Lawrence Livermore National Laboratory

Auxiliary-field Monte Carlo methods for Nuclear Structure

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UCRL-PRES-

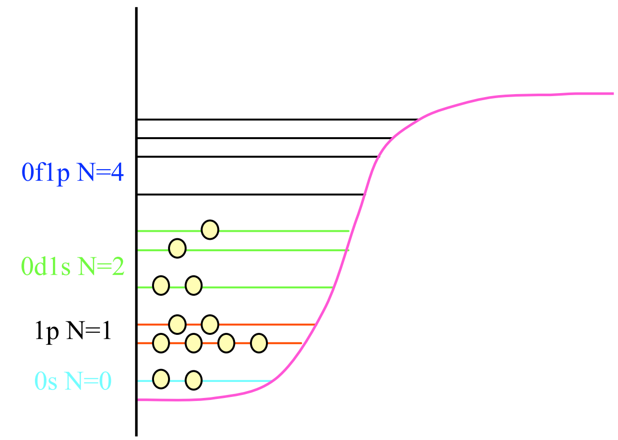
Traditional CI methods

- Typical eigenvalue problem

$$H\Psi_i = E_i \Psi_i$$

- Construct many-body basis states $|\phi_i\rangle$ so that

$$\Psi_i = \sum_n C_{in}\phi_n$$



$$\phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \ldots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \ldots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \ldots a_j^+ a_i^+ |0\rangle$$

Traditional CI methods

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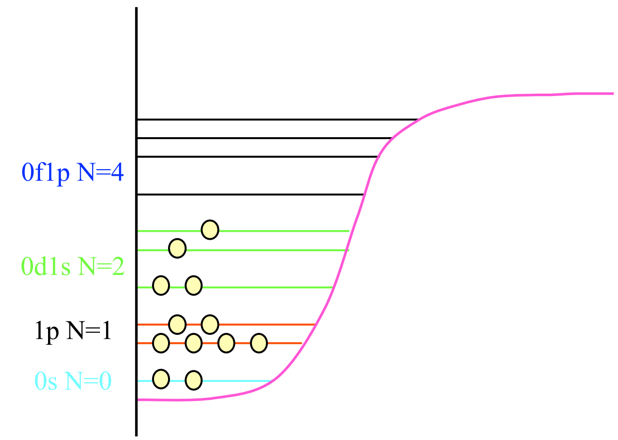
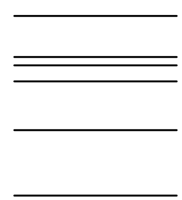


- Calculate Hamiltonian matrix $H_{ij}=\langle\phi_j|H|\phi_i\rangle$
  - Diagonalize to obtain eigenvalues

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \dots & H_{NN} \end{pmatrix} \longrightarrow$$



$$\phi = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \dots a_j^+ a_i^+ |0\rangle$$

Current computational capability of the order 10^{10} states

Traditional methods suffer from computational overload

- Effective interaction needs to be derived!
- Large dimensions
  - Grows dramatically with number of particles
  - Consider half-filled fp-gsd

$$\mathrm{Dim} \approx \begin{pmatrix} N_{sps}^{p} \\ n^{p} \end{pmatrix} \begin{pmatrix} N_{sps}^{n} \\ n^{n} \end{pmatrix} \qquad \begin{pmatrix} 50 \\ 25 \end{pmatrix} \begin{pmatrix} 50 \\ 25 \end{pmatrix} = 1.9 \times 10^{28}$$

Current computational capability of the order 10^{10} states

Even 10^{15} states would require a computer ~ 10^{6} times more powerful than any computer available today

10^{20} IS NOT AN OPTION!

Auxiliary-Field Monte Carlo

- Try something different

Thermal filter

$$E_{GS} = \lim_{\beta\to\infty} \frac{\langle \psi_{trial} | e^{-\beta\hat{H}/2} \hat{H} e^{-\beta\hat{H}/2} | \psi_{trial} \rangle}{\langle \psi_{trial} | e^{-\beta\hat{H}} | \psi_{trial} \rangle}$$

Thermal trace, T=1/β

$$E(\beta) = \frac{Tr\left[\hat{H} e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]}$$

- The Hamiltonian is two-body and the exponential $e^{-\frac{1}{2}\beta\sum_\alpha V_\alpha \hat{O}_\alpha^2}$ is impossible to deal with, so try

$$\int d\sigma_\alpha e^{-\frac{1}{2}\beta V_\alpha\left(\hat{O}_\alpha - s\sigma_\alpha\right)^2} = \sqrt{\frac{2\pi}{\beta|V_\alpha|}}$$

$$s = \begin{cases} \pm 1 & \text{if } V_\alpha \le 0 \\ \pm i & \text{if } V_\alpha > 0 \end{cases}$$

Auxiliary-Field Monte Carlo

- Try something different

Thermal filter

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$$e^{-\beta V_\alpha \hat{O}_\alpha^2} = \sqrt{\frac{\beta|V_\alpha|}{2\pi}} \int d\sigma_\alpha e^{\underbrace{-\beta\,|V_\alpha|\sigma_\alpha^2}_{\text{Gaussian factor}} + \underbrace{2\beta s \sigma_\alpha V_\alpha \hat{O}_\alpha}_{\text{One-body operator}}}$$

- Known as the Hubbard-Stratonovich transformation
- Two-body transformed to one-body - VERY GOOD
- Introduced integral over an auxiliary field σ
  - Many σ fields, also $e^{-\beta\hat{H}} \rightarrow \underbrace{e^{-\Delta\beta\hat{H}} \cdots e^{-\Delta\beta\hat{H}}}_{N_t \text{ time slices}}$

Auxiliary-Field Monte Carlo

- Path-integral approach in Fock space
- C. W. Johnson, S. E. Koonin, G. H. Lang, and W. E. Ormand, Phys. Rev. Lett. **69**, 3157 (1992)
- G. H. Lang, C. W. Johnson, S. E. Koonin, and W. E. Ormand, Phys. Rev. C**48**, 1518 (1993)
- W. E. Ormand, Prog. Theo. Phys. Supp. No. **124**, 37 (1996)
- S.E. Koonin, D.J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997).

Path integral formulation

$$e^{-\frac{1}{2}\Delta\beta\hat{H}} = \prod_{\alpha}\sqrt{\frac{|V_\alpha|}{2\pi}}\int\prod_{\alpha}d\sigma_\alpha e^{-\frac{1}{2}\Delta\beta\sum_{\alpha}|V_\alpha|\sigma_\alpha^2} e^{-\Delta\beta\sum_{\alpha}(\varepsilon_\alpha - V_\alpha s_\alpha\sigma_\alpha)}$$

- Transformed the many-body trace into a path integral and a trace over a one-body Hamiltonian

$$\langle\hat{O}\rangle = \frac{\int D(\vec{\sigma})e^{-\frac{1}{2}\Delta\beta\sum_{\alpha,n}|V_\alpha|\sigma_{\alpha,n}^2} Tr\left[e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\ldots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]\frac{Tr\left[\hat{O}e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\ldots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}{Tr\left[e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\ldots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]}}{\int D(\vec{\sigma})e^{-\frac{1}{2}\Delta\beta\sum_{\alpha,n}|V_\alpha|\sigma_{\alpha,n}^2} Tr\left[e^{-\Delta\beta\hat{h}(\vec{\sigma}_{N_t})}\ldots e^{-\Delta\beta\hat{h}(\vec{\sigma}_{N_t})}\right]}$$

$$= \frac{\int D(\vec{\sigma})W(\vec{\sigma})\langle\hat{O}\rangle_{\vec{\sigma}}}{\int D(\vec{\sigma})W(\vec{\sigma})}$$

Some useful information I

- $h(\sigma)$ is an N_sxN_s matrix

$$\mathbf{U}_{\vec{\sigma}_i} = e^{-\Delta\beta\hat{h}(\vec{\sigma}_i)} = 1 - \Delta\beta\mathbf{h}(\vec{\sigma}_i) + \frac{1}{2}\left(\Delta\beta\mathbf{h}(\vec{\sigma}_i)\right)^2 + \ldots$$

$$\mathbf{U}_{\vec{\sigma}}(\tau_2,\tau_2) = \mathbf{U}_{\vec{\sigma}_{\tau_2}} \ldots \mathbf{U}_{\vec{\sigma}_{\tau_1}}$$

- Overlaps and Grand-canonical trace

$$\left\langle \psi_t \middle| U_{\vec{\sigma}}(\beta,0) \middle| \psi_t \right\rangle = \det\left[\Psi_L^{+}\Psi_R\right]$$

$$Tr_G = \det\left[1 + \mathbf{U}_{\vec{\sigma}}(\beta,0)\right]$$

  - Project particle number for Canonical trace

- Density matrix

$$\left\langle a_i^{+} a_j \right\rangle_{\vec{\sigma}} = \left[\Psi_R\left(\Psi_L^{+}\Psi_R\right)^{-1}\Psi_L^{+}\right]_{ij}$$

$$= \left[\left(1 + \mathbf{U}_{\vec{\sigma}}(\beta,0)\right)^{-1}\mathbf{U}_{\vec{\sigma}}(\beta,0)\right]_{ij}$$

Some useful information II

- Maximum - Hartree solution

$$\frac{\partial \ln W(\vec{\sigma})}{\partial \sigma_{\alpha,n_t}} = 0$$

$$\sigma_\alpha^{MF} = -s_\alpha \operatorname{sgn}(V_\alpha) \frac{Tr\left[\hat{O}_\alpha e^{-\Delta\beta \hat{h}(\vec{\sigma}_{N_t})} \ldots e^{-\Delta\beta \hat{h}(\vec{\sigma}_{N_t})}\right]}{Tr\left[e^{-\Delta\beta \hat{h}(\vec{\sigma}_{N_t})} \ldots e^{-\Delta\beta \hat{h}(\vec{\sigma}_{N_t})}\right]} = -s_\alpha \operatorname{sgn}(V_\alpha) \left\langle \hat{O}_\alpha \right\rangle_{\vec{\sigma}^{MF}}$$

- Curvature

$$\frac{\partial^2 \ln W(\vec{\sigma})}{\partial \sigma_{\alpha,n_t} \partial \sigma_{\alpha',n_{t'}}} = -\Delta\beta |V_\alpha| \delta_{\alpha\alpha'} \delta_{n_t n_{t'}} + \Delta\beta^2 V_\alpha V_{\alpha'} \left(\left\langle \hat{O}_\alpha \left(\Delta\beta |n_t - n_{t'}|\right) \hat{O}_{\alpha'} \right\rangle_{\vec{\sigma}^{MF}} - \left\langle \hat{O}_\alpha \right\rangle_{\vec{\sigma}^{MF}} \left\langle \hat{O}_{\alpha'} \right\rangle_{\vec{\sigma}^{MF}} \right) = -C_{(\alpha n_t)(\alpha' n_{t'})}$$

- Gaussian approximation

$$W(\vec{\sigma}) \approx \exp\left[-\frac{1}{2} \sum_{(\alpha,n_t)(\alpha',n_{t'})} C_{(\alpha,n_t)(\alpha',n_{t'})} \left(\sigma_{\alpha,n_t} - \sigma_\alpha^{MF}\right)\left(\sigma_{\alpha',n_t'} - \sigma_{\alpha'}^{MF}\right) \right]$$

Auxiliary-Field Monte Carlo

- We now have a multi-dimensional (many thousands!) integral

$$\left\langle \hat{O} \right\rangle = \frac{Tr\left[\hat{O}e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]} = \frac{\int D[\vec{\sigma}]W(\vec{\sigma})\left\langle \hat{O} \right\rangle_{\vec{\sigma}}}{\int D[\vec{\sigma}]W(\vec{\sigma})}$$

10^{22} states → 2×10^{5} fields

Auxiliary-Field Monte Carlo

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$$\langle \hat{O} \rangle = \frac{Tr\left[\hat{O}e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]} = \frac{\int D[\vec{\sigma}]W(\vec{\sigma})\langle \hat{O} \rangle_{\vec{\sigma}}}{\int D[\vec{\sigma}]W(\vec{\sigma})} \qquad \rightarrow \qquad \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{1}{N}\sum_k \langle \hat{O} \rangle_{\vec{\sigma}_k \in W(\sigma)}$$

10^{22} states → 2×10^5 fields

But W(σ) must be positive

Auxiliary-Field Monte Carlo

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$$\langle \hat{O} \rangle = \frac{Tr\left[\hat{O}e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]} = \frac{\int D[\vec{\sigma}]W(\vec{\sigma})\langle \hat{O} \rangle_{\vec{\sigma}}}{\int D[\vec{\sigma}]W(\vec{\sigma})} \rightarrow \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{1}{N}\sum_k \langle \hat{O} \rangle_{\vec{\sigma}_k \in W(\sigma)}$$

10^{22} states $\rightarrow$ 2×10^5 fields

But W(σ) must be positive

But, in general, W(σ) is not positive definite

$$\langle \hat{O} \rangle = \frac{\int D[\vec{\sigma}]\left|W(\vec{\sigma})\right|\langle \hat{O} \rangle_{\vec{\sigma}} W(\vec{\sigma})/\left|W(\vec{\sigma})\right|}{\int D[\vec{\sigma}]\left|W(\vec{\sigma})\right| W(\vec{\sigma})/\left|W(\vec{\sigma})\right|} \rightarrow \langle \hat{O} \rangle_{\mathrm{MC}} = \frac{\sum_k \langle \hat{O} \rangle_{\vec{\sigma}_k} W(\vec{\sigma}_k)/\left|W(\vec{\sigma}_k)\right|}{\sum_k W(\vec{\sigma}_k)/\left|W(\vec{\sigma}_k)\right|}$$

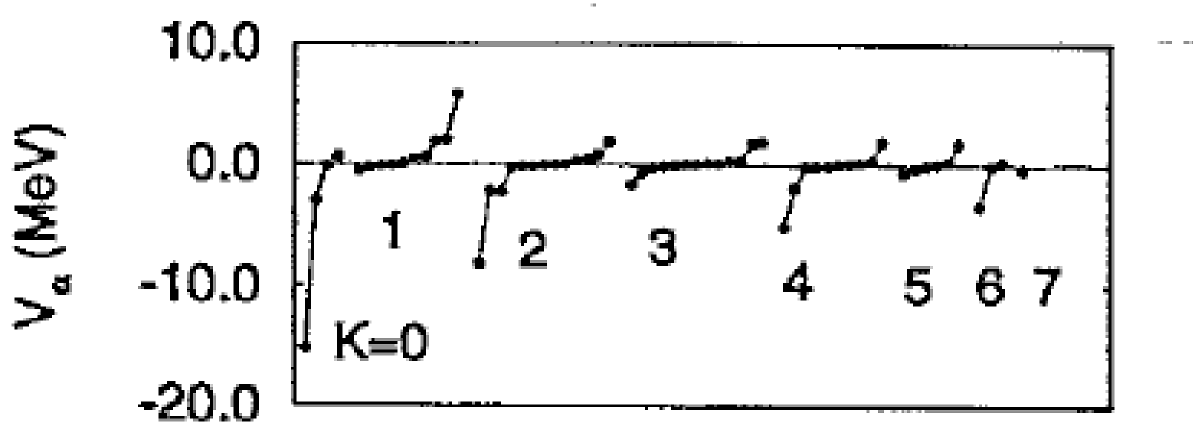
The Sign-problem

- Problem: In general, W(σ) has bad sign

$$H = \frac{1}{2}\sum_{\alpha K\pi} E_\alpha^\pi(\alpha)\sum_M (-1)^M \rho_{\alpha,\pi}^{KM}\rho_{\alpha,\pi}^{K-M}$$

- Good sign when

$$\mathrm{sgn}\left(E_\alpha^\pi\right) = \pi(-1)^{K+1}$$

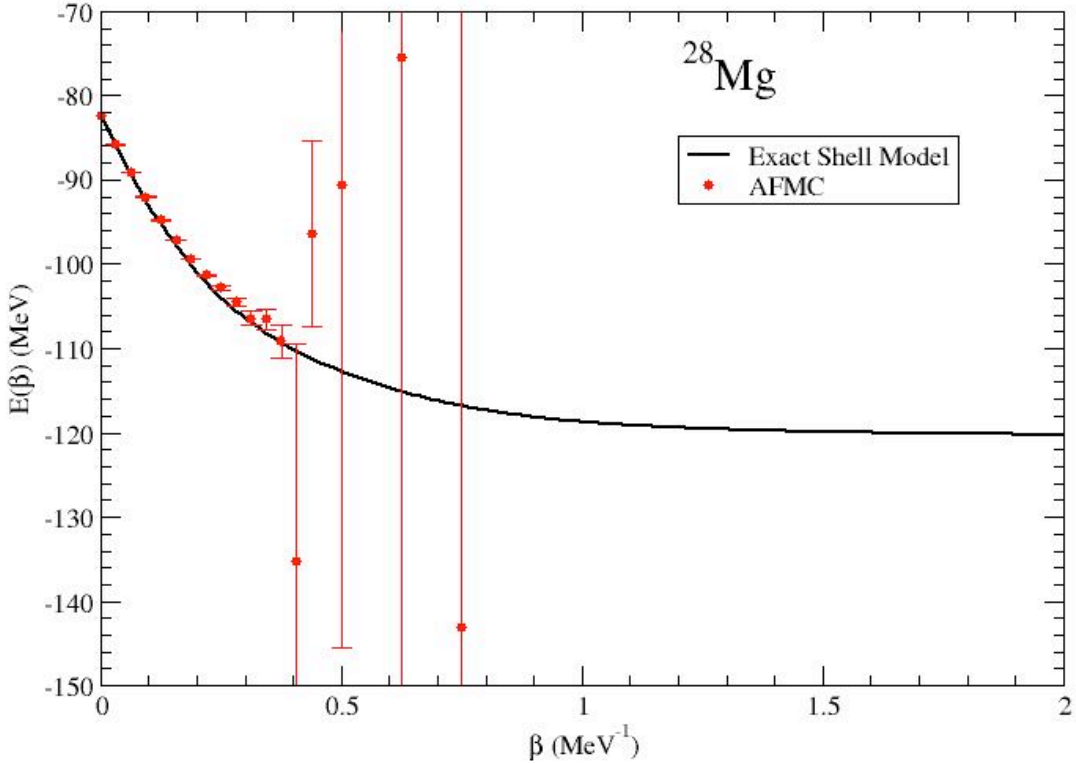


Eigenvalues of Brown-Richter fp-shell interaction

The Sign-problem

- Problem: In general, $W(\sigma)$ has bad sign

Thermal Energy for ^{28}Mg



AFMC was essentially useless for realistic interactions

Defeating the Sign Problem?

- Introduce a shift in the Hamiltonian [maximum of $W(\sigma)$]

$$H = \sum_\alpha V_\alpha \left(\hat{O}_\alpha - \tilde{\sigma}_\alpha\right)^2 + 2V_\alpha \tilde{\sigma}_\alpha \hat{O}_\alpha - V_\alpha \tilde{\sigma}_\alpha^2$$

$$e^{-\frac{1}{2}\beta V_\alpha \left(\hat{O}_\alpha - \tilde{\sigma}_\alpha\right)^2} = \int d\sigma e^{-\frac{1}{2}\beta |V_\alpha| \sigma_\alpha^2} e^{-\beta V_\alpha s_\alpha \left(\hat{O}_\alpha - \tilde{\sigma}_\alpha\right)}$$

$$e^{-\frac{1}{2}\Delta\beta \hat{H}} = \prod_\alpha \sqrt{\frac{|V_\alpha|}{2\pi}} \int \prod_\alpha d\sigma_\alpha e^{-\frac{1}{2}\beta \sum_\alpha \left(|V_\alpha| \sigma_\alpha^2 - V_\alpha \tilde{\sigma}^2 - 2V_\alpha s_\alpha \tilde{\sigma}_\alpha \sigma_\alpha\right)} e^{-\Delta\beta \sum_\alpha \left(\varepsilon_\alpha - V_\alpha \left(s_\alpha \sigma_\alpha + \tilde{\sigma}_\alpha\right)\right)}$$

- New maxima:

$$\sigma_\alpha = -s_\alpha \operatorname{sgn}(V_\alpha)\left(\left\langle \hat{O}_\alpha \right\rangle - \tilde{\sigma}_\alpha\right)$$

$$\tilde{\sigma}_\alpha = \left\langle \hat{O}_\alpha \right\rangle$$

$$\rightarrow \sigma_\alpha = 0$$

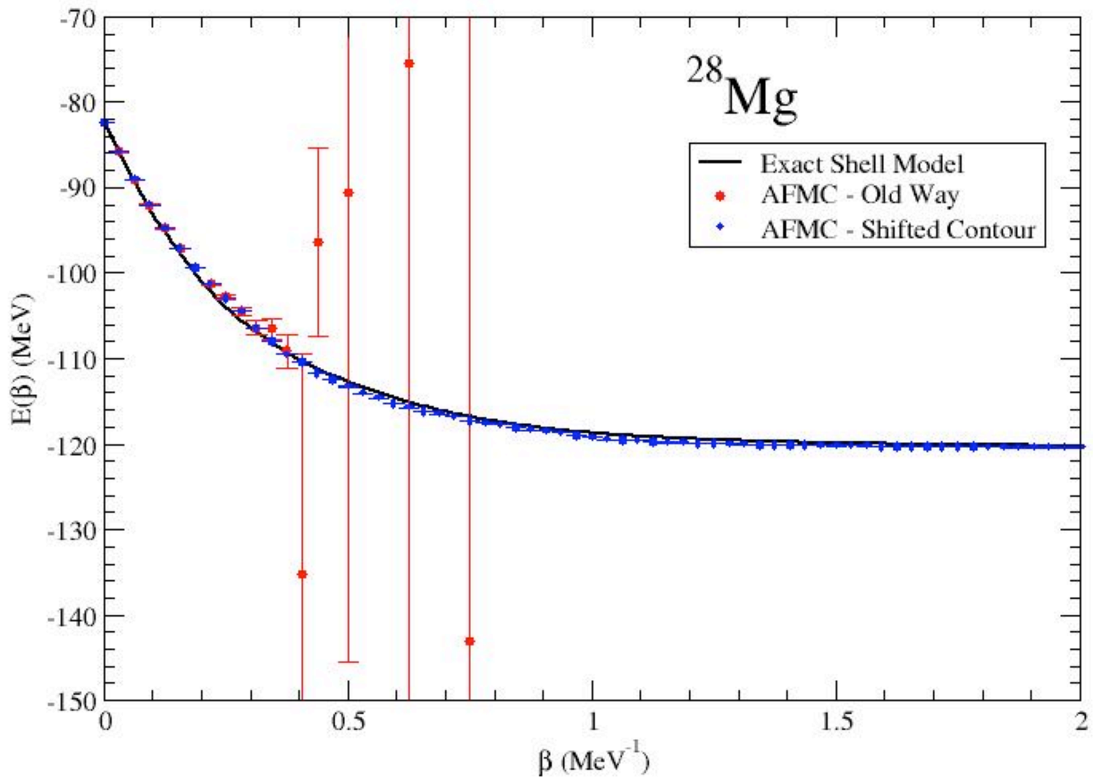
Sample with Gaussian factor

$$G(\vec{\sigma}) = e^{-\frac{1}{2}\Delta\beta \sum_{\alpha,n} |V_\alpha| \sigma_{\alpha,n}^2}$$

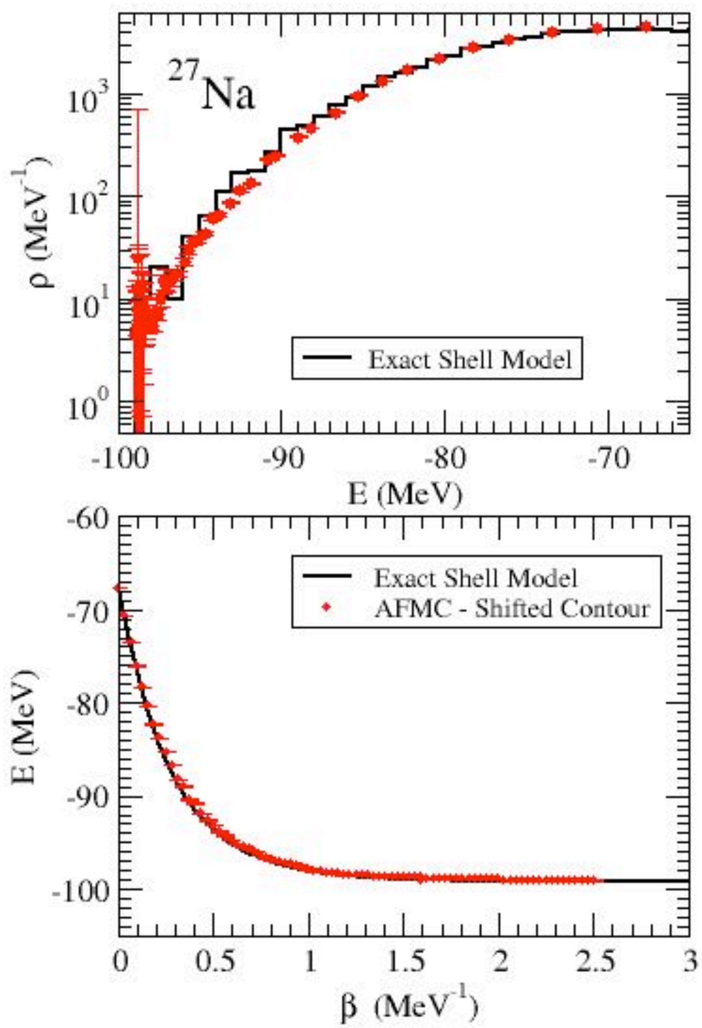
Defeating the Sign Problem

- Introduce a shift in the Hamiltonian [maximum of $W(\sigma)$]

$$H = \sum_\alpha V_\alpha \left(\hat{O}_\alpha - \tilde{\sigma}_\alpha\right)^2 + 2V_\alpha \tilde{\sigma}_\alpha \hat{O}_\alpha - V_\alpha \tilde{\sigma}_\alpha^2$$



Auxiliary-Field Monte Carlo



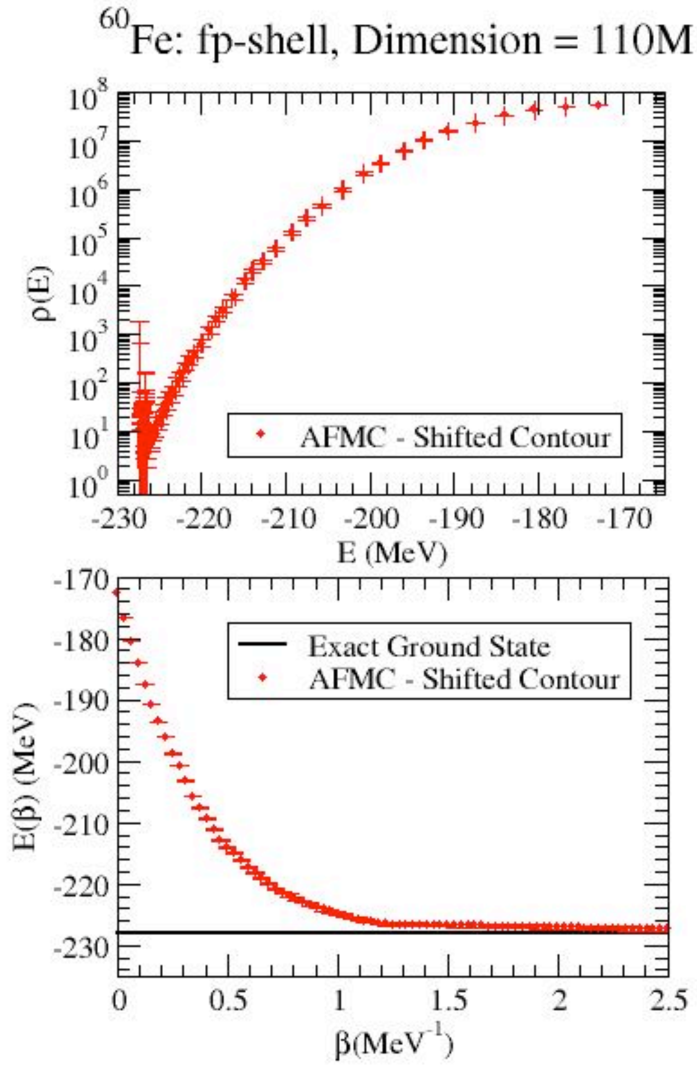
$$Z(\beta) = \int_0^\beta E(\beta')d\beta' + Z(0)$$

$$\rho(E) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{-\beta E} Z(\beta)$$

$$\rho(E) \approx \frac{e^{\ln Z(\beta)+\beta E}}{\sqrt{-2\pi \frac{\partial E}{\partial \beta}}}$$

We can solve the general CI problem exactly

Auxiliary-Field Monte Carlo



What we can calculate?

1. Binding energy
2. Level densities
3. Strength functions
   1. $\langle O^{+}(\tau)O(0)\rangle$
   2. Electro-magnetic
   3. Weak
   4. Thermally averaged
4. Even and Odd nuclei
5. Angular Momentum?

Can we do something far more general?

- Couple Hartree-Fock mean-field with CI
- We can start with Skyrme-like, Gogny, or even an EFT interaction

Two-body interaction - Skyrme potential

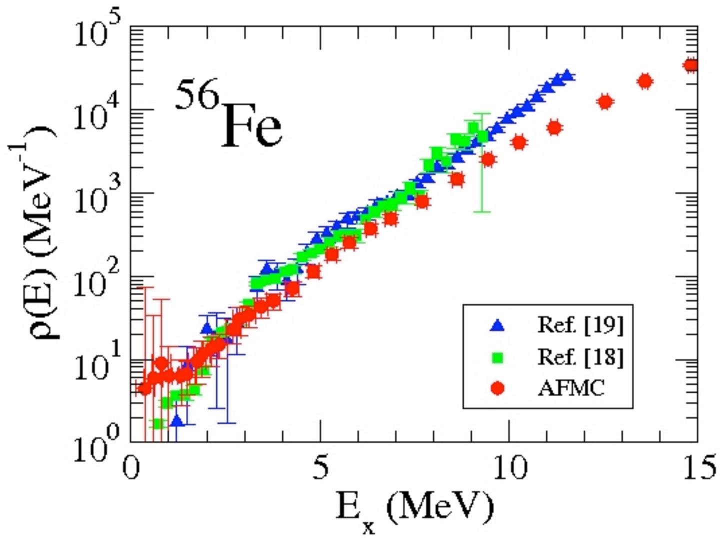
$$v_{12} = t_0\left(1 + x_0 P_\sigma\right)\delta\left(\vec{r}_1 - \vec{r}_2\right) + \frac{1}{2} t_1\left(1 + x_1 P_\sigma\right)\left[\delta\left(\vec{r}_1 - \vec{r}_2\right)\frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right) + \frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\delta\left(\vec{r}_1 - \vec{r}_2\right)\right] +$$
$$t_2\left(1 + x_2 P_\sigma\right)\frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\cdot\delta\left(\vec{r}_1 - \vec{r}_2\right)\frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right) + W_0\left(\vec{\sigma}_1 + \vec{\sigma}_2\right)\cdot\frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\times\delta\left(\vec{r}_1 - \vec{r}_2\right)\frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$
$$t_3\delta\left(\vec{r}_1 - \vec{r}_2\right)\delta\left(\vec{r}_2 - \vec{r}_3\right)$$

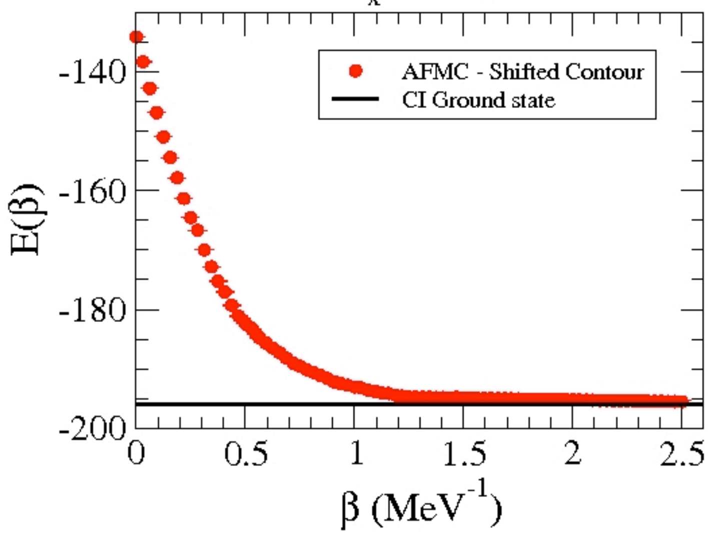
- Typically we fit the potential parameters to experimental binding energies
- But, it is very difficult to include quantum correlations

Three-body interaction - Density-dependent two-body

$$\frac{1}{6} t_3\left(1 + x_3 P_\sigma\right)\delta\left(\vec{r}_1 - \vec{r}_2\right)\rho^\alpha\left(\left(\vec{r}_1 + \vec{r}_2\right)/2\right)$$

Results: ^{56}Fe





18. A. Schiller *et al.*, Phys. Rev. C **68**, 054326 (2003).
19. A. V. Voinov *et al.*, Phys. Rev. C **74**, 014314 (2006).

$$E_{CI} = -195.901 \qquad \approx 1000 \text{ CPU hr}$$

$$E_{AFMC} = -195.687(107) \qquad \approx 12 \text{ CPU hr}$$

Application to the Hubbard Model

The Hamiltonian:

$$\hat{H} = -t\sum_{i,j}\sum_{\sigma} c^{+}_{\sigma_j} c_{\sigma_i} + U\sum_{j} n_{\uparrow j} n_{\downarrow j}$$

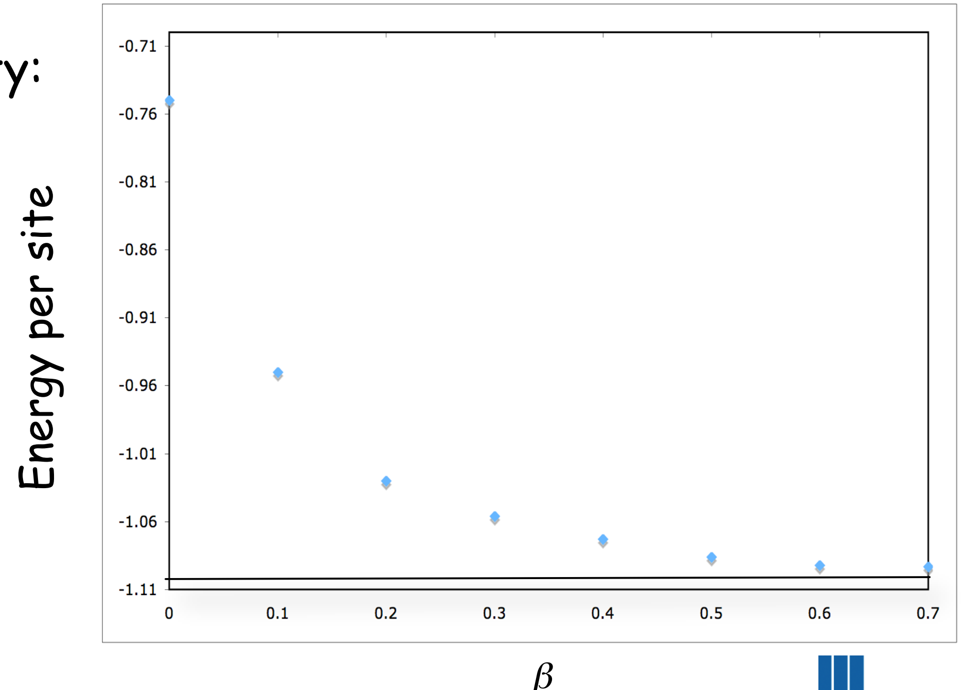
One-body term

electron number operator

$$n_{js} = c^{+}_{js} c_{js}$$

The shift is just the electron density:

$$\sigma_i = n_i = \frac{N_e}{N}$$

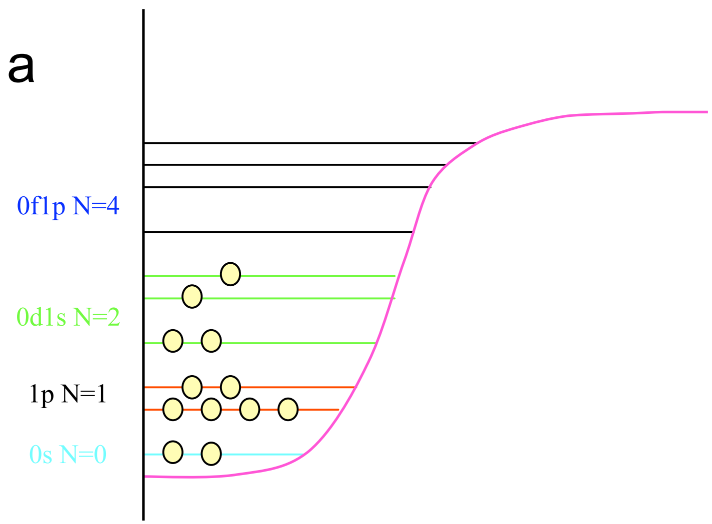


Exact Energy: -1.0944

E=-1.0933+/-0.0005

Can we do something far more general?

- Solve Hartree-Fock problem
- Use Hartree-Fock single-particle states to compute two-body matrix elements within a CI basis
- Use AFMC to compute ground state energy
- Fit interaction parameters



- Challenges:
    - Three-nucleon interaction
    - Continuum
    - Center-of-mass
    - Numerical stability for heavy nuclei (large scale on diagonal of U)

Summary

- Shifted contour seems to offer a pathway to solving the sign problem
- Calculations performed in the fp-shell with Gaussian sampling are competitive with CI
- Full confirmation coming after data recovery
  - Check convergence with $\Delta\beta$
- Couple Hartree-Fock mean-field with CI methods, attempt to perform a universal fit that includes quantum correlations