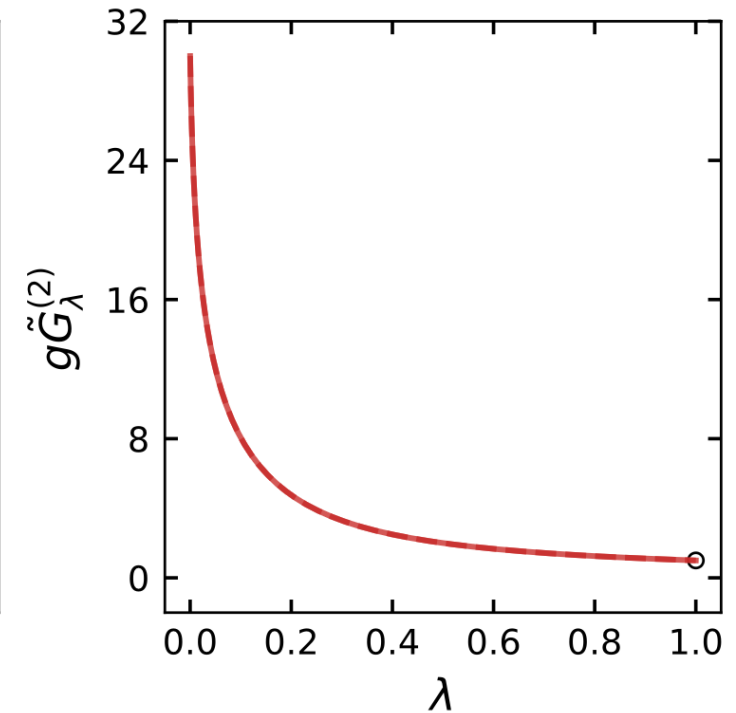
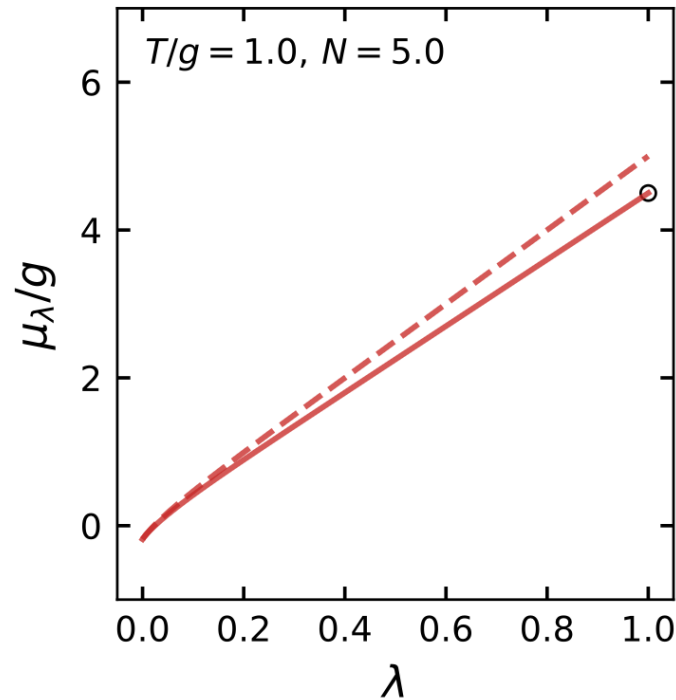
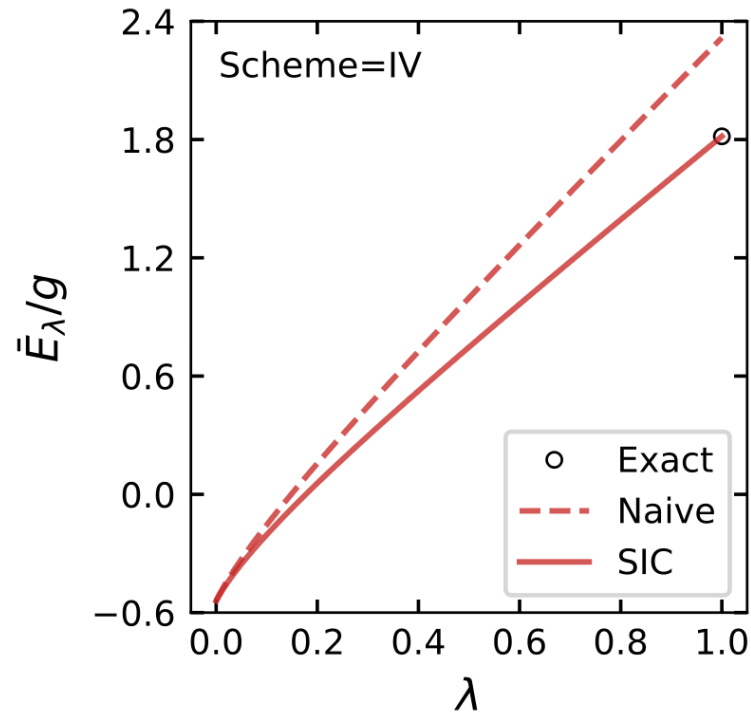
$$\tilde{G}_\lambda^{(4)} = \beta^3 [\langle (N - \langle N \rangle)^4 \rangle - 3 \langle (N - \langle N \rangle)^2 \rangle]$$

Solution with Scheme IV: Maximum entropy closure

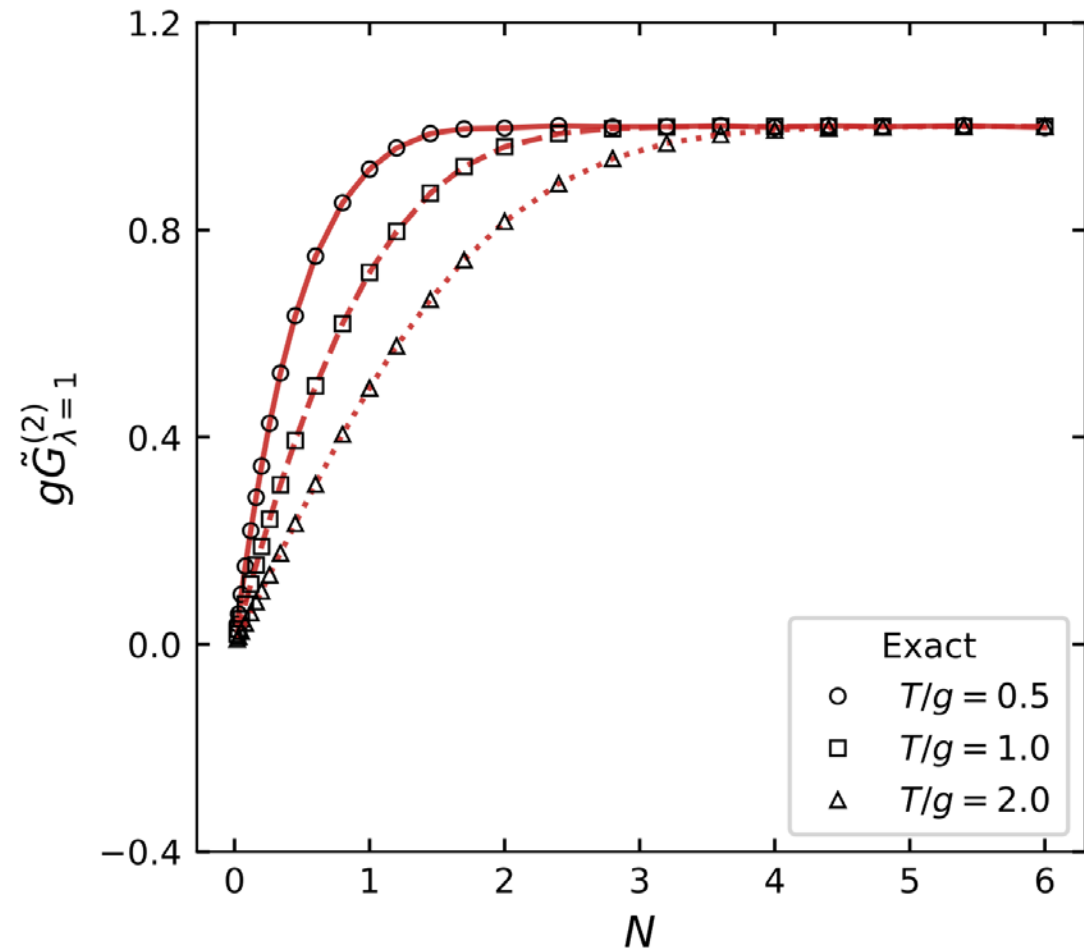
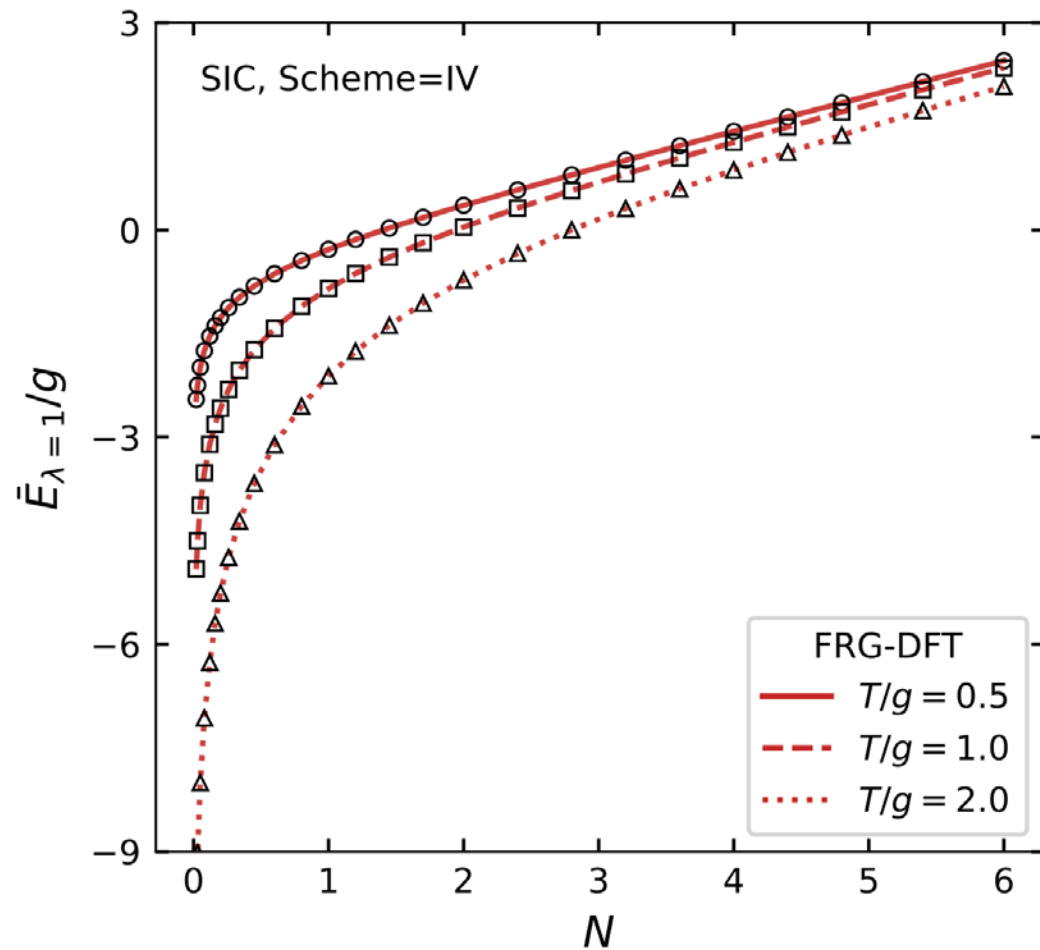
$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)}$$

$$\partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \tilde{G}_\lambda^{(3)}$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2 - \frac{g}{2} \frac{1}{\beta} \tilde{G}_\lambda^{(4)} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \left(\tilde{G}_\lambda^{(3)} \right)^2 \quad \text{Via maximum entropy principle}$$

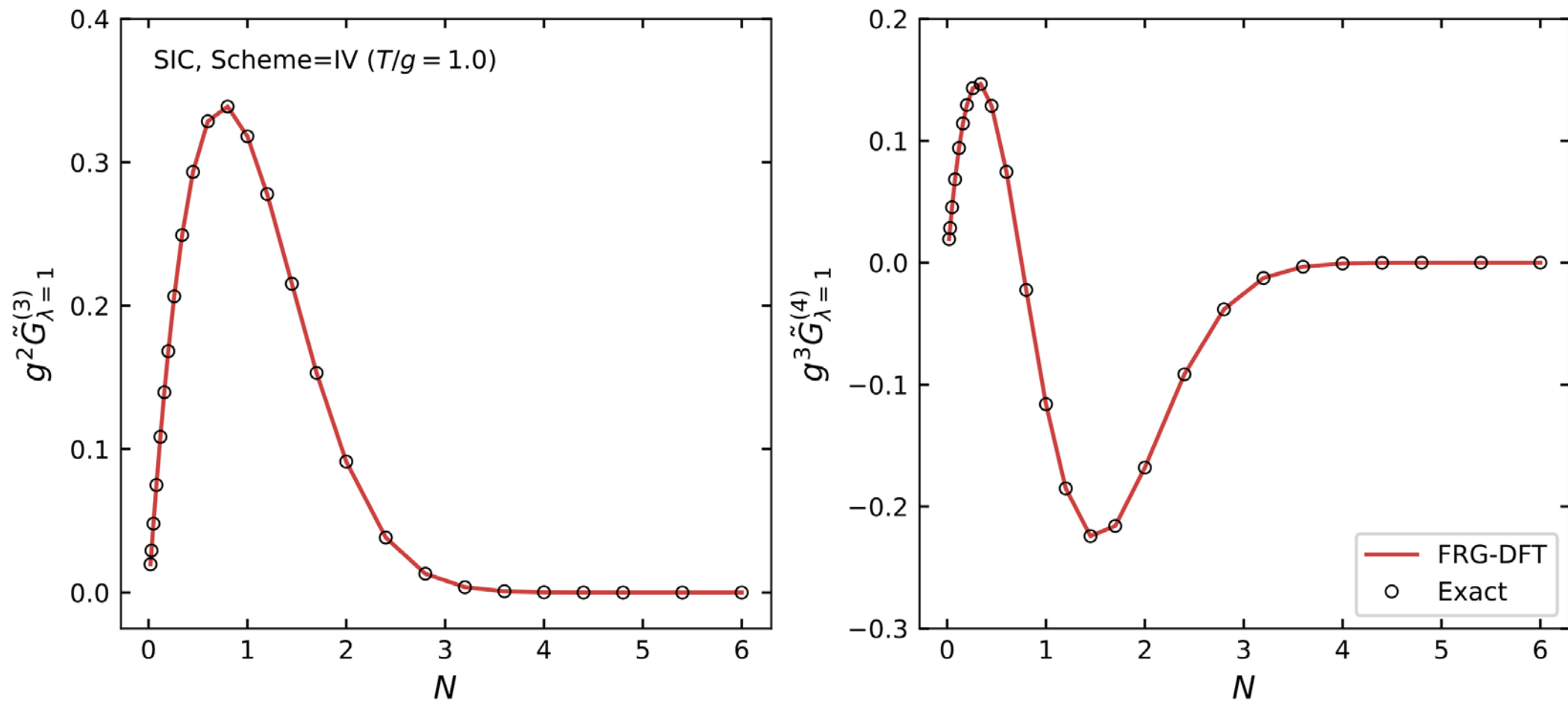


Solution with Scheme IV: Maximum entropy closure



✓ Satisfactory results are obtained with the maximum entropy closure.

Three- and four-density correlators: Scheme IV



✓ Higher-order density correlators are also reproduced satisfactorily.

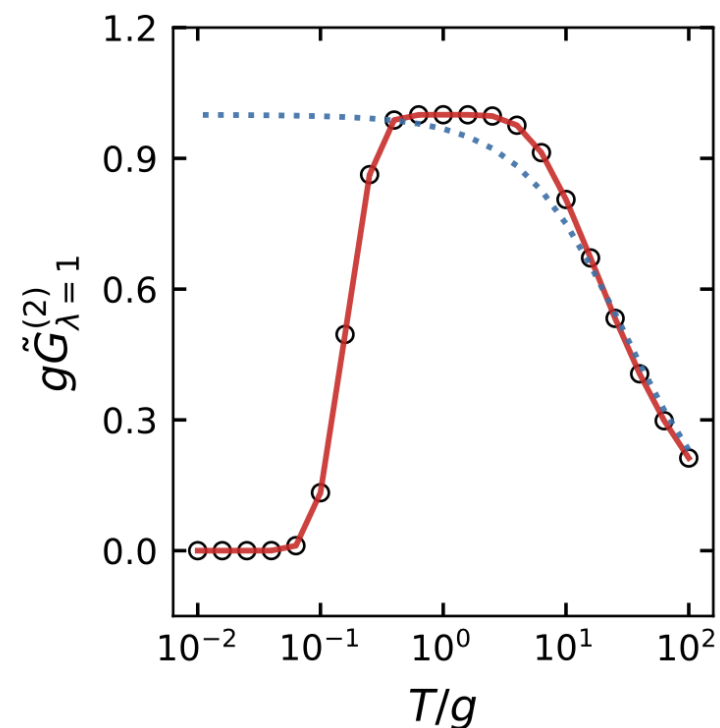
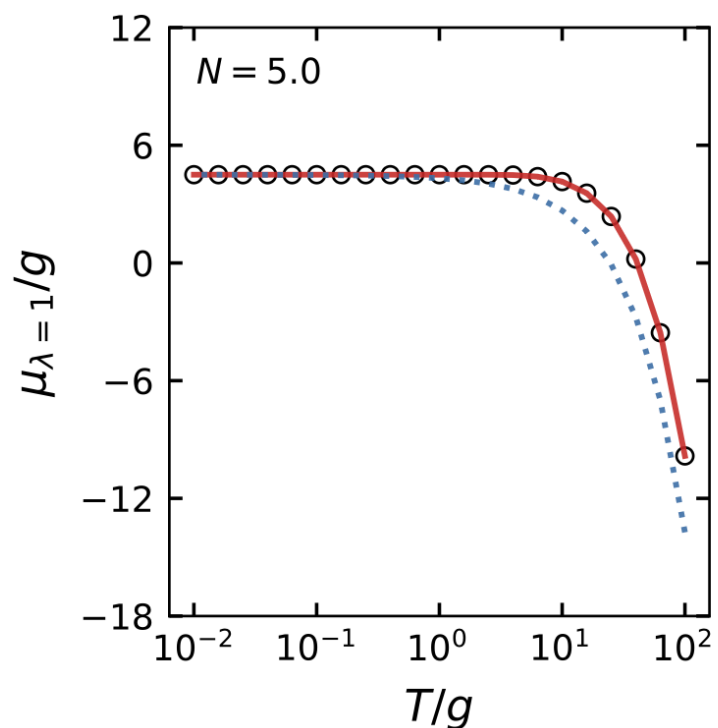
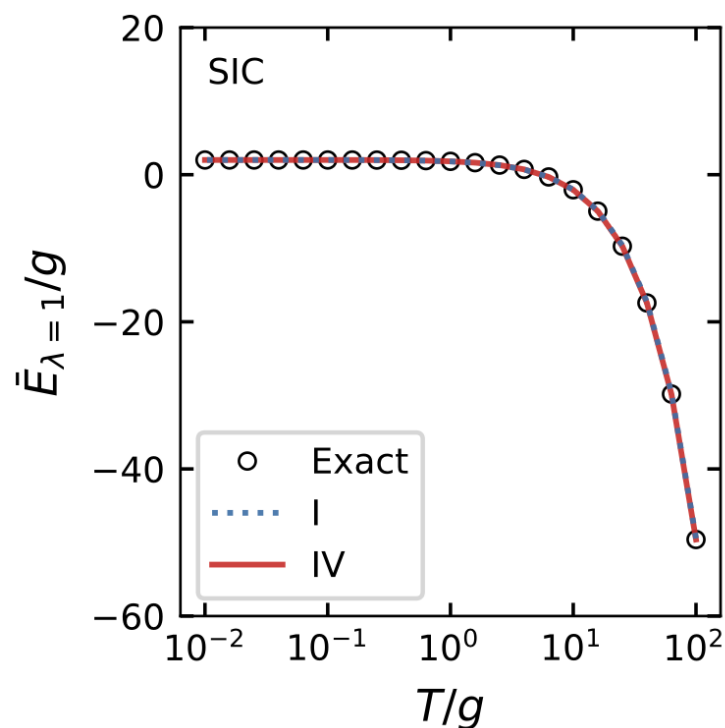
Performance over a broad range T/g

① Scheme I: Minimal closure

$$\tilde{G}_\lambda^{(3,4)} = 0$$

④ Scheme IV: Maximum entropy closure

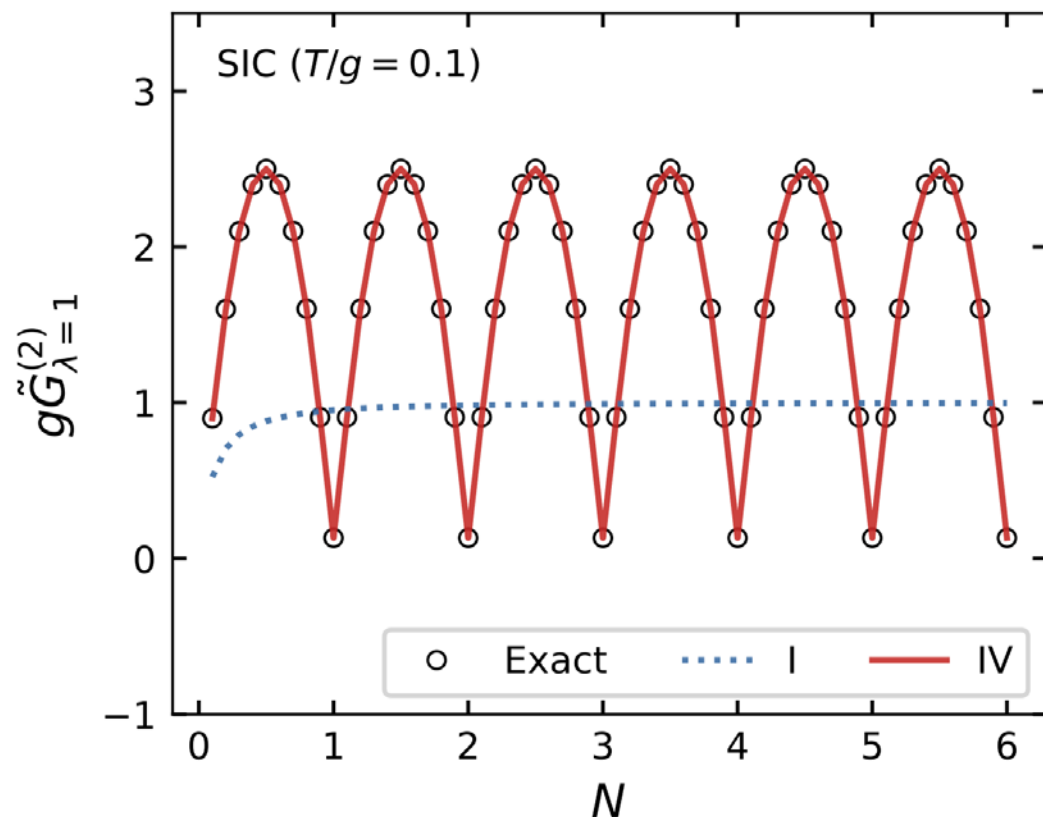
$$\tilde{G}_\lambda^{(3,4)} \text{ from maximum entropy}$$



Low-temperature oscillatory of two-density correlator

□ At low temperature ($T \ll g$), the dominant number states are N and $N + 1$

$$\mathcal{Z} \simeq e^{-\beta(E_N - \mu N)} + e^{-\beta[E_{N+1} - \mu(N+1)]}$$



✓ Define probability $\delta \equiv p_{N+1} \in [0,1]$

$$\langle N \rangle = Np_N + (N+1)p_{N+1} = N + \delta$$

$$\text{Var}(N) = \langle N^2 \rangle - \langle N \rangle^2 = \delta(1 - \delta)$$

$$g\tilde{G}^{(2)} = g\beta\text{Var}(N) = (T/g)^{-1}\delta(1 - \delta)$$

✓ $\delta = 0.5 \rightarrow g\tilde{G}_{\max}^{(2)} = (T/g)^{-1}/4 = 2.5$

✓ $\delta = 0$ or $1 \rightarrow g\tilde{G}_{\min}^{(2)} = 0$

Summary

□ Benchmarking studies of **collective quantum tunneling**

- ✓ TDGCM was successfully applied to the two-particle two-well model.
- ✓ TDGCM agrees perfectly with exact solutions without the self-trapping effect.
- ✓ $\langle \theta \rangle$ and $\langle \phi \rangle$ extraction methods reveal systematic method-dependence.

□ Benchmarking studies of **density functionals**

- ✓ FRG-DFT provides a feasible route to quantum thermodynamics.
- ✓ Exact flow equation identifies the indispensable SIC term.
- ✓ Closure should preserve consistency among density cumulants.