Finite-temperature Canonical-Ensemble Quantum Monte Carlo for Fermi Gases and Nuclei

Christopher N. Gilbreth

Institute for Nuclear Theory
University of Washington

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Collaborators

Yoram Alhassid
Yale University

Scott Jensen
Yale University

George Bertsch
INT, UW

Funding and Compute Time

Institute for Nuclear Theory

Outline

- Motivation
- Finite-temperature auxiliary-field Monte Carlo
- Canonical projection at finite temperature (technical aspects)
  - Discrete Fourier Transform
  - Stabilized diagonalization
  - Reduction of dimension
  - Optimization of two-body observables
- Applications to the unitary Fermi gas
- Applications to nuclei

Motivation

- The canonical ensemble is important for studying finite-size systems and even-odd effects in large systems
- Examples include atomic nuclei, metallic grains, finite-size systems of cold atoms; pairing in cold atoms
- Ground-state quantum Monte Carlo (QMC) calculations automatically work in the canonical ensemble
- Finite temperature usually done in the grand-canonical ensemble
- Canonical projection typically increases the computational scaling of finite-temperature QMC
- We have developed methods for finite-temperature QMC in the canonical ensemble which are competitive with grand-canonical calculations in computational time.

Finite-temperature AFMC

- Hubbard-Stratonovich transformation

$$e^{-\Delta\beta V\hat{O}^2/2} = \sqrt{\frac{\Delta\beta|V|}{2\pi}} \int_{-\infty}^{\infty} d\sigma e^{-\Delta\beta|V|\sigma^2/2} e^{\pm\Delta\beta s V\sigma\hat{O}} \qquad s = \begin{cases} 1, & V < 0 \\ i, & V > 0 \end{cases}$$

- Trotter decomposition $\beta = 1/(\text{temperature})$

$$e^{-\beta\hat{H}} = \left(e^{-\Delta\beta\hat{H}}\right)^{N_\tau}, \quad N_\tau = \beta/\Delta\beta \qquad e^{-\Delta\beta\hat{H}} = e^{-\Delta\beta\hat{H}_0/2} e^{-\Delta\beta\hat{V}} e^{-\Delta\beta\hat{H}_0/2} + O((\Delta\beta)^3)$$

- Path integral

$$e^{-\beta\hat{H}} = \int D[\sigma] \underbrace{G_\sigma}_{} \underbrace{\hat{U}(\sigma)}_{}$$

imaginary-time dependent auxiliary fields $\boldsymbol{\sigma}(\tau)$

One-body propagator

Gaussian weight

- One-body propagator $\hat{U}(\sigma) = \hat{U}_{N_\tau} \cdots \hat{U}_1$

- Observables $\langle\hat{O}\rangle = \dfrac{\mathrm{Tr}(\hat{O}e^{-\beta\hat{H}})}{\mathrm{Tr}(e^{-\beta\hat{H}})} = \dfrac{1}{N_{\mathrm{samp}}} \displaystyle\sum_{i=1}^{N_{\mathrm{samp}}} \langle\hat{O}\rangle_{\sigma^{(i)}}$

  - $\langle\hat{O}\rangle_{\sigma^{(i)}}$ calculated using matrix algebra in the single-particle space

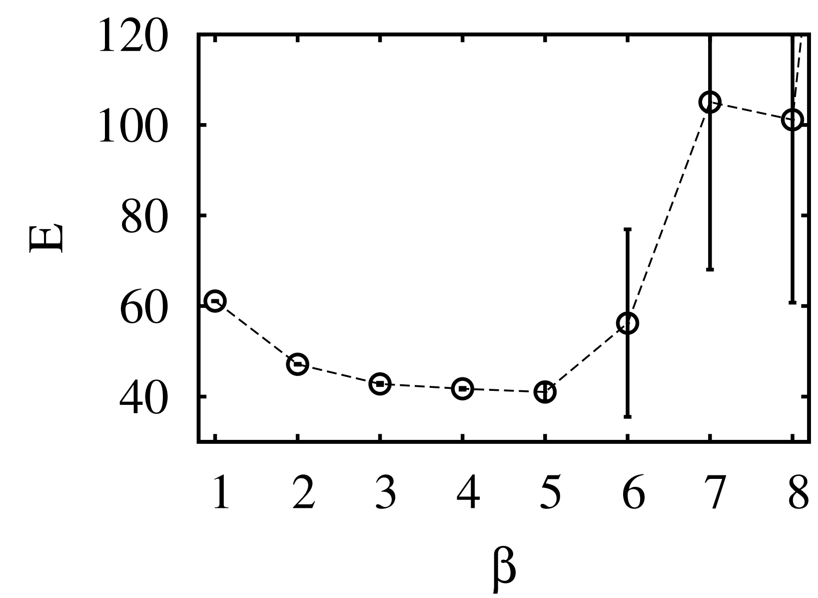
Numerical Stabilization

- Numerical scales grow and mix as time slices multiply

$$U = U_{N_\tau} \cdots U_1 \qquad\qquad U_t \sim N_s \times N_s$$

- At low temperatues, smaller scales are lost

$$\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \longrightarrow \begin{pmatrix} X & X & X \\ X & X & X \\ X & X & X \end{pmatrix} \longrightarrow \begin{pmatrix} \mathcal{X} & \mathcal{X} & \mathcal{X} \\ \mathcal{X} & \mathcal{X} & \mathcal{X} \\ \mathcal{X} & \mathcal{X} & \mathcal{X} \end{pmatrix}$$



- To manage, accumulate the decomposition

$$U = QDR = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} \mathcal{X} & & \\ & X & \\ & & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}$$

Q unitary, $D > 0$ diagonal, R unit upper triangular.

- Keeps track of varying scales within the propagator

- Similar to orthogonalization of the s.p. wavefunctions in ground-state calculations

Exact canonical projection

- Discrete Fourier transform of particle number

$$\frac{1}{M}\sum_{m=1}^{M} e^{i\varphi_m(N-N')} = \delta_{N,N'} \pmod{M} \qquad \varphi_m = 2\pi m/M$$

Fermions: setting M = (number of single-particle states) yields an exact projection

$$\hat{P}_N = \frac{1}{N_s}\sum_{m=1}^{N_s} e^{i\varphi_m(\hat{N}-N)}$$

- Number-projected trace

Chemical potential inserted for numerical stability

Number of single-particle states N_s

$$\mathrm{Tr}_N(\hat{U}) = \frac{e^{-\beta\mu N}}{N_s}\sum_{m=1}^{N_s} e^{-i\varphi_m N}\,\mathrm{Tr}_{\mathrm{GC}}(\hat{U}e^{\beta\mu\hat{N}}e^{i\varphi_m\hat{N}})$$

Number of particles

- Grand-canonical trace: $\mathrm{Tr}_{\mathrm{GC}}(\hat{U}e^{\beta\mu\hat{N}}e^{i\varphi_m\hat{N}}) = \det(I + Ue^{\beta\mu}e^{i\varphi_m})$

- Direct implementation requires N_s determinants, requiring $O(N_s^4)$ operations

Stabilized diagonalization

*CG, Y. Alhassid, Comp. Phys. Comm. **188**, 1 (2015)*

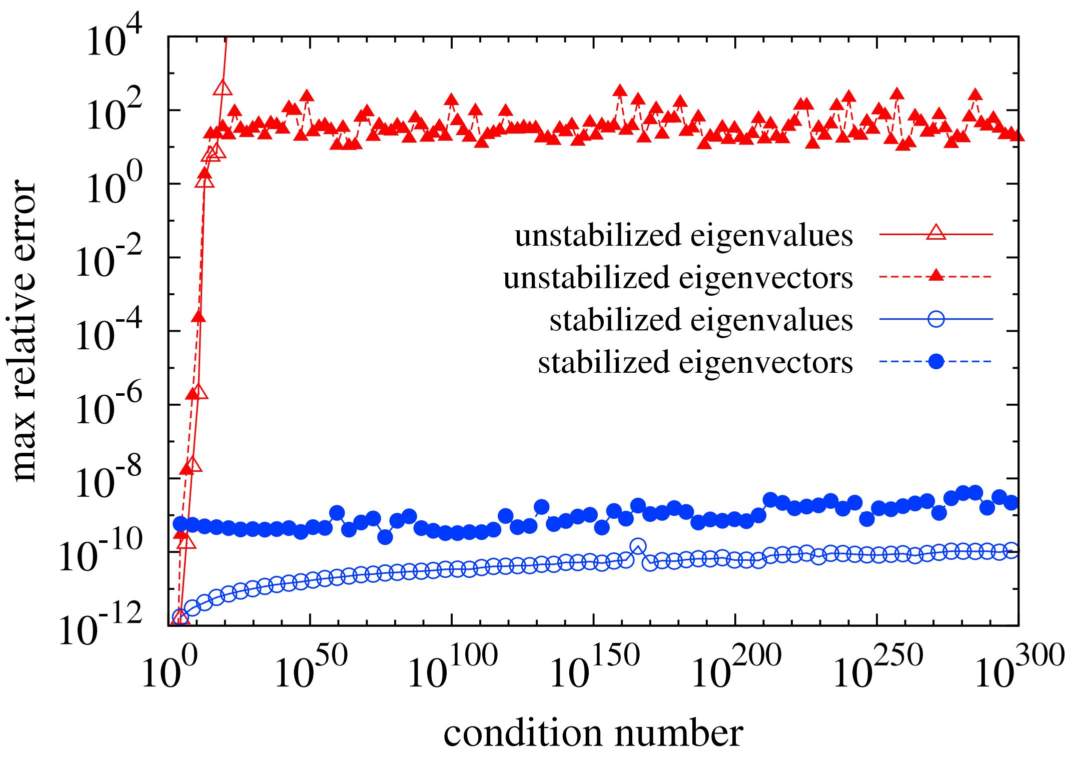
- Need to compute $\det(1 + e^{i\varphi_m} QDR)$ for each *m*

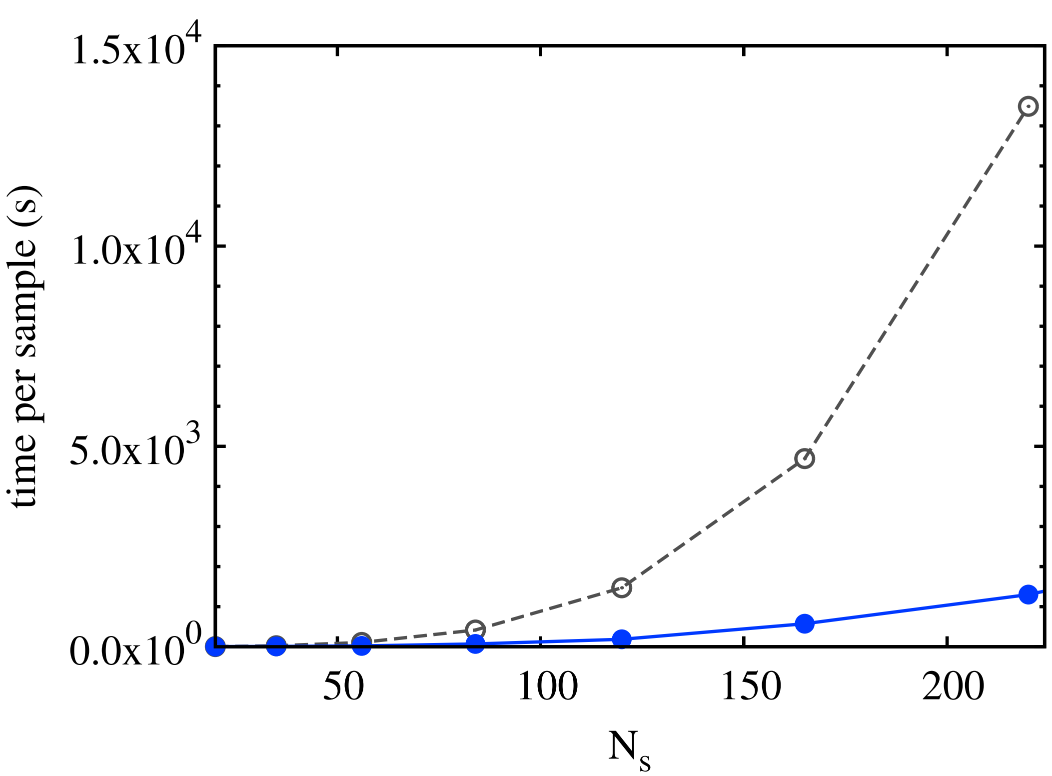
- Can stably diagonalize DRQ to obtain eigenvalues & eigenvectors of QDR

$$QDRx = \lambda x \;\Leftrightarrow\; DRQy = \lambda y \qquad (x = Qy)$$

$$\mathrm{Tr}_N(\hat{U}) = \frac{1}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m N} \prod_{k=1}^{N_s} (1 + \lambda_k e^{i\varphi_m})$$

- Reduces computational scaling to $O(N_s^3)$





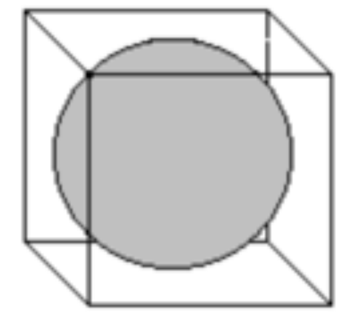
Model space truncation

- Cubic scaling is still problematic for larger systems

- Spherical cutoff in momentum space $\Lambda = \pi/\delta x$:

[Bulgac, Drut, Magierski, Phys. Rev. A **78**, 023625 (2008)]

$$\hat{H} = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} + \hat{V} \qquad \epsilon_{\boldsymbol{k}} = \begin{cases} \hbar^2 k^2/2m\,, & k \leq \Lambda \\ \infty\,, & \text{otherwise} \end{cases}$$



Reduces N_s by ~ 1/2 but affects two-body physics.

- We can find a rigorous way to reduce the model space dimension with a controllable error.

- Make use of the decomposition

$$U = Q\,D\,R = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} X & & \\ & X & \\ & & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}$$

U - Unitary
D - Diagonal
R - Unit upper triangular

to identify and remove unimportant states (for a given field configuration).

Eigenvalues $|\lambda_i| \sim D_{ii}$ **Occupations** $n_i \sim \dfrac{|\lambda_i|}{1 + |\lambda_i|}$

Truncated diagonalization

- Transform to $S = e^{\beta\mu} DRQ$ and zero out small scales: $S' = S + (\text{small perturbation})$

$$S = e^{\beta\mu} DRQ = \begin{pmatrix} X & X & X & X & X \\ X & X & X & X & X \\ x & x & x & x & x \\ x & x & x & x & x \\ . & . & . & . & . \end{pmatrix}_{N_s \times N_s}$$

$\tilde{S}$

$$S' = e^{\beta\mu} D' RQ = \left(\begin{array}{ccc|cc} X & X & X & X & X \\ X & X & X & X & X \\ x & x & x & x & x \\ \hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right)_{N_s \times N_s} = S + E$$

- Choose number of rows to zero so that $||E|| < \varepsilon$ (small parameter)

- Nonzero eigenvalues & eigenvectors of S' can be obtained from $\tilde{S}$

$$S'y = \lambda y\,, \qquad y = \begin{pmatrix} y_1 \\ \vdots \\ y_{N_r} \\ 0 \\ \vdots \end{pmatrix}, \qquad (\lambda \neq 0)$$

Truncated diagonalization cont.

- Transformation matrices have the form (for $S' = P'\Lambda P^{-1}$, $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots)$)

$$P' = \begin{pmatrix} \boxed{\tilde{P}} & \boxed{\text{basis for } \mathrm{Null}(S')} \\ \begin{matrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{matrix} & \end{pmatrix} \qquad P'^{-1} = \begin{pmatrix} \boxed{\tilde{P}^{-1}} & \boxed{A} \\ \begin{matrix} x & x & x \\ x & x & x \end{matrix} & \begin{matrix} x & x \\ x & x \end{matrix} \end{pmatrix}$$

- The the only physically relevant part of P' is $\tilde{P}$, which is obtained automatically.

- The matrix A is unknown, so P'^{-1} needs to be determined from matrix algebra:

$$P'^{-1}_{ij} = \sum_{k=1}^{N_s} X^{-1}_{ik} (RQ)_{kj}, \qquad X_{ik} = \sum_{l=1}^{N_s} (RQ)_{il} P'_{lk}, \qquad i, k = 1{:}\, N_s,\; j = 1{:}\, N$$

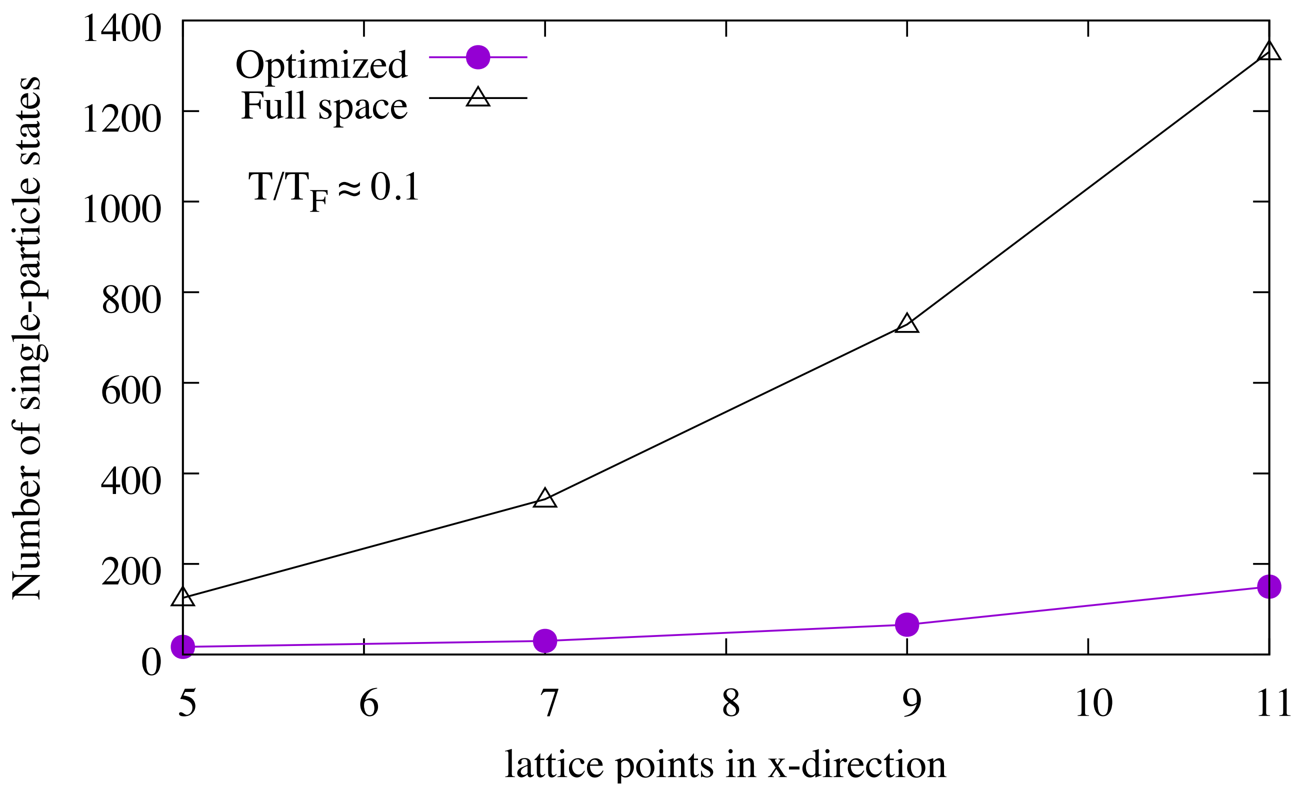
- This procedure effectively reduces the dimension of the propagator by omitting unoccupied states.

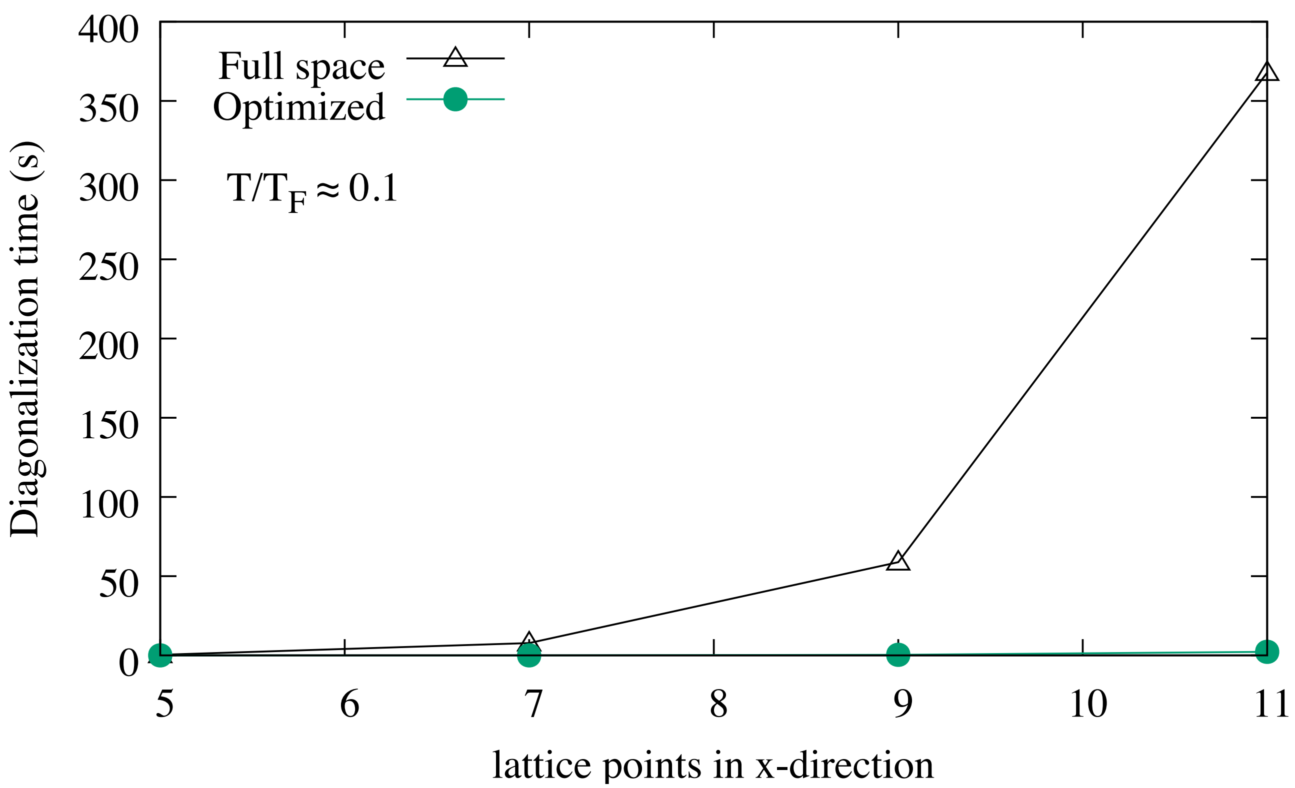
- Typical dimensions $(2\text{-}4) \times (\text{number of particles})$ at temperatures of interest

- Particularly relevant at low densities

Timing - unitary Fermi gas

- At fixed filling $\nu \approx 0.06$





- Canonical projection becomes effectively negligible in cost for most observables in dilute systems

Two-body observables

- General matrix elements $\langle a_i^\dagger a_j a_k^\dagger a_l \rangle$. For e.g., spin susceptibility.

$$\langle a_i^\dagger a_j a_k^\dagger a_l \rangle_\sigma = \frac{e^{-\beta\mu}}{Z N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m N} \langle a_i^\dagger a_j a_k^\dagger a_l \rangle^{(m)} \eta_m \ , \quad \gamma_{ij}^{(m)} = \sum_\alpha P_{i\alpha} (1 + \lambda_\alpha^{-1} e^{-\beta\mu} e^{-i\varphi_m})^{-1} P_\alpha^{-1}$$

$O(N_s^4)$ to compute all $\gamma^{(m)}$ matrices.

1. Reduce number of points in Fourier transform: approximate projection

$$\frac{1}{N_{\mathrm{FT}}} \sum_{m=1}^{N_{\mathrm{FT}}} e^{i\varphi_m (N - N')} = \begin{cases} 1, & N = N' \pmod{N_{\mathrm{FT}}} \\ 0, & \text{otherwise} \end{cases}$$

[L. Fang, Y. Alhassid]

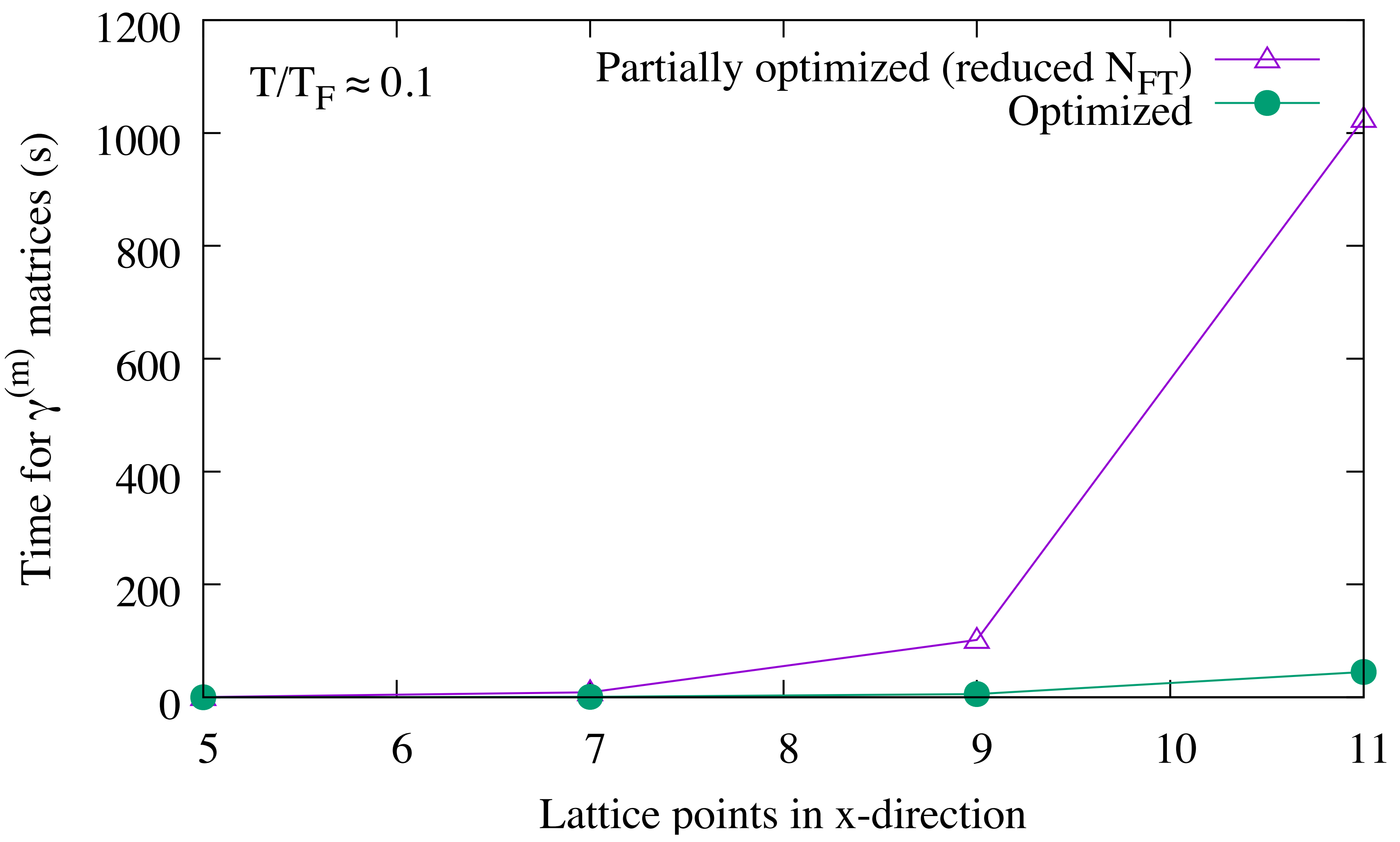
2. Omit unoccupied states α such that $(1 + \lambda_\alpha^{-1} e^{-\beta\mu})^{-1} \ll 1$

3. Optimize calculations for states far from the Fermi surface:

$$1 + \lambda_\alpha^{-1} e^{-\beta\mu} e^{-i\varphi_m} = \begin{cases} \lambda_\alpha e^{\beta\mu} e^{i\varphi_m} (1 - \lambda_\alpha e^{\beta\mu} e^{i\varphi_m} + \ldots), & \lambda_\alpha e^{\beta\mu} < 1 \\ 1 - (\lambda_\alpha e^{\beta\mu} e^{i\varphi_m})^{-1} + \ldots & \lambda_\alpha e^{\beta\mu} > 1 \end{cases}$$

Contributions from $\lambda_\alpha e^{\beta\mu} e^{i\varphi_m}$ are more efficient to compute than those from $(1 + \lambda_\alpha^{-1} e^{-\beta\mu} e^{-i\varphi_m})$.

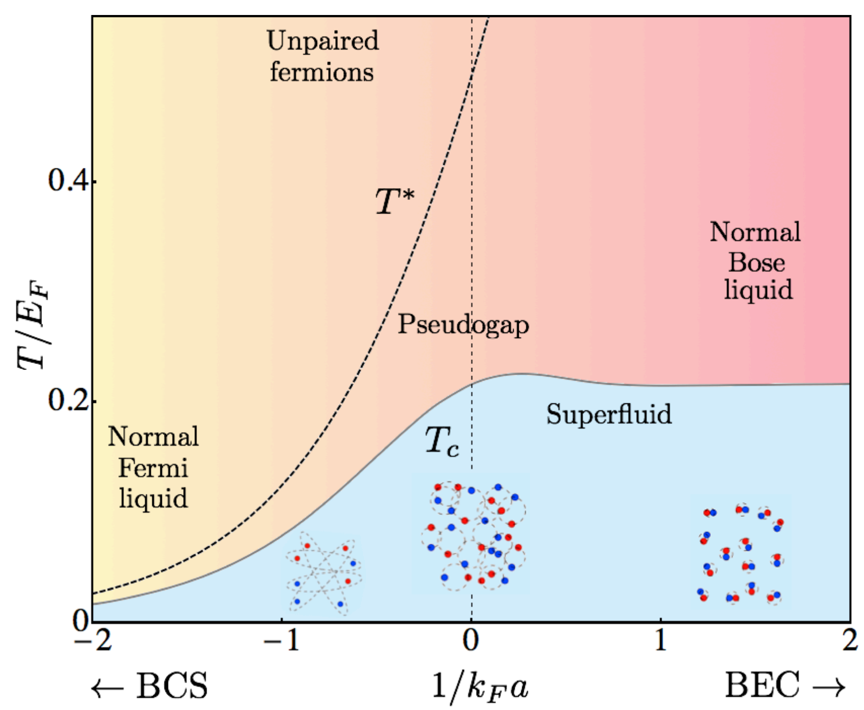
Timing— two-body observables



Enables otherwise impractical canonical two-body observables.

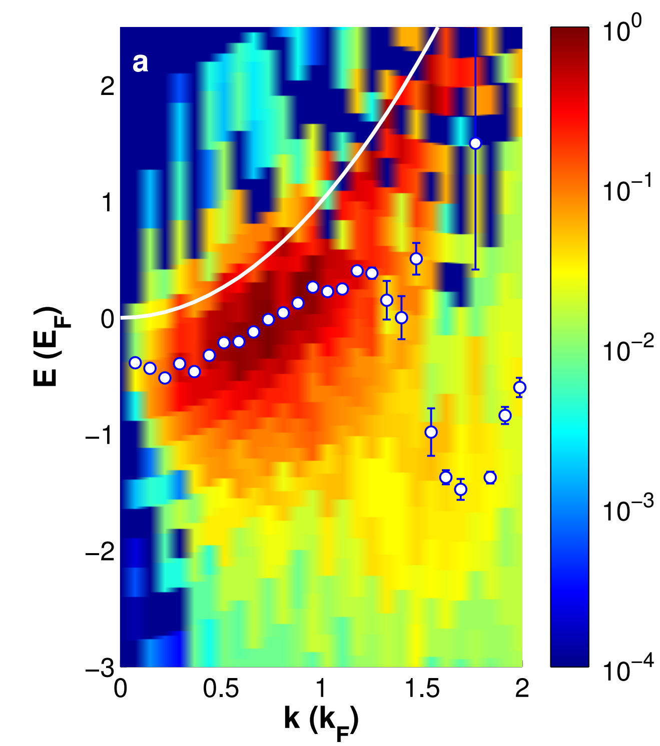
Finite-temperature unitary Fermi gas

- Spin-1/2 particles interact in 3D with range $r_0 \ll k_F^{-1}$ (pure *s*-wave scattering)
- Only length scales: k_F, s-wave scattering length a, thermal wavelength λ_T
- Universal physics independent of the short-range structure of the particles
- BCS-BEC crossover obtained as a function of $1/(k_F a)$



Randeria and Taylor (2014)

Unitary limit



Photoemission spectroscopy at unitarity
Sagi, et al. (PRL 2015)

- **Pseudogap regime:** pairing without condensation $T_c < T < T^*$.
  There is a long-running debate about its existence in the unitary limit.
  See our review: *S. Jensen, CG, Y. Alhassid arXiv:1807.03913*

Lattice model

- Fixed number $N = N_\uparrow + N_\downarrow$ of particles interact at finite temperature, on a cubic lattice (N_x^3 points), with periodic boundary conditions, and an on-site interaction.

- Length scales: L (box volume), $1/k_F$ (Fermi wavelength), δx (lattice spacing), λ_T (thermal wavelength)

- Homogeneous unitary gas obtained in the limits $N/(N_x^3) \to 0, \quad N \to \infty$

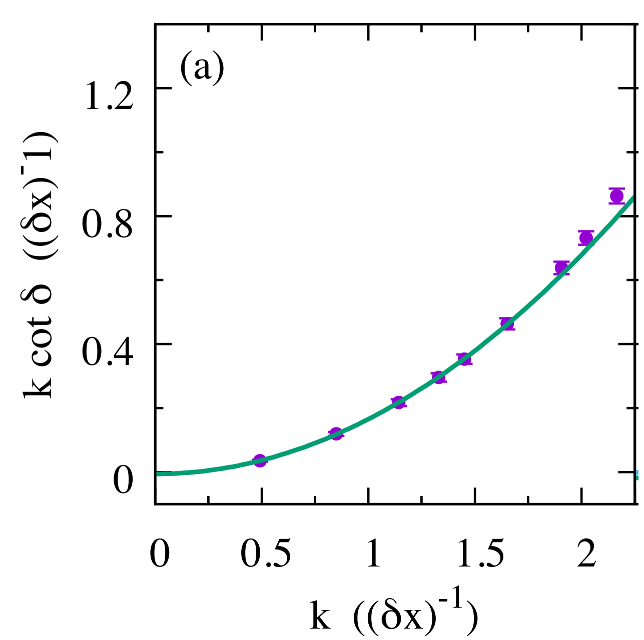
$$\hat{H} = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{V_0}{(\delta x)^3} \sum_{\mathbf{x}} \hat{n}_\uparrow(\mathbf{x}) \hat{n}_\downarrow(\mathbf{x}) \qquad \frac{1}{V_0} = \frac{m}{4\pi\hbar^2 a} - \int_B \frac{d^3k}{(2\pi)^3 2\epsilon_{\mathbf{k}}}$$

- Single-particle model space $\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \quad n_i = -K, \ldots, K$

- This lattice model has an effective range $r_e = 0.337\, \delta x$ *(Werner, Castin 2012)*

  Effective range expansion:

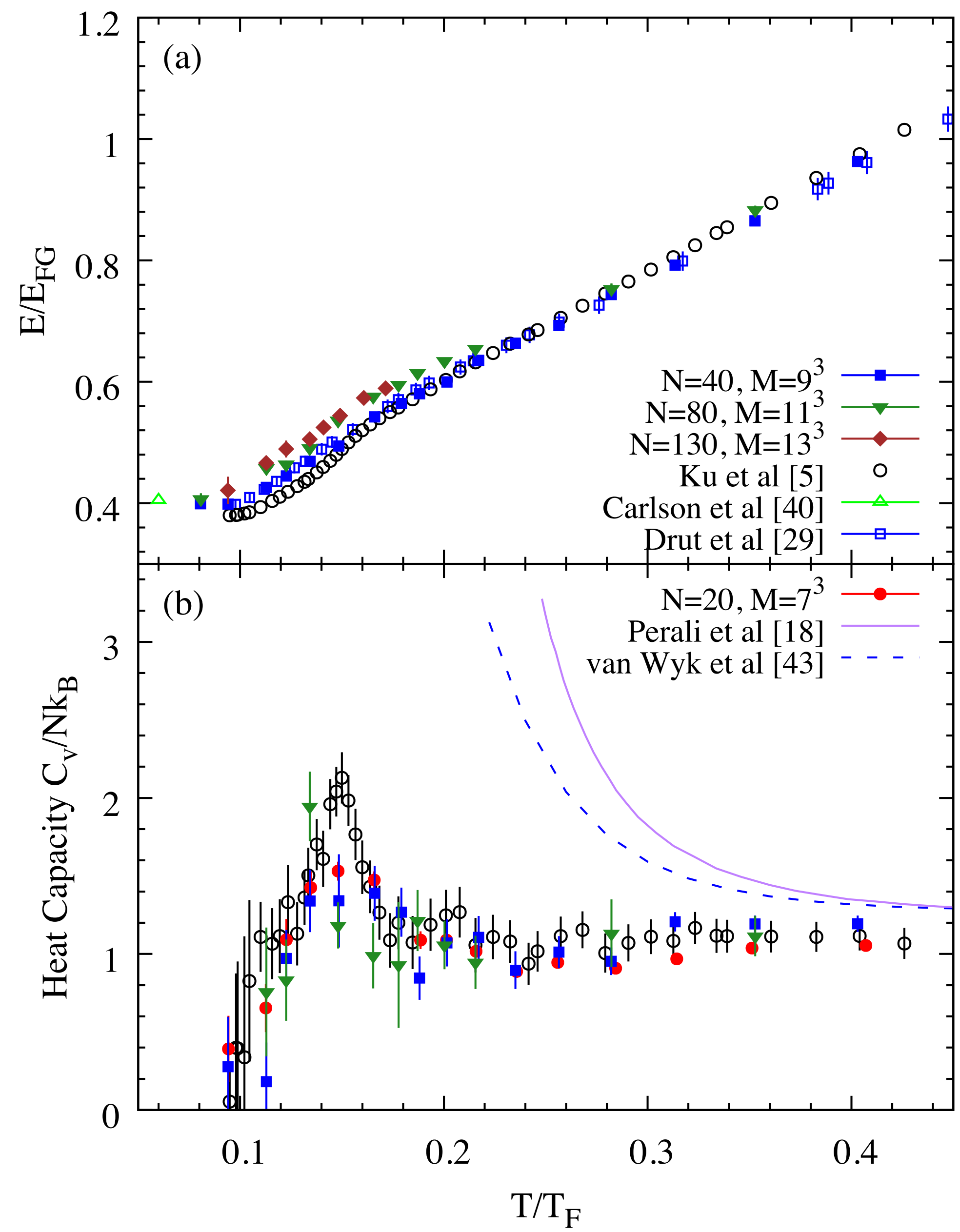
$$k \cot(\delta) = -a^{-1} + \frac{1}{2} r_e k^2 + \ldots$$



Thermodynamics of the unitary Fermi gas

S. Jensen, CG, Y. Alhassid, arxiv:1801.06163

- Energy and heat capacity



- First calculation of the heat capacity across the superfluid phase transition

Pairing correlations across the phase transition

S. Jensen, CG, Y. Alhassid, arxiv:1801.06163

- At finite density with $k_F r_e \simeq 0.4$
- Condensate fraction

  $n = \lambda_{\max}/(N/2)$

  by diagonalizing $\langle a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} a_{-\mathbf{q},\downarrow} a_{\mathbf{q},\uparrow} \rangle$

- Finite-temperature pairing gap

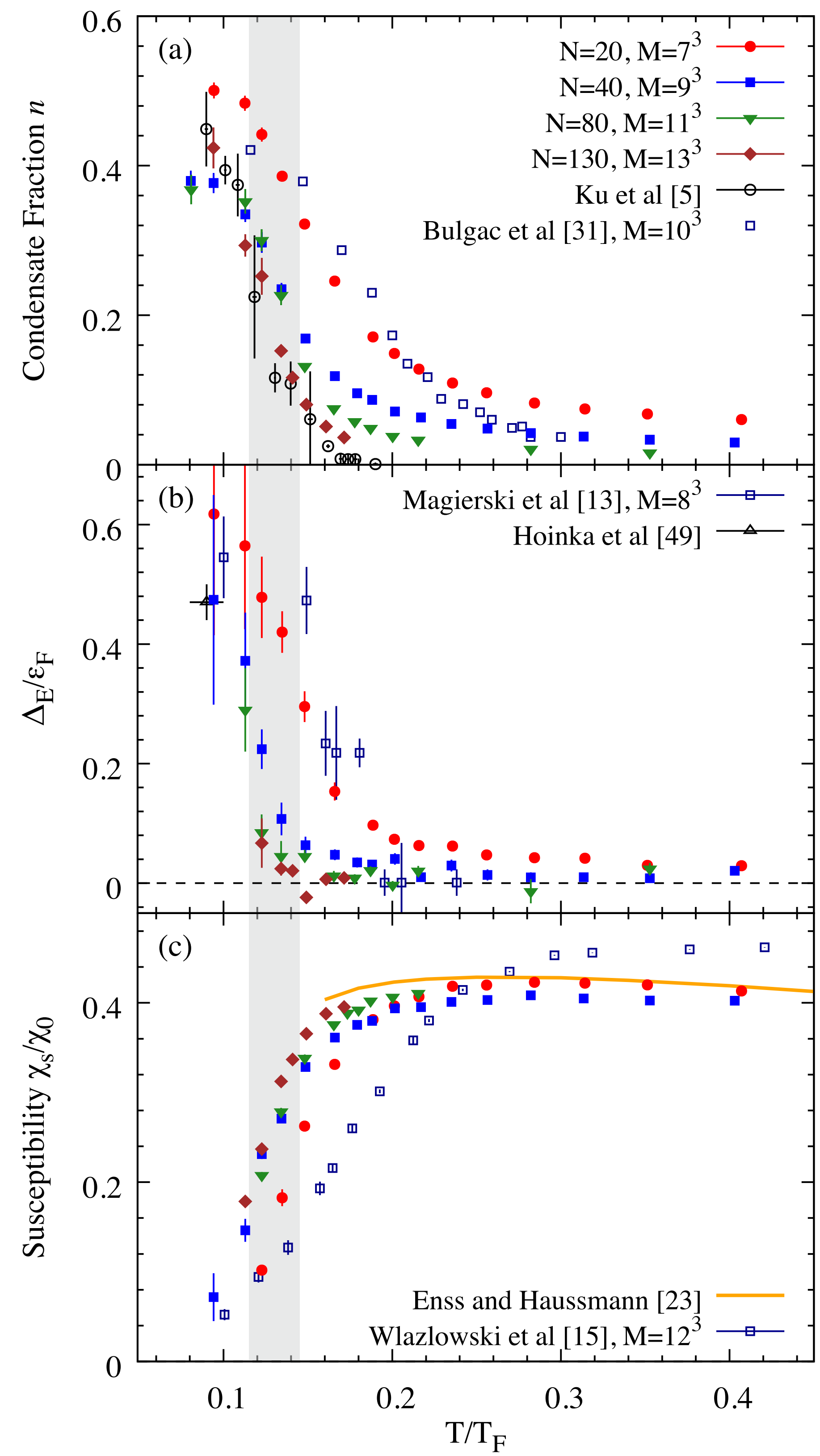
  $$\Delta_E = [2E(N_\uparrow, N_\downarrow - 1) - E(N_\uparrow, N_\downarrow) - E(N_\uparrow - 1, N_\downarrow - 1)]/2$$

- Static spin suscptibility

  $$\chi_s = \frac{\beta}{V} \langle (\hat{N}_\uparrow - \hat{N}_\downarrow)^2 \rangle$$

  using a single number projection onto $N_\uparrow + N_\downarrow$

- $T_c \simeq 0.13(15) T_F$ estimated at this finite density
- No clear signature of the pseudogap at unitarity



Spin susceptibility

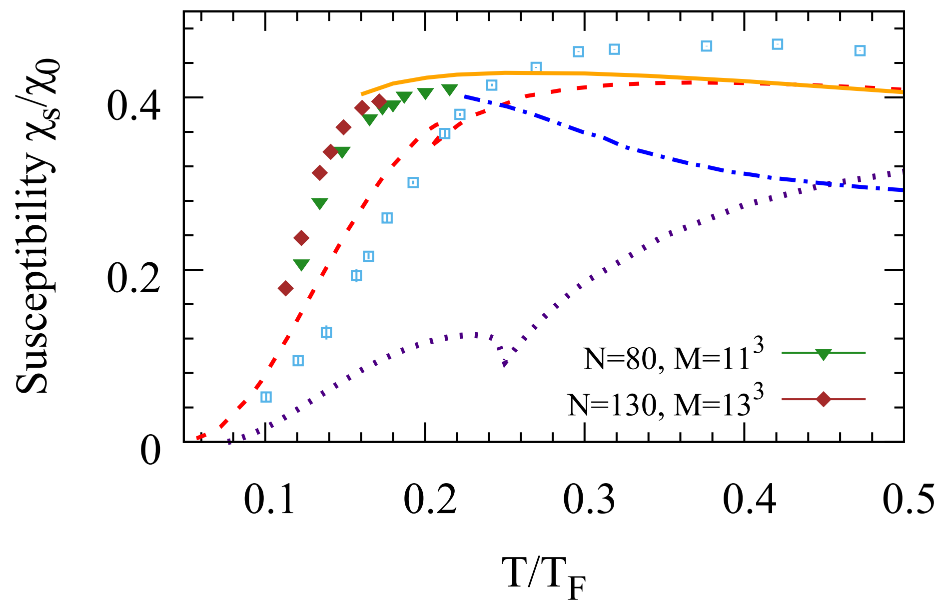


Fig. 13: Spin susceptibility χ_s for the uniform gas computed using our canonical-ensemble AFMC (solid symbols), the AFMC result of Ref. [97] (open squares), the T-matrix result of Ref. [52] (dotted line), the T-matrix result of Ref. [67] (dashed line), the fully self-consistent Luttinger-Ward result of Ref. [51] (solid line), and the self-consistent NSR result of Ref. [120] (dashed-dotted line).

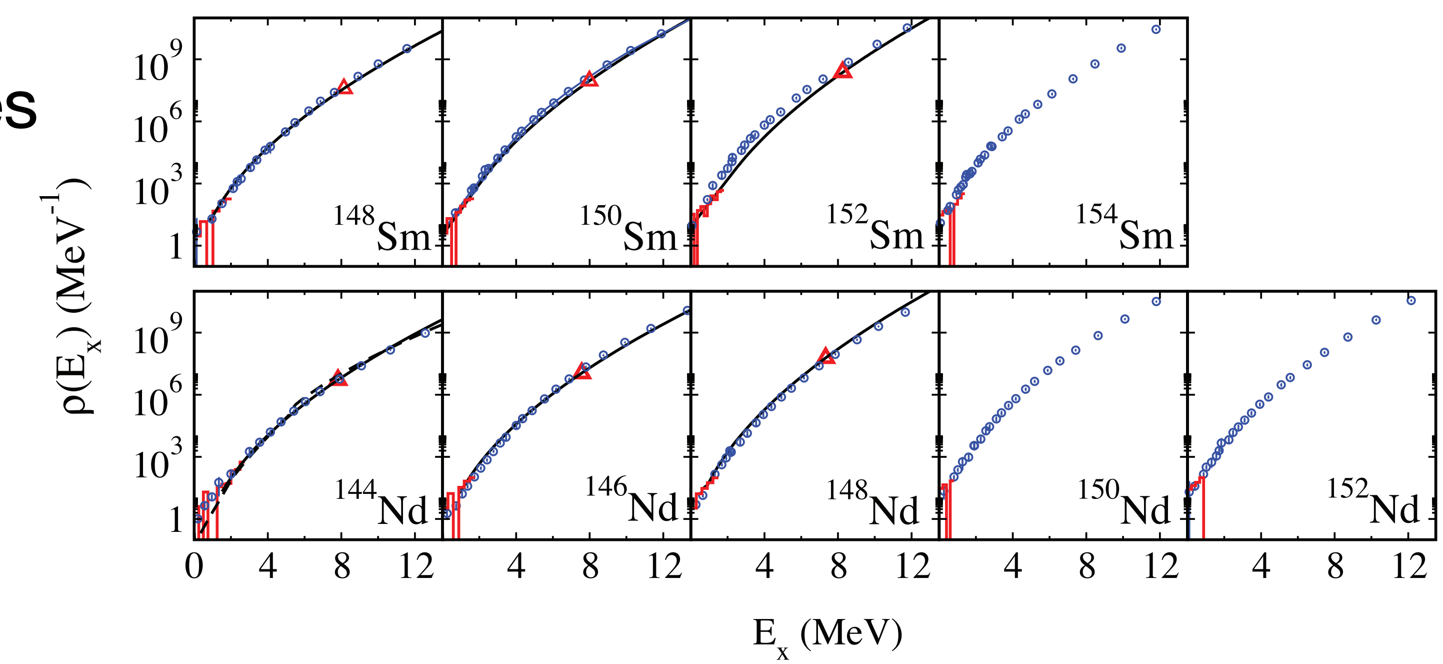
S. Jensen, CG, Y. Alhassid arXiv:1807.03913

Auxiliary-field quantum Monte Carlo for heavy nuclei

- Shell Model Monte Carlo (SMMC): N_p protons and N_n neutrons interact in a valence space outside a frozen core.
- Canonical-ensemble observables $\langle \hat{O} \rangle = \dfrac{\mathrm{Tr}_{N_p,N_n}(\hat{O} e^{-\beta \hat{H}})}{\mathrm{Tr}_{N_n,N_p} e^{-\beta \hat{H}}}$ computed using AFMC
- Phenomenological pairing + multipole interaction

$$\hat{H} = \hat{H}_0 - \sum_{\nu=p,n} g_\nu \hat{P}_\nu^\dagger \hat{P}_\nu - \sum_{\lambda=2,3,4} \chi_\lambda : (\hat{O}_{\lambda;p} + \hat{O}_{\lambda;n}) \cdot (\hat{O}_{\lambda;p} + \hat{O}_{\lambda;n}) :$$

- Rare-earth nuclei ($^{148\text{-}154}$Sm, $^{144\text{-}152}$Nd, ^{162}Dy)
  proton orbitals: $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$ $1f_{7/2}$
  neutron orbitals: $0h_{11/2}$, $0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$
- Successful model for level densities & collective properties of medium-mass and heavy nuclei



Book chapter: Y. Alhassid, in "Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling: a Symmetry-Guided Perspective," ed. K. D. Launey

Nuclear deformations in AFMC

CG, Alhassid, Bertsch, PRC ***97****, 014315 (2018); Alhassid, CG, Bertsch, PRL* ***113****, 262503 (2014)*

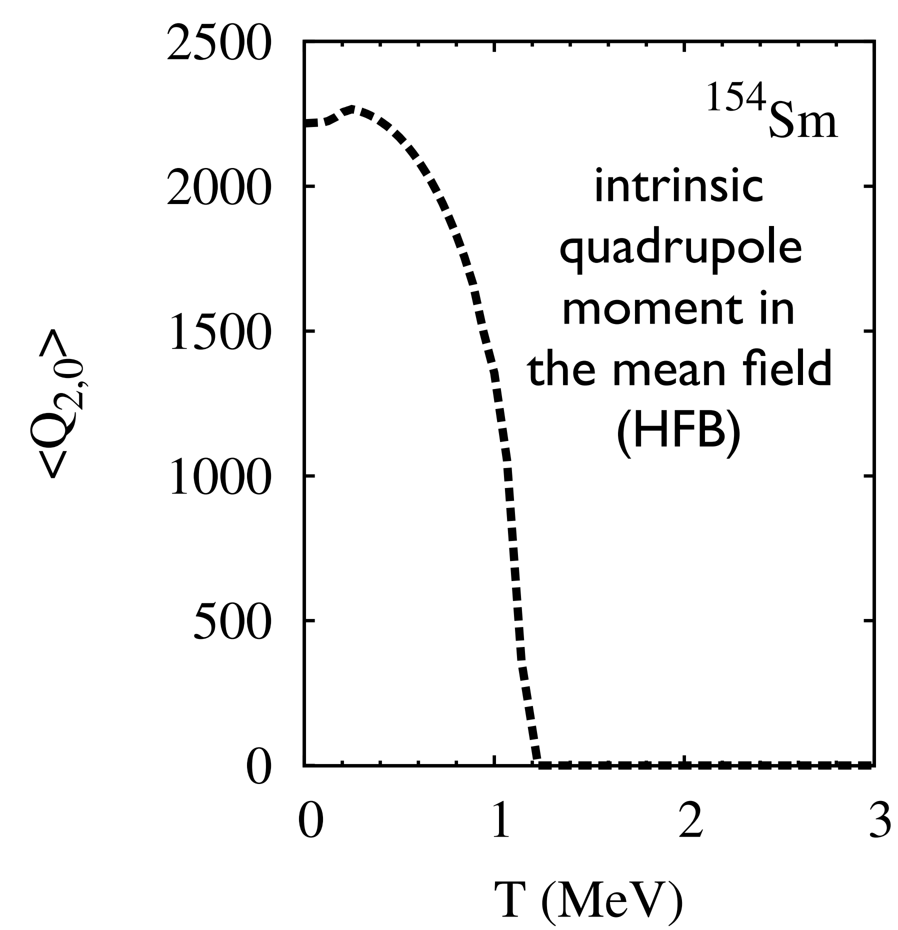
- Mean-field theory is a convenient framework for the study of the intrinsic structure of deformed nuclei, but breaks rotational invariance.
- It also predicts sharp phase transitions, which are washed out in finite systems.
- The challenge is to study nuclear deformation in a framework which *preserves rotational invariance* and captures *finite-size effects*.

Nuclear shapes

$$R = R(\theta,\phi) = R_0\left(1 + \sum_{\lambda,\mu} a^*_{\lambda,\mu} Y_{\lambda,\mu}(\theta,\phi)\right)$$

- The most important nuclear deformation is the quadrupole ($\lambda = 2$), characterized by the mass quadrupole operator

$$Q_{2,\mu} = \sqrt{\frac{16\pi}{5}} \sum_i r_i^2\, Y_{2\mu}(\Omega_i)$$ (sum over particles)



Quadrupole projection

- We study the distribution of $\hat{Q}_{2,0}$ by discretizing the Fourier transform

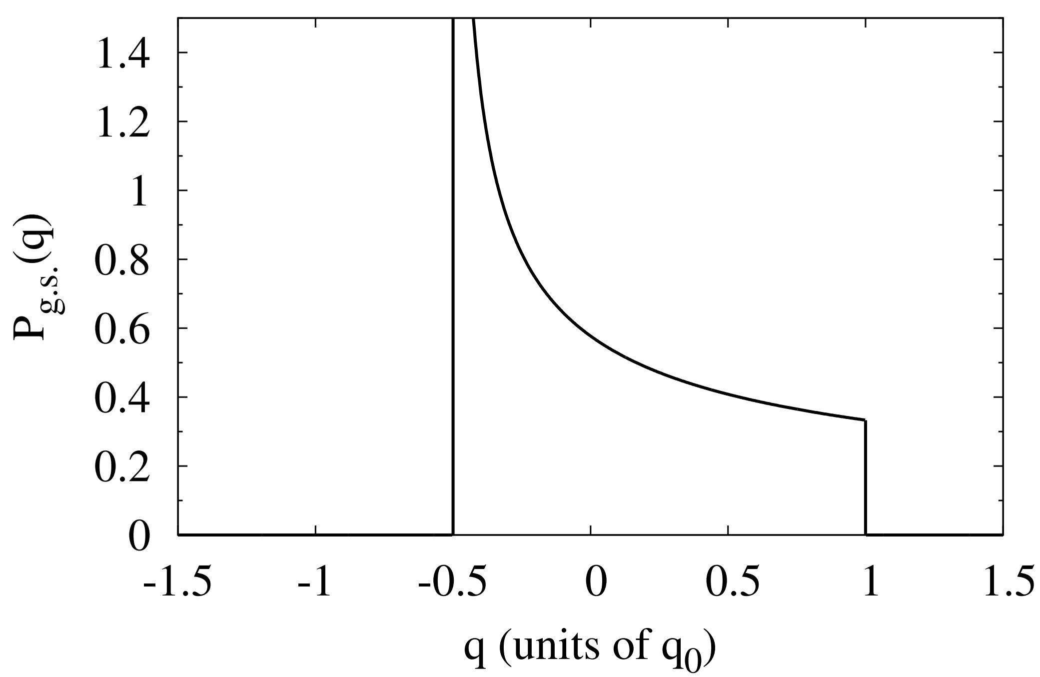
$$\delta(\hat{Q}_{2,0} - q) \approx \frac{1}{2q_{\max}} \sum_{m=1}^{2M+1} e^{i\varphi_m(\hat{Q}_{2,0}-q)}, \qquad q \in [-q_{\max}, q_{\max}], \quad 2M+1 \text{ grid points}, \quad \varphi_m = 2\pi m/(2q_{\max})$$

- Since $\hat{Q}_{2,0}$ is a one-body operator, we can compute its distribution.
- $[\hat{Q}_{2,0}, \hat{H}] \neq 0$, unlike in other projections (e.g., particle number, spin):

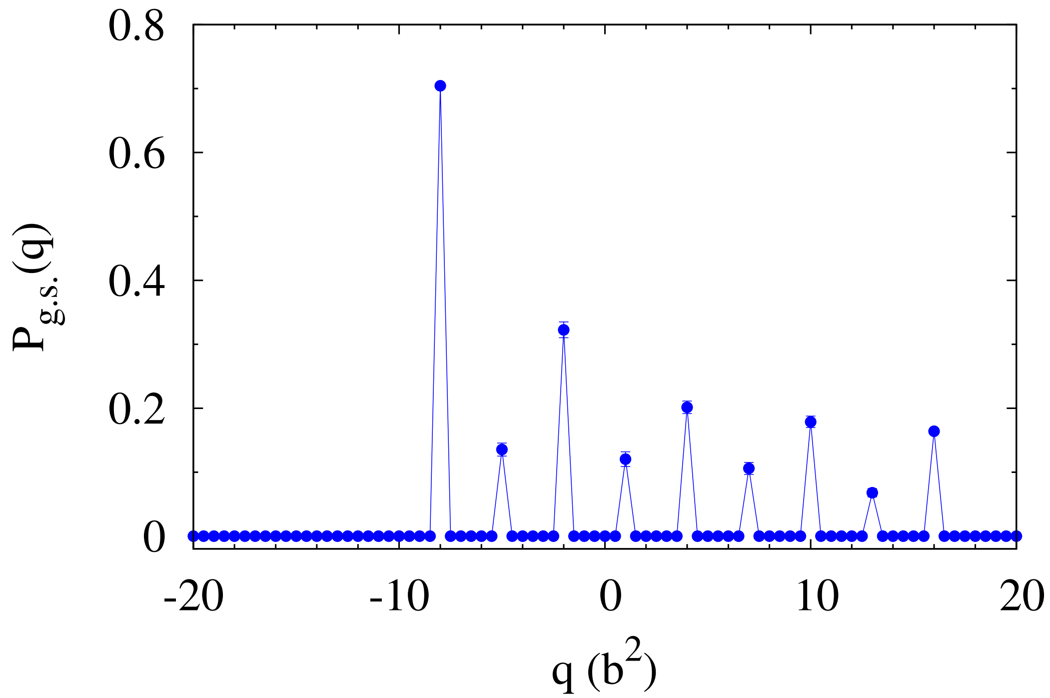
$$P_\beta(q) = \sum_n \delta(q - q_n) \sum_m \langle q, n | e, m \rangle^2 e^{-\beta e_m}$$

- The distribution $P_\beta(q)$ is slow to equilibrate (long decorrelation times). To resolve this problem, we average $P_\beta(q)$ over carefully chosen rotations of the system

Prolate rigid rotor with intrinsic quadrupole moment q_0

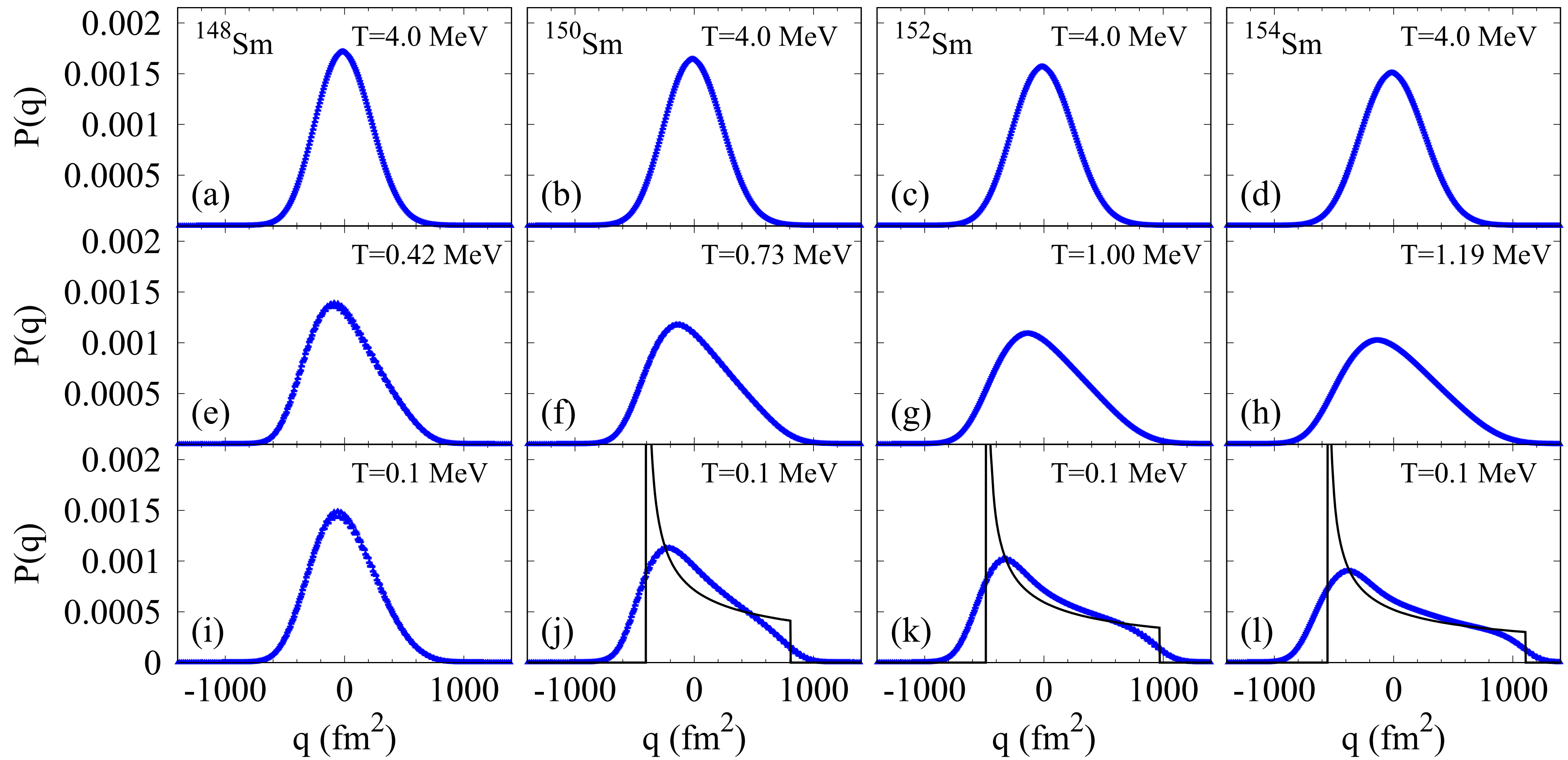


Test case: ^{20}Ne ($Q_{2,0}$ has a discrete spectrum)



Spherical-to-deformed shape transitions in samarium

*CG, Alhassid, Bertsch, PRC **97**, 014315 (2018);*



- High temperatures: quadrupole distribution $P_\beta(q)$ is close to Gaussian
- Intermediate temperatures: ^{148}Sm is close to Gaussian, while $^{150\text{-}154}$Sm show skewed distributions
- Low temperatures: ^{148}Sm is still Gaussian, while $^{150\text{-}154}$Sm distributions are similar to that of a rigid rotor, a clear signature of deformation.
- Applications to level densities: *Mustonen, Gilbreth, Alhassid, arxiv:1804.01617 (PRC, in press)*

Summary

- The canonical ensemble is essential for certain observables, such as the pairing gap, and finite-size systems such as atomic nuclei.
- We have introduced methods to reduce overall scaling:
  - Stabilized diagonalization
  - Reduction of model space for each auxiliary field configuration
  - Reduced number of quadrature points
  - "Fermi surface optimizations" for two-body observables
- These methods make canonical-ensemble calculations competitive with the grand-canonical ensemble.
- Applications to cold atoms & nuclei: pseudogap, level densities, deformation properties of nuclei
- For an alternative approach, see recent work of [Wang, Assad, Toldin, PRE **96**, 042131 (2017)]