Stabilizing Canonical-Ensemble Calculations in the Auxiliary-Field Monte Carlo Method

C. N. Gilbreth
In collaboration with Y. Alhassid
Yale University

Advances in quantum Monte Carlo techniques for non-relativistic many-body systems
Institute for Nuclear Theory
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Outline

- Auxiliary-field quantum Monte Carlo (AFMC) in the configuration-interaction framework
  - Exact particle-number projection
- Numerical stabilization
  - More efficient method for particle-number projection
- Application: Thermodynamic properties of a trapped finite cold atomic Fermi gas
  - Heat capacity, condensate fraction, pairing gap
  - Spatial density
  - Density due to an “extra” particle

Auxiliary-field Quantum Monte Carlo (AFMC)

- A method for studying highly-correlated systems which is free of systematic errors
- Benefits:
  - Permits finite-temperature calculations
  - No fixed-node approximations (for good sign interactions)
  - Useful in different contexts (electronic structure, nuclear physics, atomic physics, chemistry)
  - Allows calculation of any one- or two-body observable
- Challenges:
  - Sign problem -- for repulsive interactions and certain projections
  - Scaling is $N_s^3 \times N_t$ or $N_s^4 \times N_t$, depending on the application
  - Numerical stability at low temperatures / large model spaces

AFMC in Configuration (Fock) Space

- Goal: compute the thermal expectation

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

  for a collection of fermions.

- Steps to formulate AFMC:

  (a) Formulation of the Configuration-Interaction (CI) Hamiltonian as a sum of quadratic one-body operators

  (b) Trotter decomposition (imaginary time discretization)

  (c) Path-integral representation

  (d) Calculation of observables for a given set of fields

  (e) Monte Carlo evaluation

(a) Hamiltonian and (b)Trotter decomposition

- Single-particle basis: $|i\rangle, i = 1, \ldots, N_s$
- Model space: set of all Slater determinants from the s.p. basis
- Hamiltonian:

$$\hat{H} = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

- Rewrite in terms of one-body densities $a_i^\dagger a_k, a_j^\dagger a_l$ and diagonalize the matrix v_{ijkl} to obtain

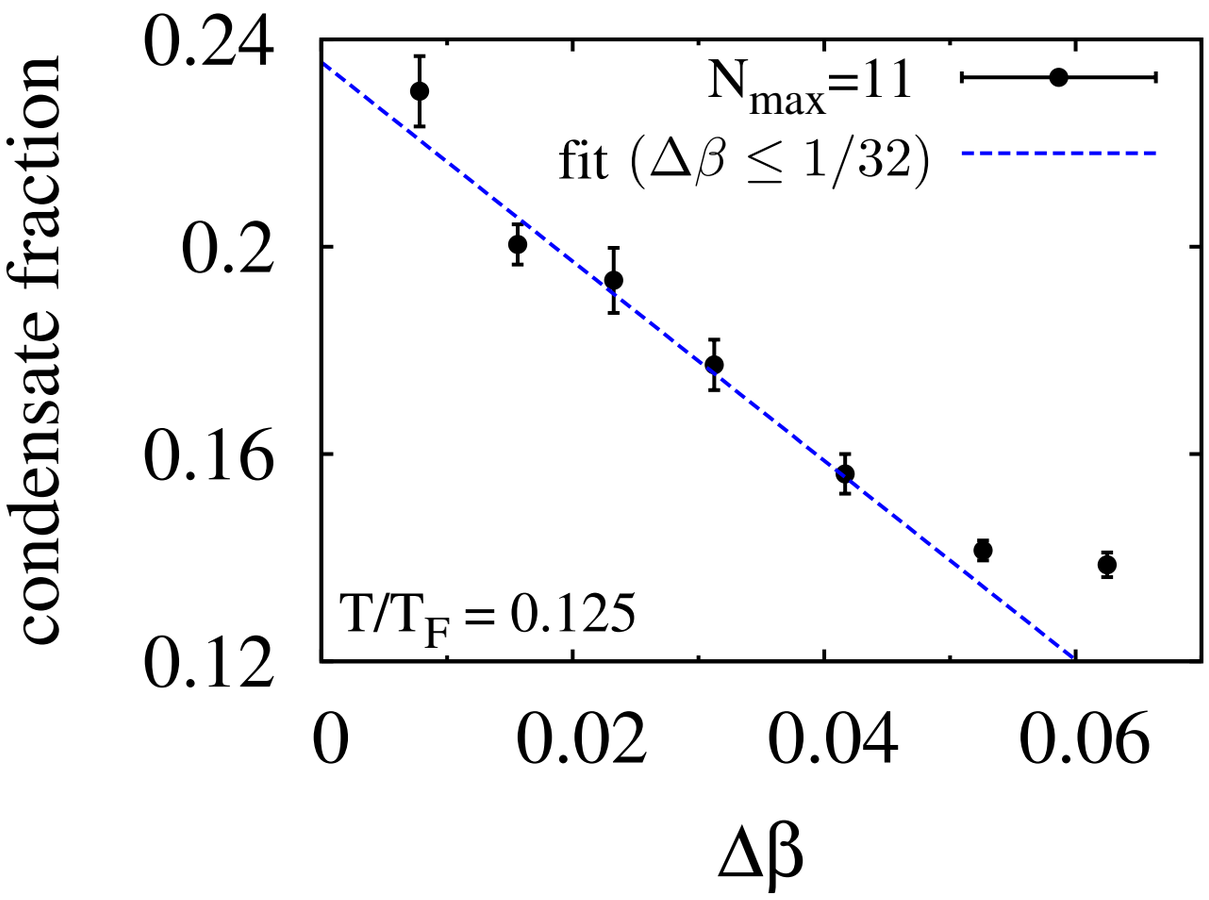
$$\hat{H} = \hat{H}_0 + \frac{1}{2} \sum_\alpha \lambda_\alpha \hat{O}_\alpha^2$$

where $\hat{H}_0$ and $\hat{O}_\alpha$ are one-body operators.

- Trotter decomposition: $e^{-\beta \hat{H}} = (e^{-\Delta\beta \hat{H}})^{N_t}$, $\Delta\beta \equiv \beta / N_t$ and

$$e^{-\Delta\beta \hat{H}} = e^{-\Delta\beta \hat{H}_0} \prod_\alpha e^{-\Delta\beta \lambda_\alpha \hat{O}_\alpha^2 / 2} + O((\Delta\beta)^2)$$

Discretization error in observables



- The error due to the Trotter decomposition scales as $\Delta\beta$
- We perform a linear fit and extrapolate to $\Delta\beta \to 0$

(c) Path-Integral Formulation

- Hubbard-Stratonovich (HS) transformation:

$$e^{-\Delta\beta\lambda\hat{O}^2/2} = \int_{-\infty}^{\infty} d\sigma e^{-\Delta\beta|\lambda|\sigma^2/2} e^{-\Delta\beta s\lambda\sigma\hat{O}}, \quad s = \begin{cases} 1, & \lambda < 0 \\ i, & \lambda > 0 \end{cases}$$

  - This linearizes the two-body part of the Hamiltonian into a one-body operator, with the addition of an auxiliary field σ.

- End result of the HS transformation:

$$e^{-\beta\hat{H}} = \int \underbrace{D[\sigma]}_{\text{Integration measure}} \underbrace{G_\sigma}_{\text{Gaussian weight}} \underbrace{\hat{U}(\sigma)}_{\text{Non-interacting propagator}}$$

Time-dependent auxiliary fields (many)

- A path integral of a non-interacting propagator with respect to fluctuating time-dependent auxiliary fields.

(d) Observables in the Canonical Ensemble

- Want to compute: $\int D[\sigma] G_\sigma \mathrm{Tr}[\hat{U}(\sigma)\hat{O}]$
- $\hat{U}(\sigma)$ is a non-interacting propagator and $\hat{O}$ is a one-or two-body operator.
- To compute traces for fixed particle number, we use exact particle-number projection:

$$\mathrm{Tr}_N[\hat{O}\hat{U}(\sigma)] = \frac{1}{N_s}\sum_{m=1}^{N_s} e^{-i\varphi_m N}\mathrm{Tr}_{\mathrm{GC}}[\hat{O}\hat{U}(\sigma)e^{i\varphi_m \hat{N}}]\,.$$

Number of single-particle states

Canonical trace
N = number of particles

$\varphi_m \equiv 2\pi m/N_s$

Grand-canonical trace

- Can be derived by writing $\mathrm{Tr}_{\mathrm{GC}}$ as a sum of canonical traces

[W. E. Ormand, et al., Phys. Rev. C **49**, 1422 (1994)]

(d) Canonical ensemble cont.

- To compute grand-canonical quantities, can use matrix algebra in the single particle space (of order ~100-1000):
  - $\mathrm{Tr}_{\mathrm{GC}}(\hat{U}(\sigma)e^{i\varphi_m\hat{N}}) = \det(1+Ue^{i\varphi_m})$
  - $$\frac{\mathrm{Tr}_{\mathrm{GC}}[a_i^\dagger a_j \hat{U}(\sigma)e^{i\varphi_m\hat{N}}]}{\mathrm{Tr}_{\mathrm{GC}}[\hat{U}(\sigma)e^{i\varphi_m\hat{N}}]} = \left(\frac{1}{1+U^{-1}e^{-i\varphi_m}}\right)_{ji}$$

    where U is the matrix representing $\hat{U}$ in the single-particle space.

(e) Monte Carlo evaluation

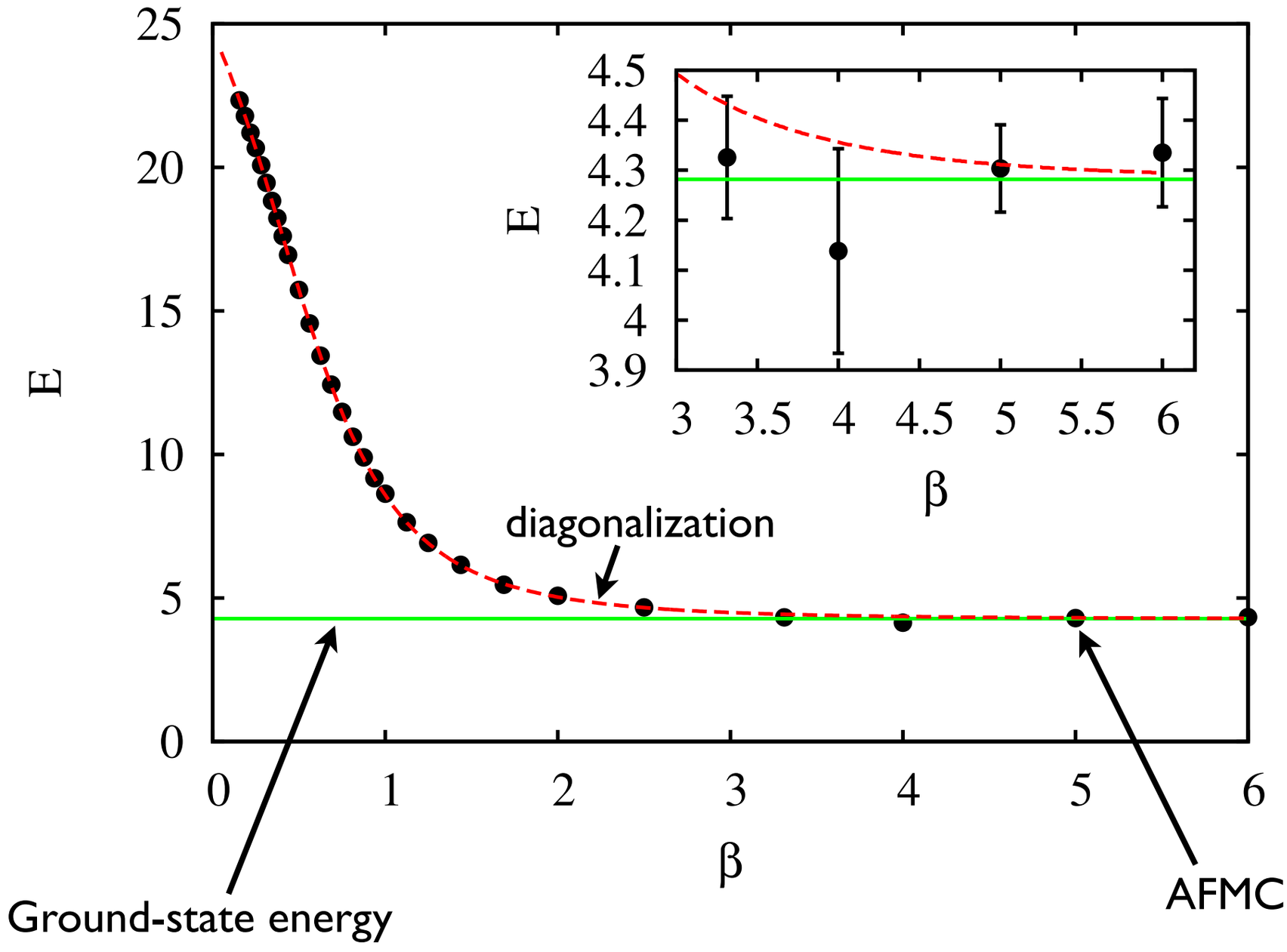
- Discretize the integrals over the auxiliary fields:

$$\int D[\sigma]G_\sigma \hat{U}(\sigma) \longrightarrow \sum_\sigma w(\sigma)\hat{U}(\sigma)$$

- Apply the Metropolis algorithm.

[Koonin, et al., Phys. Rep. **278**, 1 (1997)]

Accuracy of AFMC: Three cold atoms



AFMC vs. diagonalization for a fixed interaction with three cold atoms $(\uparrow\uparrow\downarrow)$ in a harmonic trap

Numerical Stabilization

Numerical Stabilization

- Need to compute, for each *m*,

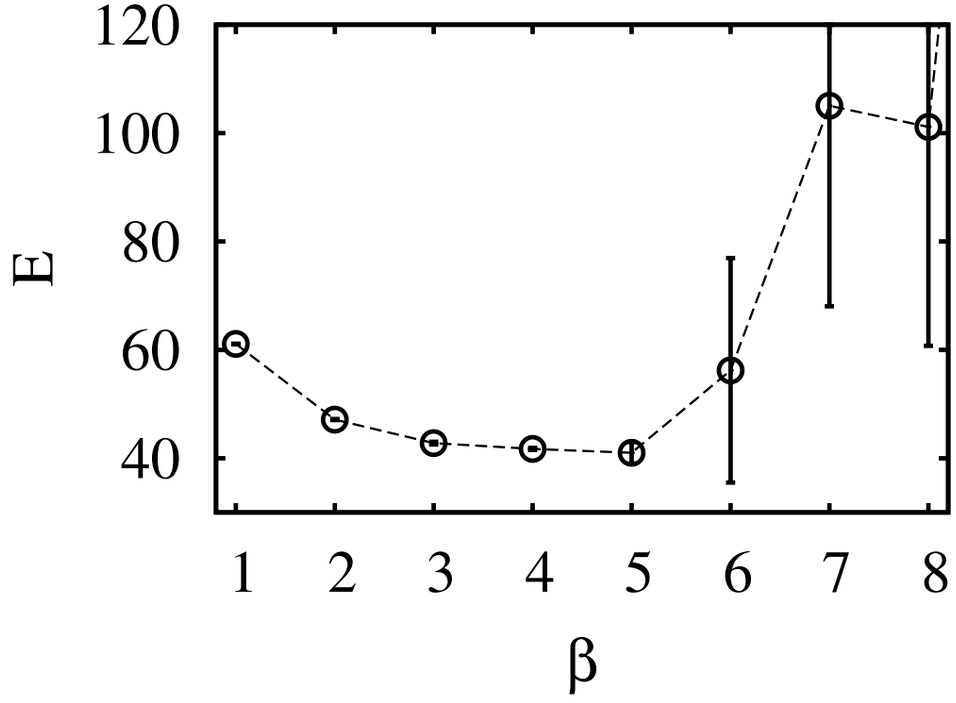
$$\mathrm{Tr}_{\mathrm{GC}}[\hat{U}(\sigma)e^{i\varphi_m \hat{N}}] = \det(1 + Ue^{i\varphi_m})$$

  where $U =$ matrix representing $\hat{U}$ in the single-particle space.

- At long imaginary times, the propagator U becomes unstable.
- (1) Compute U:
  - (a) Unstabilized method
  - (b) Stabilized method
- (2) Compute determinant:
  - (i) Unstabilized method
  - (ii) Standard stabilized method
  - (iii) New stabilized method (faster)

Unstabilized calculation of U

- As N_t grows large, the matrix product $U = U(\sigma_{N_t}) \cdots U(\sigma_2) U(\sigma_1)$ becomes ill-conditioned: ratio of largest to smallest eigenvalues becomes very large.
- The matrix elements of *U*, however, *all* become large, and it is impossible to extract smaller scales (those near the Fermi surface) accurately.



Energy vs. inverse temperature β for 20 cold atoms in the unitary limit.

At low temperatures, calculation becomes unreliable.

- Unstabilized calculation is only good for high temperatures (small β)

Stabilized Calculation of U

- Stabilized calculation of U: Use method of [E.Y. Loh Jr. and J. E. Gubernatis, in *Electronic Phase Transitions*, 1992]
- Instead of computing U, compute a decomposition $U = ADB$ of U which explicitly displays all numerical scales.
- A and B are well-conditioned, and D is diagonal with positive entries:

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

- E.g., singular value decomposition or QR decomposition

Stabilized Matrix Multiplication

- To compute $U = U_{N_t} \cdots U_2 U_1$, begin with an initial decomposition of U_1 and carefully update when multiplying in each new factor:

$$
\begin{aligned}
U_1 &= A_1 D_1 B_1 && \text{(decompose)} \\
&\vdots \\
U_{n+1}(A_n D_n B_n) &= ((U_{n+1} A_n) D_n) B_n && \text{(group terms)} \\
&= (A_{n+1} D_{n+1} B') B_n && \text{(decompose)} \\
&= A_{n+1} D_{n+1} (B' B_n) && \text{(group terms)} \\
&= A_{n+1} D_{n+1} B_{n+1} \\
&\vdots \\
U &= A_{N_t} D_{N_t} B_{N_t}
\end{aligned}
$$

- The intermediate matrix $(U_{n+1} A_n) D_n$ is column-stratified and therefore can be decomposed stably

Stabilized Matrix Multiplication cont.

- A column-stratified matrix displays its scales in the columns:

$$U_{n+1}A_nD_n = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} X & & \\ & x & \\ & & x \end{pmatrix} = \begin{pmatrix} X & x & x \\ X & x & x \\ X & x & x \end{pmatrix}$$

- Similarly, a row-stratified matrix displays its scales in the rows:

$$DBA = \begin{pmatrix} X & & \\ & x & \\ & & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} = \begin{pmatrix} X & X & X \\ x & x & x \\ x & x & x \end{pmatrix}$$

- Stratified matrices are much more stable for decomposition and diagonalization than general matrices with widely varying scales.

(2) Calculation of the Determinant

- Wish to compute $\det(1 + Ue^{i\varphi_m})$ for each $m = 1, 2, \ldots, N_s$
- (i) Unstabilized calculation:
  - Compute $U = U_{N_t} \cdots U_1$ using standard matrix multiplication
  - Diagonalize U and compute $\det(1 + Ue^{i\varphi_m}) = \prod_{k=1}^{N_s} (1 + \lambda_k e^{i\varphi_m})$
  - Only for high temperatures. Scales as $O(N_s^3)$ (diagonalization)
- (ii) Standard stabilized calculation: [Alhassid et al., **101**, 082501 (2008)]
  - Cannot multiply out ADB to diagonalize, as this would destroy information. Instead:

$$\begin{aligned} 1 + ADBe^{i\varphi_m} &= A(A^{-1}B^{-1} + De^{i\varphi_m})B \\ &= A(A'D'B')B \qquad \text{(decompose)} \end{aligned}$$

  - Requires decomposition for each $m = 1, \ldots, N_s$, so scales as $O(N_s^4)$

Stabilized Matrix Diagonalization

[Gilbreth & Alhassid, arXiv:1210.4131]

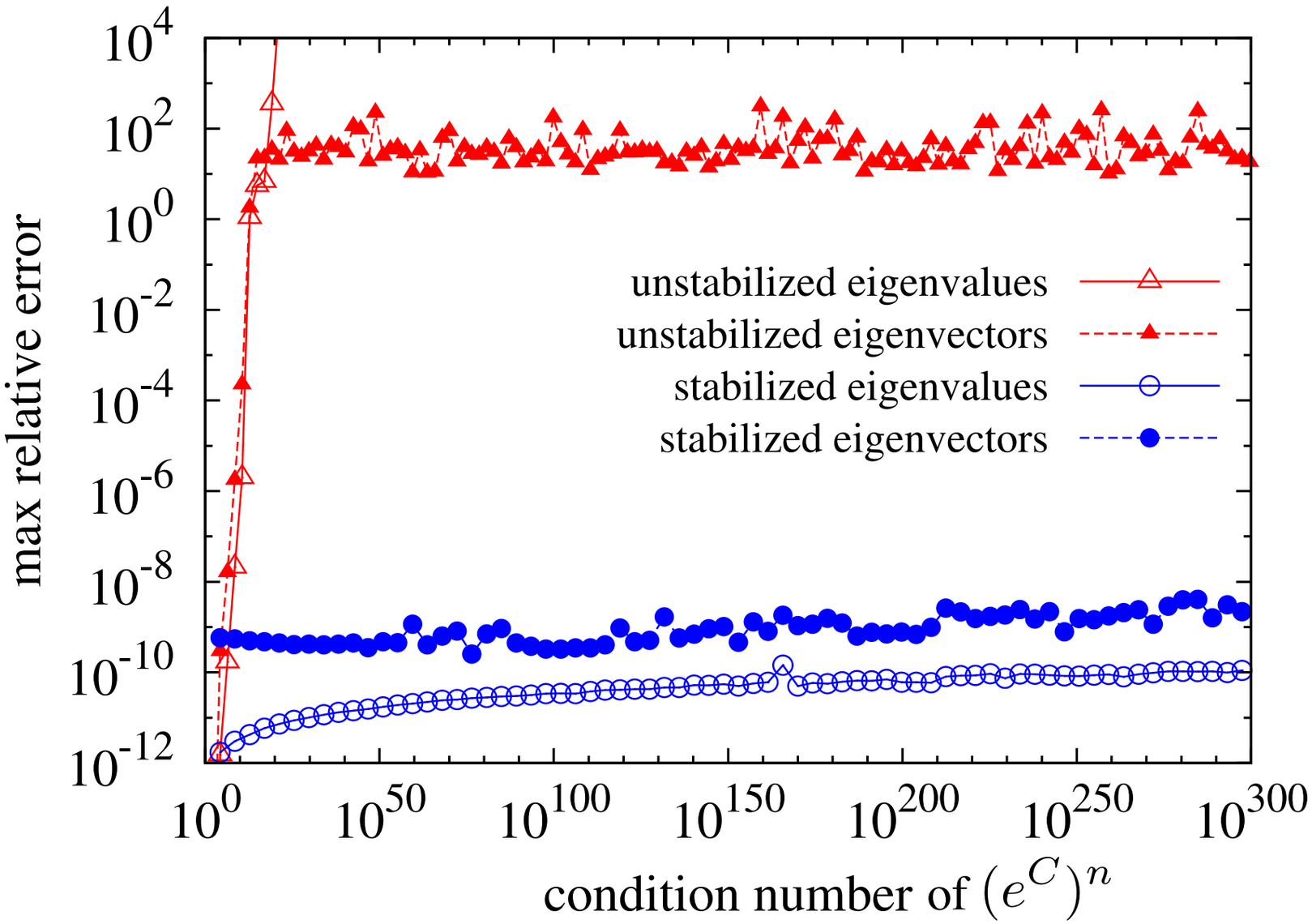
- (iii) New method: Transform

$$ADBx = \lambda x \qquad \text{Let } x = Ay$$
$$\Leftrightarrow DBAy = \lambda y$$

  - The matrix DBA is row-stratified and can be multiplied out & diagonalized stably
  - Eigenvalues are identical to those of ADB.
  - Reduces time back to $O(N_s^3)$

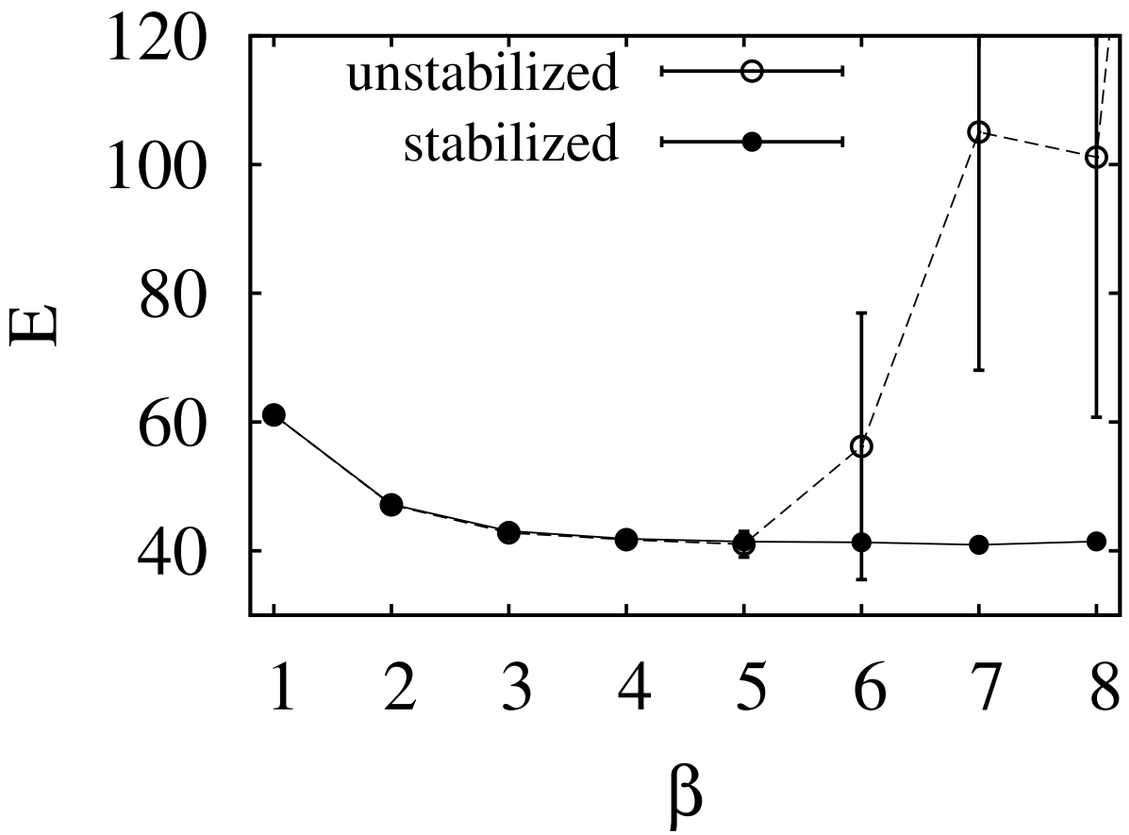
- Test 1: Compute eigenvectors and eigenvalues of $(e^C)^n$, where C is a random complex matrix, and $n = 1, 2, 3, \ldots$
- Test 2: Compare to standard stabilization method

Accuracy of Diagonalizing an ill-conditioned Matrix

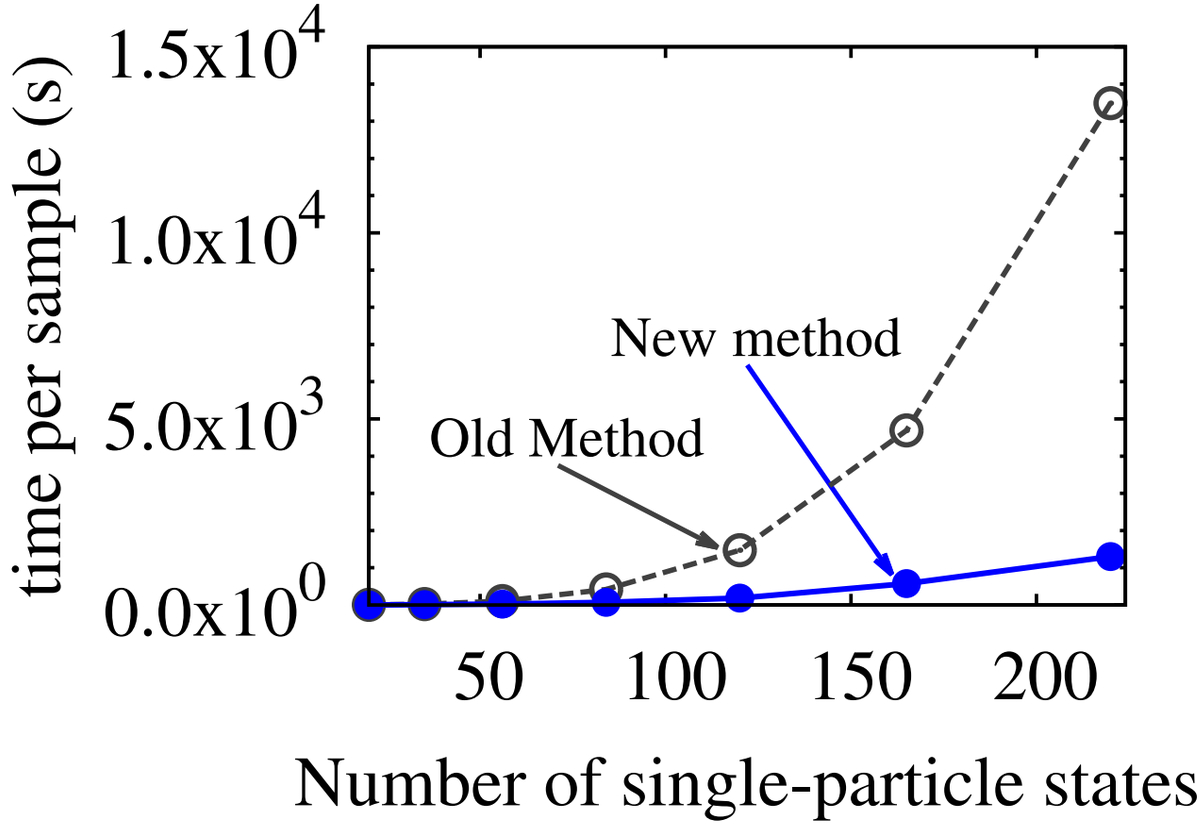


Error in stabilized and unstabilized eigenvalues and eigenvectors of the matrix $(e^C)^n$

Numerical Stabilization -- Accuracy and Timing



Accuracy



Timing

Summary

- AFMC method in the configuration-interaction framework
- Strongly-interacting systems with arbitrary good-sign interactions can be studied
- Calculations in the canonical ensemble
- A new stabilization method in the canonical ensemble
  - Much faster, scales as $O(N_s^3)$ instead of $O(N_s^4)$

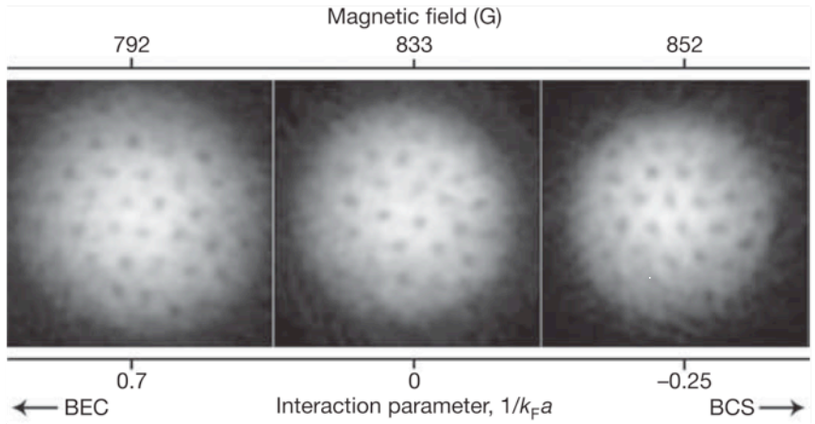
Thermodynamics of a finite trapped cold atomic Fermi gas

Advances with Atomic Fermi Gases

- 1999: First realization of an ideal degenerate Fermi gas (^{40}K). Evaporative cooling to $T = 0.5\ T_F$ (JILA, CO)

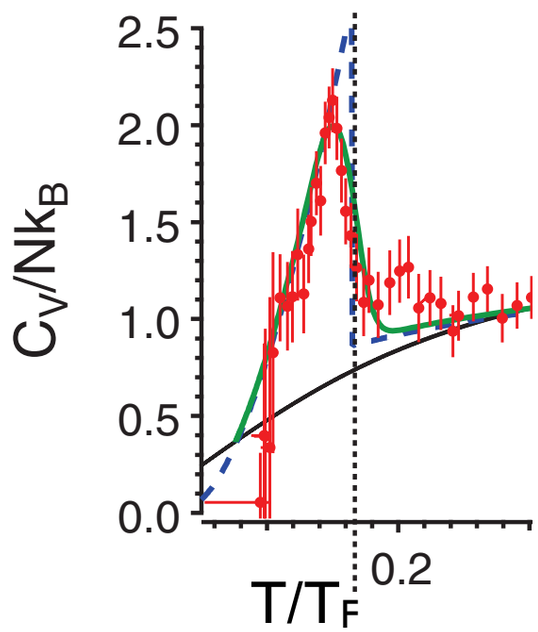
- 2002: Feshbach resonance allows tuning to strongly-interacting regime (^{6}Li, Duke Univ.)

- 2005: Observation of vortex lattice after "stirring" confirms superfluidity (MIT) [Zwierlein, M.W. et al., Nature **435**, 1047 (2005)]



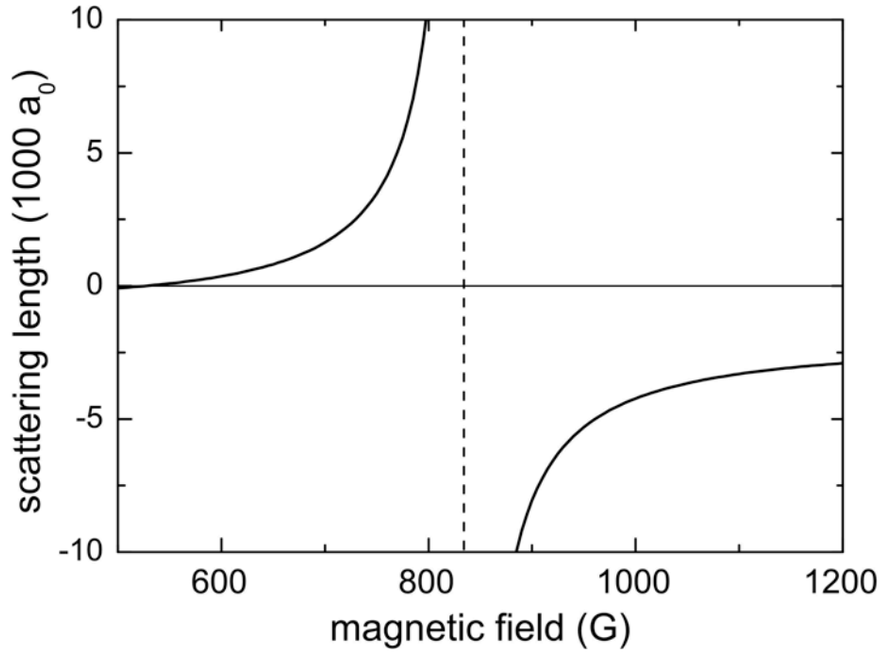
- 2012: Measurement of "lambda" peak in heat capacity (MIT)

[Ku, et al., Science **335**, 563 (2012)]



Clean, strongly interacting, tunable systems

- Two species ("↑" and "↓") of Fermions interact at very short range in a harmonic trap.
- Zero-range (s-wave) interactions
- s-wave scattering length *a* controllable via external magnetic field
- Unitary limit $(a \to \infty)$ *saturates s-wave scattering cross section.*
- Strongly interacting, *nonperturbative* system when $|a|$ is large

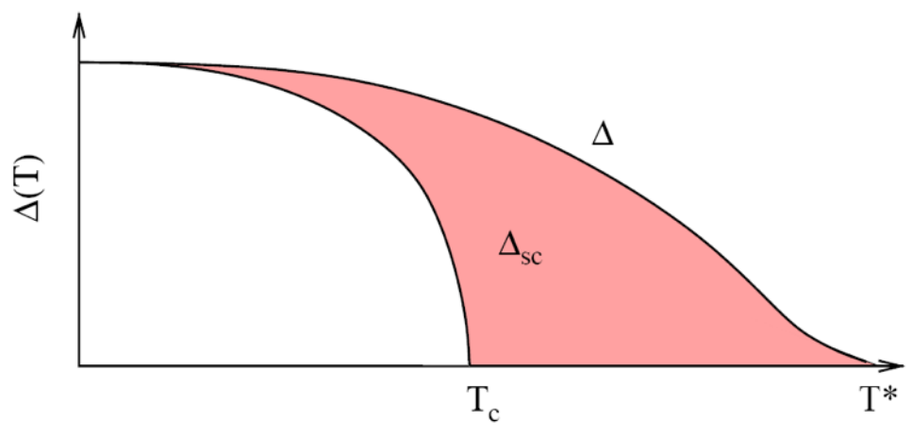


[Zwierlein, M.W. et al., Nature **435**, 1047 (2005)]

Unitary, Finite, Trapped Fermi Gas

- Goal: Describe thermodynamics of trapped finite-size (~20 particle) Fermi gas in the unitary limit.
  - Heat capacity
  - Pairing gap
  - Condensate fraction.
  - Particle density

- Questions:
  - Is the superfluid phase transition visible in a system of this size?
  - If so, is there a pseudogap effect?



[Q. Chen et al., Physics Reports **412** (2005) 1-88]

AFMC for Trapped Cold Atoms

- Hamiltonian:

$$H = \sum_{i=1}^{N_1+N_2} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}m\omega^2 r_i^2 \right) + \sum_{i<j} V(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

- Single-particle basis of harmonic-oscillator states:

$$|i\rangle = |nlm\rangle = R_{nl}(r)Y_l^m(\theta,\phi), \quad 2n + l \leq \underbrace{N_{\max}}$$

Cutoff parameter

- Interaction:

$$V(\boldsymbol{r}_i - \boldsymbol{r}_j) = V_0\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

(V_0 renormalized for each $N_{\max}$ to reproduce two-particle ground-state energy)

- Shell-model decomposition:

$$H = \sum_{i,j=1}^{N_s} h_{i,j}a_i^\dagger a_j + \frac{1}{2}\sum_{K,\pi,\alpha} \lambda_{K,\pi}(\alpha) \sum_{M=0}^{K} (\hat{Q}_{K\pi M}(\alpha)^2 + \hat{P}_{K\pi M}(\alpha)^2)$$

$\hat{Q}, \hat{P}$ one-body operators

- Our calculations are done in the *canonical ensemble*.

Monte Carlo Sign of the Contact Interaction

- It is well-known that the contact interaction $V(\boldsymbol{r}) = V_0\delta(\boldsymbol{r})$ has good Monte Carlo sign in coordinate space.
- It is not as clear in the Configuration-Interaction formalism.
- The proof proceeds as follows:
  - The Hamiltonian takes the form

$$H = \sum_{nlm\sigma} \varepsilon_{nl} a^\dagger_{nlm\sigma} a_{nlm\sigma} + \frac{1}{2}\sum (\boldsymbol{ab}|\hat{V}|\boldsymbol{cd}) a^\dagger_{\boldsymbol{a}\sigma} a^\dagger_{\boldsymbol{b}\sigma'} a_{\boldsymbol{d}\sigma'} a_{\boldsymbol{c}\sigma} \,,$$

  - and in a "time-reversed density decomposition":

$$\hat{H} = \hat{H}_1 + \frac{1}{2}\sum (\boldsymbol{a}\bar{\boldsymbol{b}}|\hat{V}|\boldsymbol{c}\bar{\boldsymbol{d}})(-)^{m_b}(-)^{m_d}\, a^\dagger_{\boldsymbol{a}\sigma} a_{\boldsymbol{c}\sigma} \bar{a}^\dagger_{\boldsymbol{b}\sigma'} \bar{a}_{\boldsymbol{d}\sigma'} \,, \qquad \bar{a}_{\boldsymbol{a},\sigma} = \text{time reverse}$$

  - One can show that the interaction matrix

$$V_{\boldsymbol{ac},\boldsymbol{bd}} = (\boldsymbol{a}\bar{\boldsymbol{b}}|\hat{V}|\boldsymbol{c}\bar{\boldsymbol{d}})(-)^{m_a}(-)^{m_b}$$

    has only nonpositive eigenvalues when $V_0 < 0$.

Sign of the Contact Interaction (cont.)

- We show this as follows:

$$\sum_{\boldsymbol{ac},\boldsymbol{bd}} v^*_{\boldsymbol{ac}}(\boldsymbol{a}\bar{\boldsymbol{b}}|\hat{V}|\boldsymbol{c}\bar{\boldsymbol{d}})(-)^{m_b+m_d} v_{\boldsymbol{bd}}$$

$$= V_0 \sum_{\boldsymbol{ac},\boldsymbol{bd}} \int d^3\boldsymbol{r}\, v^*_{\boldsymbol{ac}} \varphi^*_{\boldsymbol{a}}(\boldsymbol{r})\varphi_{\boldsymbol{c}}(\boldsymbol{r})\varphi^*_{\bar{\boldsymbol{b}}}(\boldsymbol{r})(-)^{m_b}\varphi_{\bar{\boldsymbol{d}}}(\boldsymbol{r})(-)^{m_d} v_{\boldsymbol{bd}}$$

$$= V_0 \int d^3\boldsymbol{r} \left(\sum_{\boldsymbol{ac}} v^*_{\boldsymbol{ac}}\varphi^*_{\boldsymbol{a}}(\boldsymbol{r})\varphi_{\boldsymbol{c}}(\boldsymbol{r})\right)\left(\sum_{\boldsymbol{bd}} \varphi_{\boldsymbol{b}}(\boldsymbol{r})\varphi^*_{\boldsymbol{d}}(\boldsymbol{r}) v_{\boldsymbol{bd}}\right)$$

$$= V_0 \int d^3\boldsymbol{r} \left|\sum_{\boldsymbol{ac}} v^*_{\boldsymbol{ac}}\varphi^*_{\boldsymbol{a}}(\boldsymbol{r})\varphi_{\boldsymbol{c}}(\boldsymbol{r})\right|^2 \leq 0\,.$$

- This implies $s = 1$ in the Hubbard-Stratonovich transformation:

$$e^{-\Delta\beta\lambda\hat{O}^2/2} = \int_{-\infty}^{\infty} d\sigma e^{-\Delta\beta|\lambda|\sigma^2/2} e^{-\Delta\beta\lambda\sigma\hat{O}}\,,$$

So the auxiliary-field Hamiltonian is complex-conjugation invariant.

Sign of the Contact Interaction (cont.)

- The propagator factorizes: $\hat{U} = \hat{U}_\uparrow \hat{U}_\downarrow$
- $\hat{U}_\uparrow, \hat{U}_\downarrow$ are invariant under complex conjugation:

$$K_0 \hat{U}_{\uparrow,\downarrow} K_0^\dagger = \hat{U}_{\uparrow,\downarrow}$$

$$\hat{U}_{\uparrow,\downarrow}|v\rangle = \lambda|v\rangle \quad \Rightarrow \quad K_0 \hat{U}_{\uparrow,\downarrow}|v\rangle = \hat{U}_{\uparrow,\downarrow} K_0|v\rangle = \lambda^* K_0|v\rangle$$

- Therefore, complex eigenvalues come in complex-conjugate pairs
- So

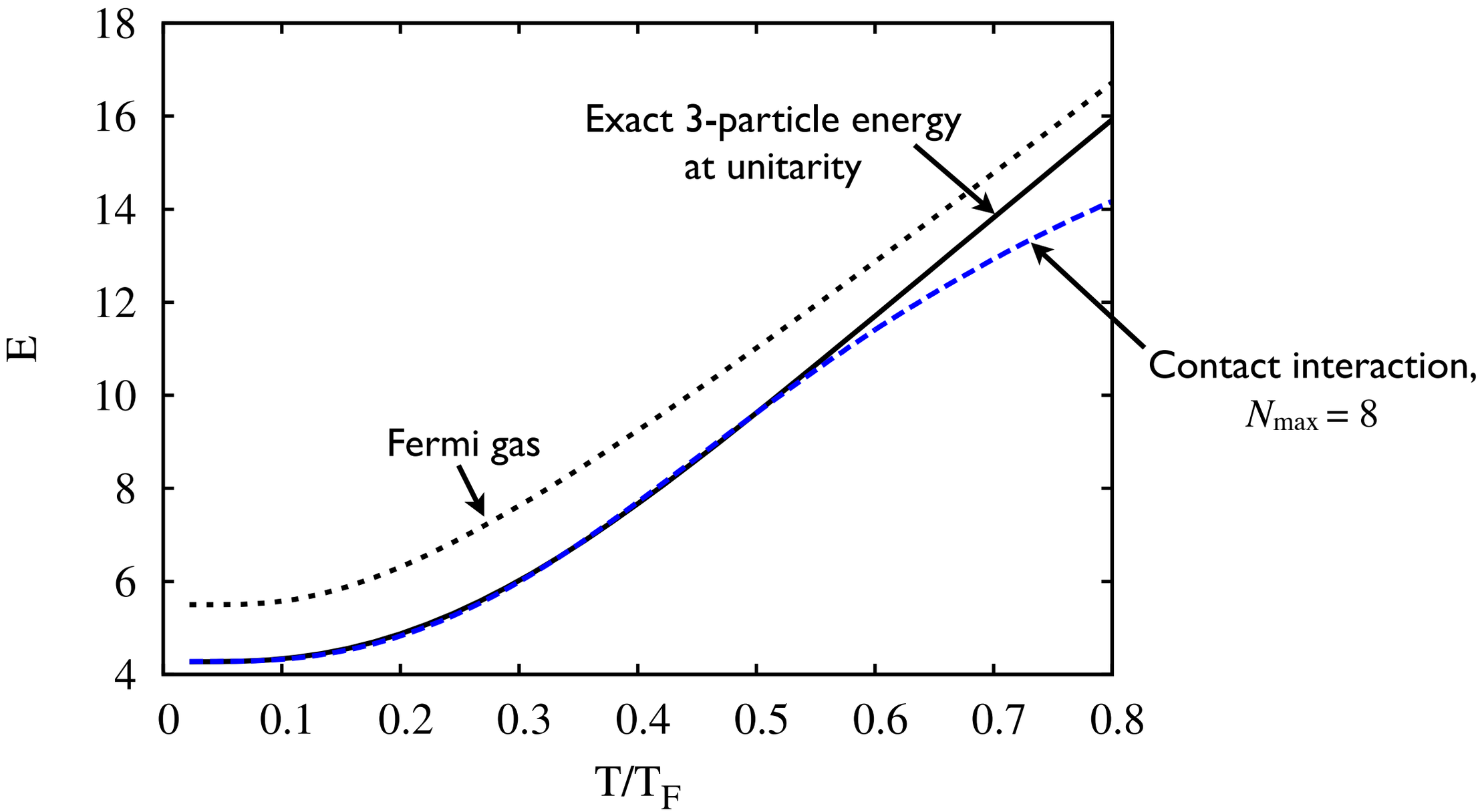
$$\mathrm{Tr}_{N_\uparrow,\downarrow}(\hat{U}_{\uparrow,\downarrow}) = \sum_i \lambda_i^{(N_{\uparrow,\downarrow})} = \mathrm{real}$$

- When $N_\uparrow = N_\downarrow$,

$$\mathrm{Tr}_{N_\uparrow,N_\downarrow}(\hat{U}) = \mathrm{Tr}_{N_\uparrow}(\hat{U}_\uparrow)\mathrm{Tr}_{N_\downarrow}(\hat{U}_\downarrow) = [\mathrm{Tr}_{N_\uparrow}(\hat{U}_\uparrow)]^2 \geq 0$$

so the calculation has good sign.

Accuracy of Renormalized Contact Interaction



Tuning V_0 to reproduce two-particle ground-state energy provides an accurate interaction for the three-particle system.

[Exact results based on S. Tan and Werner & Castin]

Heat capacity

$$C = \frac{dE(T)}{dT} \approx [E(T + \Delta T) - E(T - \Delta T)]/2\Delta T$$

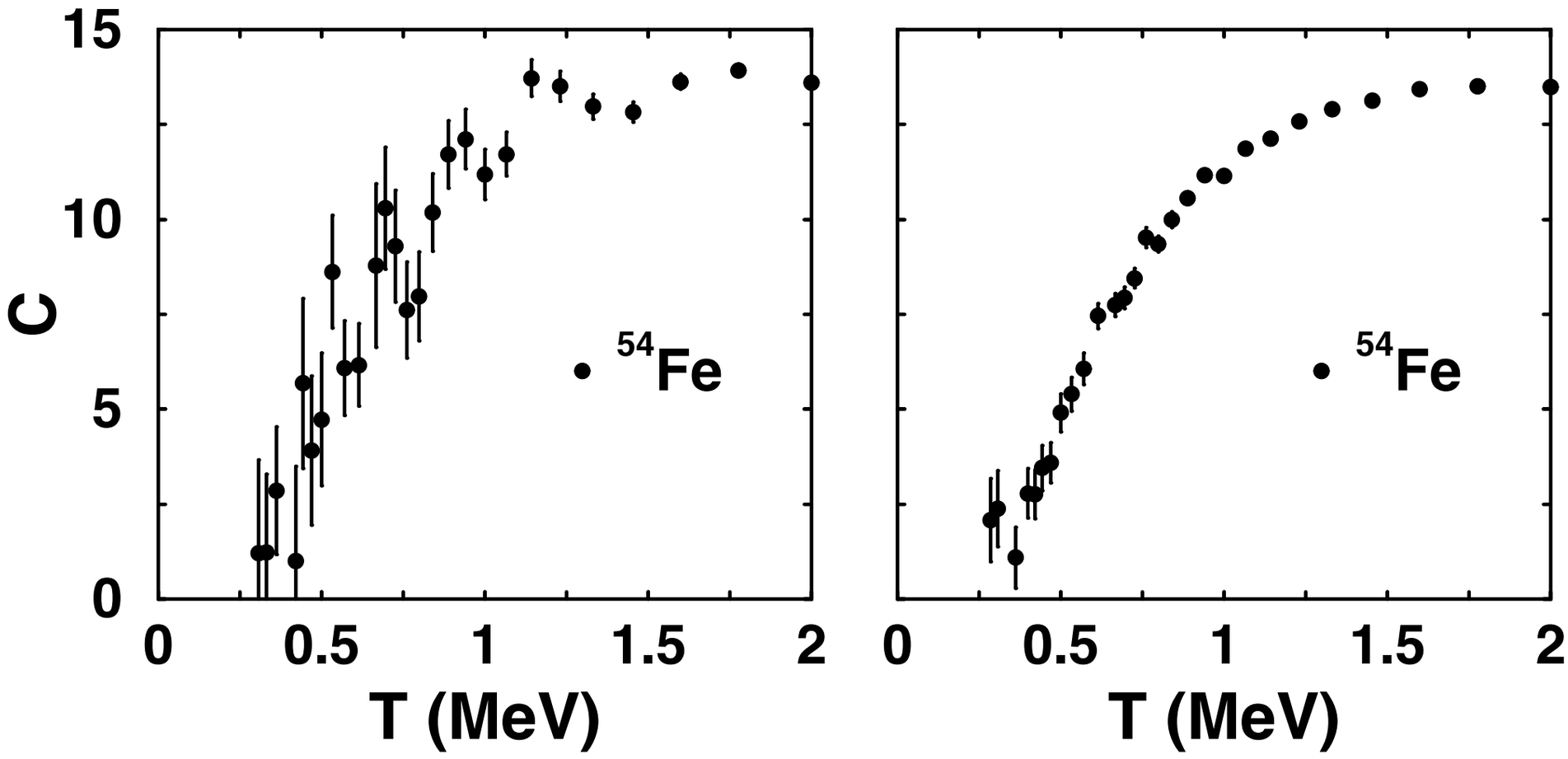
- When computing the heat capacity, the statistical error in the energy can be greatly magnified.
- We use a method of correlated errors introduced in [S. Liu and Y. Alhassid, PRL **87**, 022501 (2001)] to avoid this.
  - Sample fields at a single temperature T
  - Compute energies at $T + \Delta T$ and $T - \Delta T$ for each sample:

$$E(T \pm \Delta T) = \frac{\int D[\sigma] G_\sigma(T \pm \Delta T) \mathrm{Tr}[\hat{U}(\sigma, T \pm \Delta T)]}{\int D[\sigma] G_\sigma(T \pm \Delta T) \mathrm{Tr}\, \hat{U}(\sigma, T \pm \Delta T)}$$

  - Statistical error:

$$\mathrm{Var}(C) = \frac{1}{(2 * \Delta T)^2} \times \Big[\mathrm{Var}(\langle \hat{H}(T + \Delta T)\rangle) + \mathrm{Var}(\langle \hat{H}(T - \Delta T)\rangle) - 2 * \mathrm{Cov}(\langle \hat{H}(T + \Delta T)\rangle, \langle \hat{H}(T - \Delta T)\rangle)\Big]$$

  - Covariance greatly reduces statistical error in heat capacity



[S. Liu and Y. Alhassid, PRL **87**, 022501 (2001)]

Condensate Fraction

- "Condensate fraction" does not have a standard meaning in finite-size systems
- We define a condensate fraction from the two-body density matrix (TBDM).
- C. N. Yang (1962): Off-diagonal long-range order (ODLRO) is equivalent to the existence of a large eigenvalue in the TBDM
- Calculation:
  1. Compute $C(ij,kl) \equiv \langle a^\dagger_{i,\uparrow} a^\dagger_{j,\downarrow} a_{l,\uparrow} a_{k,\downarrow} \rangle$
  2. Diagonalize to obtain a pair wavefunction $B^\dagger \equiv \sum_{ij} \varphi_{ij} a^\dagger_{i\uparrow} a_{j\downarrow}$ corresponding to the largest eigenvalue of C.
  3. The largest eigenvalue λ satisfies (for $N_\uparrow = N_\downarrow = N/2$)

     and $\boxed{\lambda = \langle B^\dagger B \rangle}$ $\boxed{0 \le \lambda \le N/2}$ so $\boxed{n \equiv \lambda/(N/2)}$ defines a condensate fraction.

Energy-Staggering Pairing gap

- Energy-staggering pairing gap

$$\Delta_{\rm gap} \equiv [E(N_\uparrow, N_\downarrow + 1) + E(N_\uparrow + 1, N_\downarrow) - E(N_\uparrow + 1, N_\downarrow + 1) - E(N_\uparrow, N_\downarrow)]/2$$

where

$E(N_\uparrow, N_\downarrow) =$ energy of a system with $N_\uparrow$ spin-up particles and $N_\downarrow$ spin-down particles.

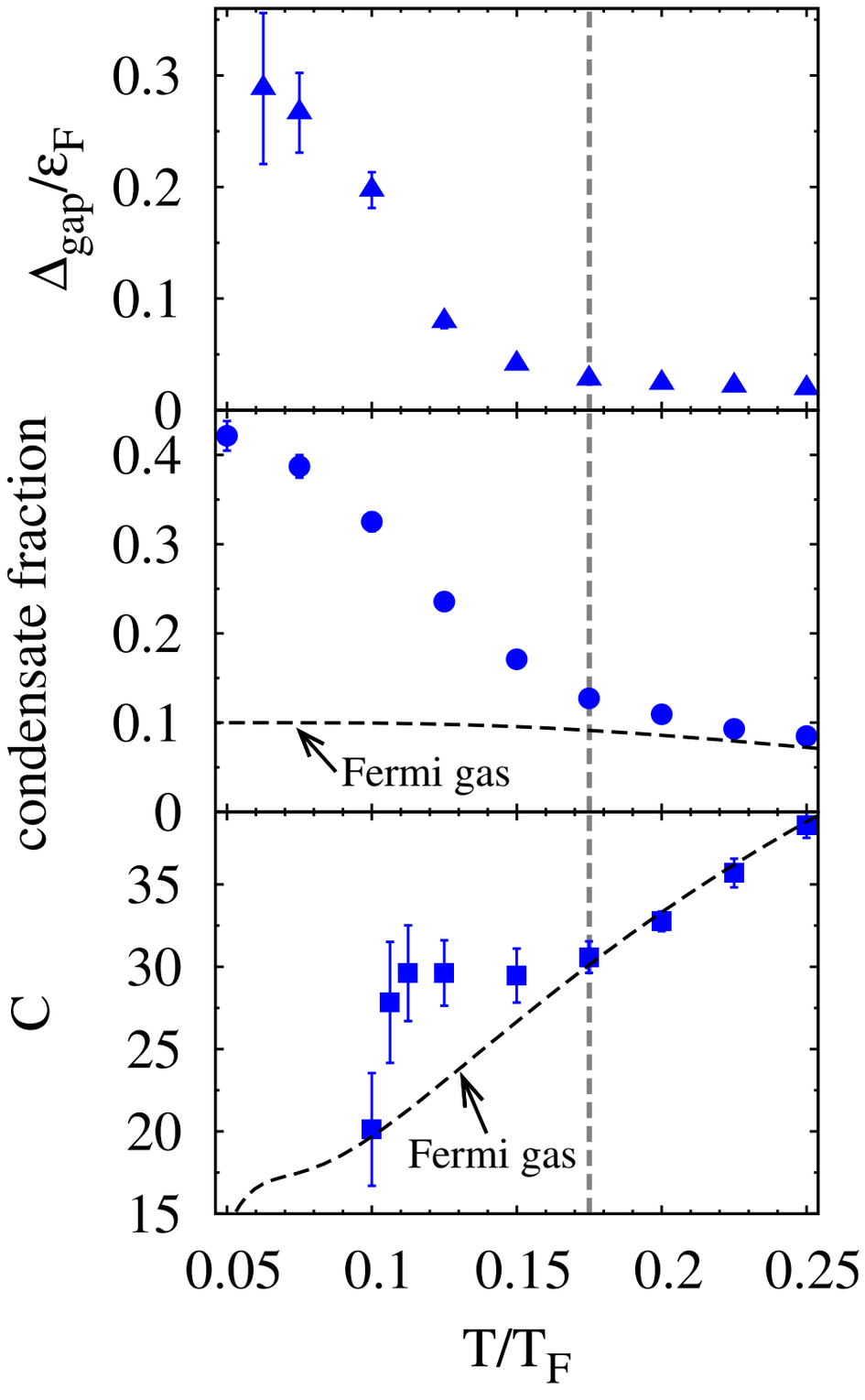
- $\Delta_{\rm gap}$ measures the difference in energy between fully paired systems and a systems with an unpaired particle.

- Calculation: (for $N_\uparrow = N_\downarrow = N/2$)

1. Sample auxiliary fields for the $(N_\uparrow, N_\downarrow + 1)$ system.
2. Compute $E(N_\uparrow, N_\downarrow)$, $E(N_\uparrow + 1, N_\downarrow) = E(N_\uparrow, N_\downarrow + 1)$, and $E(N_\uparrow + 1, N_\downarrow + 1)$ for each sample
3. Compute variance of $\Delta_{\rm gap}$ using correlated errors.

Signatures of the Phase Transition: 20 Atoms

[Gilbreth and Alhassid, arXiv:1210.4131]

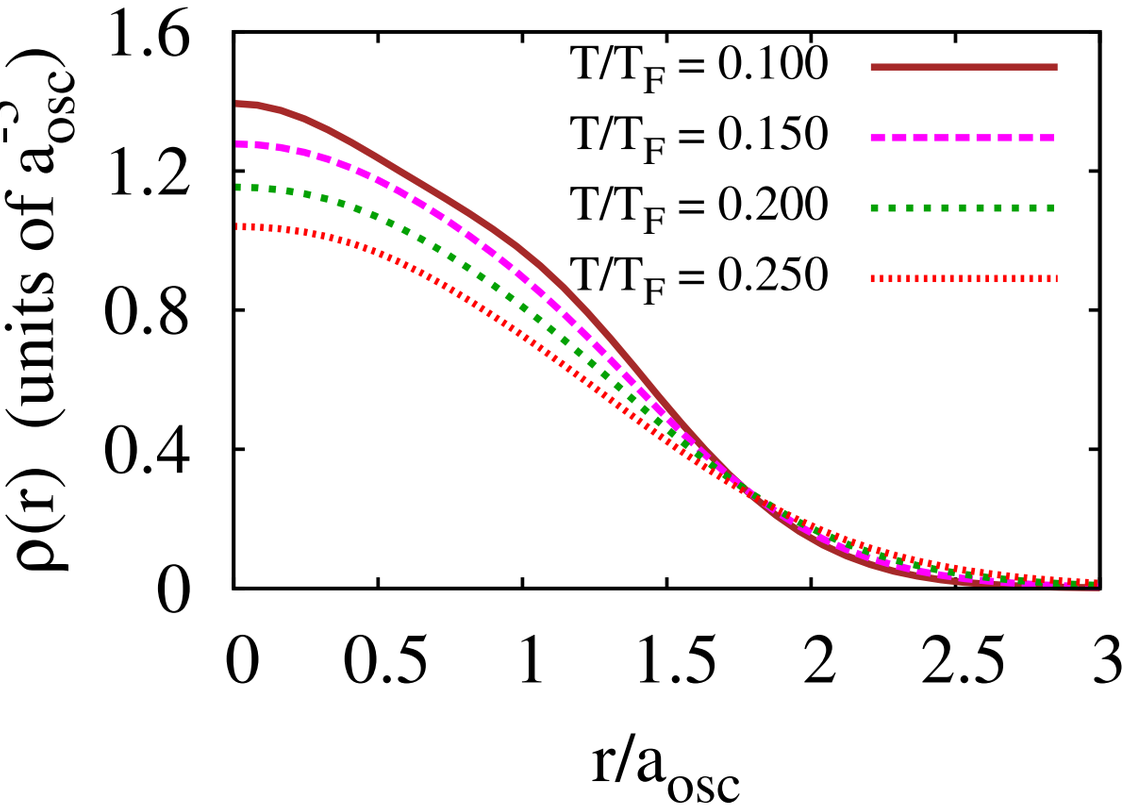


$$\Delta_{\rm gap} = [E(N_\uparrow, N_\downarrow + 1) + E(N_\uparrow + 1, N_\downarrow) - E(N_\uparrow, N_\downarrow) - E(N_\uparrow + 1, N_\downarrow + 1)]/2$$

$$C_L(ab, cd) = \langle A^\dagger_{LM}(ab) A_{LM}(cd) \rangle$$

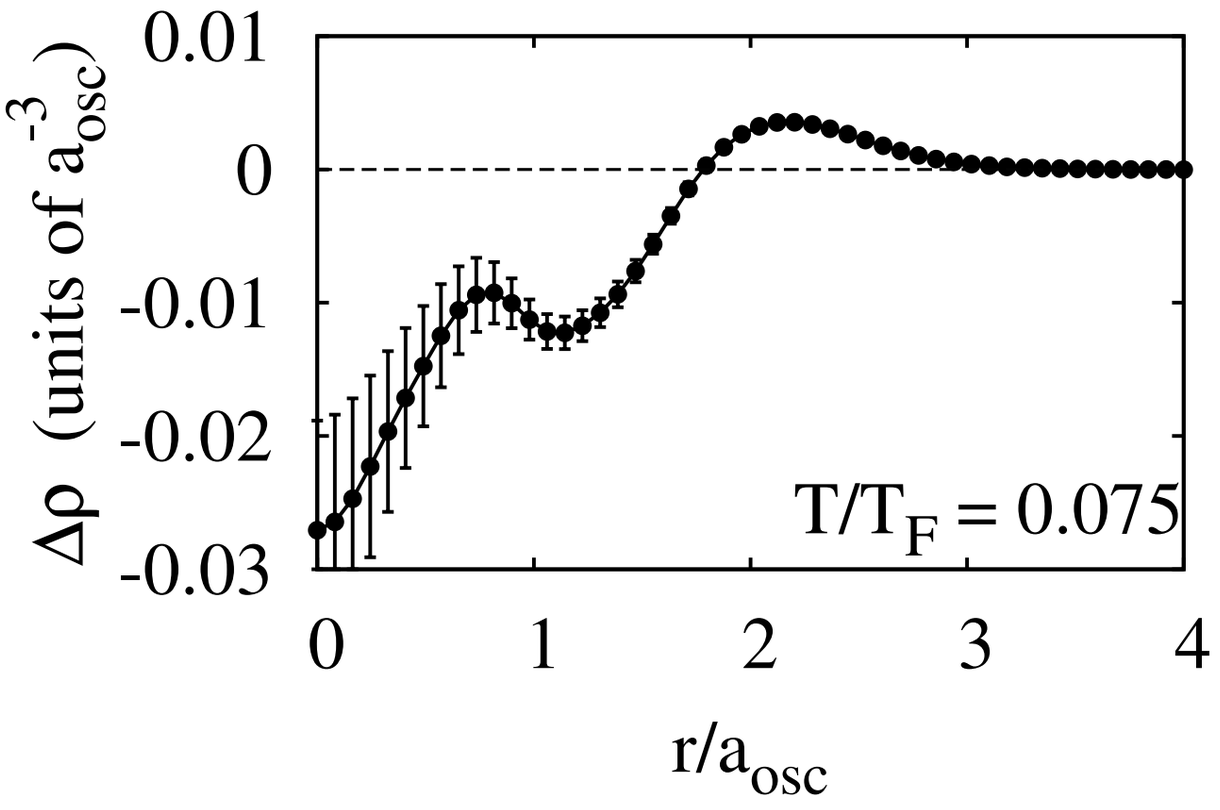
$$n = \lambda_{\rm max}/(N/2)$$

Particle Density & Odd Particle Effect



$$\rho(\boldsymbol{r}) = \left\langle \sum_\sigma \psi_\sigma^\dagger(\boldsymbol{r})\psi_\sigma(\boldsymbol{r}) \right\rangle$$

Cloud spreads out at higher temperatures



$$\Delta\rho(\boldsymbol{r}) = [\rho(\boldsymbol{r})^{(9,10)} + \rho(\boldsymbol{r})^{(10,9)}]/2 - [\rho(\boldsymbol{r})^{(10,10)} + \rho(\boldsymbol{r})^{(9,9)}]/2$$

Unpaired particle prefers the edge of the trap

Summary: AFMC in the CI Framework for Cold Atoms

- We devised a more efficient numerical stabilization method in the canonical ensemble which allows calculations in much larger model spaces.
- First *ab initio* calculations of heat capacity and energy-staggering pairing gap across the superfluid phase transition in any system of cold atoms
- Condensate fraction and particle density for a finite trapped system of cold atoms
- Clear signatures of a superfluid phase transition
- The addition of an extra particle to the spin-balanced system produces extra density at the edge of the trap.

Questions

- Questions:
  - Does $\Delta_{\rm gap}$ show a pseudogap effect in the trapped system for larger numbers of particles at unitarity?
  - Does $\Delta_{\rm gap}$ (*as opposed to the spectral function*) show a pseudogap effect in the *uniform* system?
  - How can we extend AFMC in the CI framework to larger model spaces?
    - Represent the interaction in coordinate space?
    - Optimize matrix exponential, diagonalization, etc. methods?
    - Optimize single-particle basis functions?
    - Alternatives to Metropolis?

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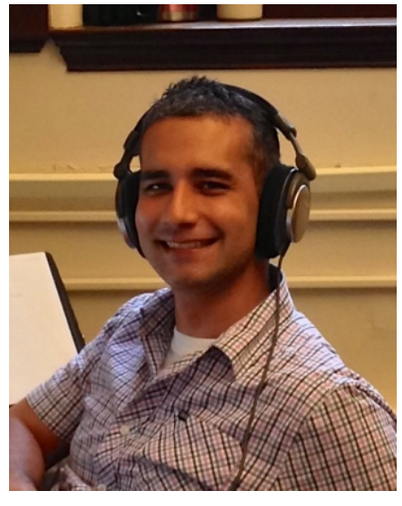
Department of Physics



Marco Bonet-Matiz