Shell model Monte Carlo approaches to nuclear level densities

H. Nakada (Chiba U.)

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I. Introduction

Nuclear structure at finite temperature

- properties under astrophysical environment
e.g. ele.-mag. & weak responses at thermal equilibrium
- statistical properties at high excitation energy ($E_x \sim 3$ MeV)
e.g. level density — key input to low-energy nuclear reaction rates

"nuclear temperature"

- microcanonical \[ T(E) = \left[ \frac{\partial}{\partial E} \ln \rho(E) \right]^{-1} \] ($\rho(E)$: level density)

- canonical \[ E(\beta) = -\frac{\partial}{\partial \beta} \ln Z(\beta) \] ($\beta = 1/T$)

⇒ $T$: external parameter controlling average excitation energy

\[ \text{both are treated within the same framework of thermodynamics} \]

(or statistical mechanics)
Nuclear level densities

- basic quantity in investigating nuclear properties at finite $T$

\[ \rho(E) \leftrightarrow Z(\beta) = \int \rho(E) e^{-\beta E} dE : \text{partition fn.} \] (in canonical formalism)

Laplace transf.

* e.g. exp. of $\rho(E) \rightarrow$ thermal properties  
  Ref.: A. Schiller et al., P.R.C63, 021316

- relevance to astrophysics — one of the critical inputs in nucleosynthesis calculations

\[ \sigma_{(n,\gamma)} \propto \sum_{J\pi} \int dE \rho_{J\pi}(E) f_{J\pi}(E) \]

\[ f: \text{transmission coeff., etc.} \]

(determined fairly well)

\[ \text{e.g. } s- \& r\text{-processes} \]

\[ \cdots (n,\gamma) \text{ vs. } \beta\text{-decay} \]

\[ \sigma_{(n,\gamma)} \propto \sum_{J\pi} \int dE \rho_{J\pi}(E) f_{J\pi}(E) \]

\[ f: \text{transmission coeff., etc.} \]

(determined fairly well)
Experimental methods to measure nuclear level densities

1. direct counting of levels — lowest-lying states or light nuclei
2. level spacing among neutron resonances ($\rho \approx \bar{D}^{-1}$) — relatively small energy range
3. Ericson fluctuation — $E_x \sim 20\text{MeV}$
4. charged particle reactions
5. $\gamma$-strength function ($\Gamma(E_x, E_\gamma) \propto F(E_\gamma)\rho(E_x)$) ← Brink-Axel hypothesis

Previous theoretical works on nuclear level densities

• backshifted Bethe formula (← Fermi-gas model) → next discussion
• distributing (spherical) s.p. levels + marginal interaction effects
  e.g. spectral averaging theory ⋯ int. → smearing (treated in terms of moments)
  ○ unable to constrain overall energy shift (↔ g.s. energy)
  ○ moderately good for spherical nuclei, but unable to handle strong collectivity
• finite-temperature methods
  e.g. mean-field approx., static-path approx. → later discussion
II. Shell model Monte Carlo approaches to nuclear level densities

Conventional approach to nuclear level densities

**Backshifted Bethe formula** ← Fermi-gas model

\[
\rho_{\text{tot}}(E_x) = \frac{\sqrt{\pi}}{12}a^{-1/4}(E_x - \Delta + t)^{-5/4} \exp \left[2\sqrt{a(E_x - \Delta)} \right] \quad (E_x - \Delta = at - t^2)
\]

\[\cdots\text{ fits well to experimental data, if the parameter } a \text{ is adjusted}\]

\[\Delta: \text{backshift, representing pairing & shell effects}\]

**Problem** \[\cdots\text{ value of } a!\quad (& \text{sometimes } \Delta, \text{also})\]

1) exp. \[\rightarrow a = A/6 \sim A/10 [\text{MeV}^{-1}] \quad \text{cf. } a \approx A/15 \text{ in Fermi-gas model}\]

2) exp. \[\rightarrow a: \text{nucleus-dependent (not only } A\text{-dependent) --- shell effects, } etc.\]

\[\Rightarrow \text{predictability?}\]
$\rho(E)$ for Ag:

\[ (n,n') \text{ at } E_n = 3.5 - 8.5 \text{ MeV} \]

Ref.: Bohr-Mottelson vol.1
Complexity due to finiteness \( \text{e.g. quantum fluctuation, shell effects, conservation, coexistence of collective \& non-coll. d.o.f.} \)

\[ \downarrow \]

**Interacting shell model** \( \cdots \) desirable for level density calculations

Both (1) **shell effects** \& (2) **2-body correlations** can fully be taken into account

(but within finite model space)

\( \text{e.g. } V = -\frac{\kappa}{2} \hat{\rho}^2 \quad (\hat{\rho} : 1\text{-body op.}) \quad \text{typically, } \kappa : \text{large} \leftrightarrow \text{collective} \)

![Diagram of interacting shell model]

To handle sufficiently large model space

\( \rightarrow \) quantum Monte Carlo method (Shell model Monte Carlo (SMMC) method)
Interacting shell model at finite $T \rightarrow$ auxiliary-fields path integral rep. 

\[ H = \sum_j \epsilon_j \hat{N}_j + \sum_{\alpha} \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2 \quad \leftarrow \text{Pandya transformation} \quad (\hat{\rho}_\alpha : 1\text{-body operator}) \]

**Suzuki-Trotter decomposition:**

\[ e^{-\beta H} = (e^{-\Delta \beta H})^{n_t} \quad \text{with} \quad \beta = n_t \Delta \beta; \]

\[ e^{-\Delta \beta H} \approx \prod_j \left[ \exp(-\Delta \beta \epsilon_j \hat{N}_j) \right] \prod_\alpha \left[ \exp(-\Delta \beta \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2) \right] + O((\Delta \beta)^2) \]

**Hubbard-Stratonovich transformation:**

\[ \exp(-\Delta \beta \frac{\kappa_\alpha}{2} \hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp \left[ -\Delta \beta \left( \frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + \sum_{\alpha} \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right]; \quad s_\alpha = \begin{cases} +1 & (\text{if} \quad \kappa_\alpha < 0) \\ +i & (\text{if} \quad \kappa_\alpha > 0) \end{cases} \]

\[ \Rightarrow \quad \text{Tr}(O e^{-\beta H}) \approx \int D[\sigma] G(\sigma) \text{Tr}(O U_\sigma); \quad G(\sigma) = \exp(-\Delta \beta \frac{|\kappa_\alpha|}{2} \sigma_\alpha^2), \quad U_\sigma = \prod_{n_t} \exp(-\Delta \beta \hat{h}_\sigma) \]

\[ \hat{h}_\sigma = \sum_j \epsilon_j \hat{N}_j + \sum_{\alpha} s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha: (\sigma\text{-dep.}) \text{ s.p. Hamiltonian} \]

Ref.: G. H. Lang et al., P.R.C 48, 1518 ('93)
\[ \langle O \rangle = \frac{\text{Tr}(O e^{-\beta H})}{\text{Tr}(e^{-\beta H})} \cong \frac{1}{N_{\text{samp}}} \sum_k \langle O \rangle_{\sigma(k)} ; \quad \langle O \rangle_{\sigma(k)} = \frac{\text{Tr}(OU_{\sigma})}{\text{Tr}(U_{\sigma})} : \text{measurement} \]
\[ \text{Tr}_{\text{GC}}(U_{\sigma}) = \text{det}(1 + U_{\sigma}) \quad U_{\sigma} : \text{s.p. matrix for } U_{\sigma} \]

\[ \ldots \text{calculable only via the s.p. matrices} \]
\[ \langle \sigma(k) \rangle \leftarrow \text{random walk under } W_{\sigma} = G(\sigma)\text{Tr}(U_{\sigma}) \]

**Level density calculation:** \[ \rho(E) = \text{Tr} \delta(E - H) \leftrightarrow Z(\beta) = \text{Tr}(e^{-\beta H}) = \int dE \rho(E)e^{-\beta E} \]

**Laplace transform** (\(\text{Tr} : \text{canonical trace}\))

**Saddle-point approx.** for the inverse Laplace transformation
\[ \Rightarrow \rho(E) \cong \frac{e^S}{\sqrt{2\pi \beta^{-2}C}} ; \quad S = \beta E + \ln Z(\beta), \quad \beta^{-2}C = -\frac{dE}{d\beta} \quad \text{cf. thermodynamics} \]

\[ S : \text{entropy, } C : \text{heat capacity} \]

\[ E(\beta) = \langle H \rangle = \frac{\text{Tr}(He^{-\beta H})}{Z(\beta)} \leftarrow \text{SMMC} \]

\[ Z \& C \leftarrow \text{numerical integration } (\ln[Z(0)/Z(\beta)] = \int d\beta' E(\beta')) \& \text{differentiation} \]
\[ E_x = E - E_0 ; \quad E_0 = \lim_{\beta \to \infty} E(\beta) \leftarrow E(\beta) \text{ for large } \beta \]
Projections:  (→ conservation, finiteness)

- **particle-number projection** (both for protons & neutrons) → canonical
  \[ \text{Tr}(U_\sigma) = \text{Tr}_{GC}(P_n U_\sigma); \quad P_n \propto \int d\phi \exp[i\phi(\hat{N} - n)] \]
  \[ \phi: \text{additional auxiliary field} \rightarrow \text{exact integration} \]

- **parity projection** → level densities for each parity
  \[ \text{Tr}(P_\pm U_\sigma) = \frac{1}{2} \text{Tr}[(1 \pm P)U_\sigma] = \frac{1}{2} [\text{Tr}(U_\sigma) \pm \text{Tr}(PU_\sigma)] \quad (P: \text{parity op.}) \]
  \[ \text{Tr}_{GC}(PU_\sigma) = \det(1 + PU_\sigma); \quad P = (-)^\ell \text{ for each s.p. state} \]

- **isospin projection** (for T-conserved Hamiltonian & model space)
  \[ \text{Ref.}: \text{H.N.} \& \text{Y. Alhassid, P.R.L. 79, 2939 ('97)} \]
  \[ \text{Ref.}: \text{H.N.} \& \text{Y. Alhassid, Proc. of 11th Int. Symp. on Cap. } \gamma \text{-Ray Spec. ('03)} \]
  \[ \rightarrow \begin{cases} \text{isospin dependence of level densities} \\
  \text{exact ‘binding energy’ correction} \quad (T\text{-splitting is not necessarily reliable}) \end{cases} \]
  \[ \text{Ref.}: \text{H.N.} \& \text{Y. Alhassid, Proc. of 11th Int. Symp. on Cap. } \gamma \text{-Ray Spec. ('03)} \]
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  - random walk with \( W_\sigma = G(\sigma)\text{Tr}_A(U_\sigma) \rightarrow \text{MC evaluation} \)
  \[ \frac{Z_{T=T_0}(\beta)}{Z_A(\beta)} = \frac{\text{Tr}_{T=T_0}(e^{-\beta H})}{\text{Tr}_A(e^{-\beta H})} \approx 1 - \frac{1 - \text{Tr}_A[U_\sigma(k)]}{N_{\text{samp}}} \sum_k \left( 1 - \frac{\text{Tr}_A[U_\sigma(k)]}{\text{Tr}_A[U_\sigma(k)]} \right) \]
  \[ \langle O \rangle_{A'} = \frac{\text{Tr}_{T=T_0}(Oe^{-\beta H})}{Z_{T=T_0}(\beta)} = \frac{\text{Tr}_A'(Oe^{-\beta H})/Z_A(\beta) - \text{Tr}_A(Oe^{-\beta H})/Z_A(\beta)}{1 - Z_{A'}(\beta)/Z_A(\beta)} \]
Relation among MFA, SPA & SMMC

- **mean-field approx.** (Hartree/Hartree-Fock)

\[ \exp(-\beta \frac{\kappa_\alpha^2}{2} \hat{\rho}_\alpha^2) \approx \exp \left[-\beta \left(\frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right] \]

\[ \sigma_\alpha = \langle \hat{\rho}_\alpha \rangle : \text{static mean-field (no fluctuation, no } \beta \text{-dependence)} \]

- **static-path approx.**

\[ \exp(-\beta \frac{\kappa_\alpha^2}{2} \hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp \left[-\beta \left(\frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right] \]

\[ \sigma_\alpha : \text{static auxiliary-field with fluctuation} \]

\[ \cdots \text{ error of } O(\beta^2) \text{ in the Trotter decomp. } \rightarrow \text{reasonable (only) for small } \beta \]

- **SMMC**

HS for \( \Delta \beta \), instead of \( \beta \rightarrow \) auxiliary-field path integral

\[ \exp(-\Delta \beta \frac{\kappa_\alpha^2}{2} \hat{\rho}_\alpha^2) \propto \int d\sigma_\alpha \exp \left[-\Delta \beta \left(\frac{|\kappa_\alpha|}{2} \sigma_\alpha^2 + s_\alpha \kappa_\alpha \sigma_\alpha \hat{\rho}_\alpha \right) \right] \]

\[ \sigma_\alpha : \beta\text{-dependent auxiliary-field with fluctuation} \]

\[ \left( \begin{array}{c} \text{MC integration of the auxiliary-fields} \\ \rightarrow \text{MC weighted sum of time-dependent ‘mean-fields’} \end{array} \right) \]
Fermion sign problem

\[ W_\sigma = G(\sigma) \text{Tr}(U_\sigma) \cdots \text{weight for the random walk of } \{\sigma\} \text{ in the MC calculation} \]

However, \( \text{Tr}(U_\sigma) \) is not always positive-definite \( \rightarrow \) “sign problem”

nuclear effective interaction \( \approx (\text{collective part}) + (\text{non-collective perturbation}) \)

\[ \uparrow \quad \downarrow \]

(almost) sign good  \quad unimportant for level densities \quad (\because \text{gross property})

\( \Rightarrow T = 1 \text{ pairing} + T = 0 \text{ multipole interaction} \)

\quad — describes collective features well (including level densities)
III. Spherical & nearly spherical nuclei — Fe-Ni region

Setup for $50 \lesssim A \lesssim 70$ nuclei

- model space — full $pf + 0g_{9/2}$ (so as to cover $S_n(\lesssim 15\text{ MeV})$)
- effective hamiltonian — $T$-conserving
  
  s.p. energies $\leftarrow$ Woods-Saxon potential (with $LS$ term)

  $T = 0$ surface-peaked multipole interactions ($\lambda = 2, 3, 4$)

  radial part ($\propto dV_{WS}/dr$) & bare strength
  $\leftarrow$ nuclear self-consistency (between density & s.p. potential)

  renormalization factors $\leftarrow$ core-polarization effects
  $\leftarrow$ comparison with a realistic interaction

  $\lambda = 2 \cdots \times 2, \lambda = 3 \cdots \times 1.5, \lambda = 4 \cdots \times 1$

  $T = 1$ pairing interaction $\leftarrow$ mass differences of $40 < A < 80$ spherical nuclei

$\Rightarrow$ uniquely determined for individual nucleus

* check of the hamiltonian for quadrupole collectivity in $^{56}\text{Fe}$

\[
E_Q \equiv \frac{\sum_i (E_i - E_0) \langle 2^+_i | Q | 0^+_g \rangle^2}{\sum_i |\langle 2^+_i | Q | 0^+_g \rangle|^2} \quad \rightarrow \quad \text{Exp. } (p, p') : 2.16, \quad \text{SMMC : } 2.12 \pm 0.11 \quad [\text{MeV}]
\]

- MC $\cdots N_{\text{samp}} \approx 4000, \Delta \beta = 1/32 [\text{MeV}^{-1}]$ (time slice)
- thermal $\cdots d\beta = 1/16 [\text{MeV}^{-1}]$ (for $Z$ & $C$)
Thermal properties of $^{56}$Fe — SMMC vs. HF & exp.

- mean-field (semi-classical) picture → signature to phase transition at $\beta_c \approx 1.3 \text{MeV}^{-1}$
  - deformed (low $T$) $\rightarrow$ spherical (high $T$)
- shell model (full quantum theory) → washed out due to quantum fluctuations!
  $\leftrightarrow$ finiteness
$E_0 \leftarrow$ a sort of extrapolation to $\beta = \infty$

* even-even nuclei

For large $\beta$, $E(\beta)$ is slightly different from $E_0$ due to the contribution of $2_1^+$

The amount of the $2_1^+$ contribution is estimated from $\langle \hat{J}^2 \rangle$

cf. This approx. will be also good, if the influence of higher states in $E(\beta)$ is compensated with that in $\langle \hat{J}^2 \rangle$

$E_x(2_1^+)$:

$$
\begin{array}{c}
\text{Fe} & \text{Ni} & \text{Zn} & \text{Ge} \\
54 & 58 & 64 & 64 \\
58 & 64 & 70 & 72
\end{array}
$$

$\Rightarrow$ check of $\left\{ \begin{array}{l}
\text{this procedure} \\
\text{the present eff. } H
\end{array} \right.$

* odd-$A$ & odd-odd nuclei

For large $\beta$, $E(\beta) \approx E_0$ (because of higher degeneracy around $E \approx E_0$)
Total level density (state density) of $^{56}$Fe

\[
\rho(E) = \frac{e^S}{\sqrt{2\pi \beta^{-2} C}}
\]

in SMMC & HF cal.

Note: Exp. total level density ← reconstructed with exp. BBF parameters

(C. C. Lu et al., Nucl. Phys. A 190, 229('72))
Total level densities of other even-even nuclei

(Exp.: C. C. Lu et al., N. P. A 190, 229(’72))

(Exp.: W. Dilg et al., N. P. A 217, 269(’73))
Parity-projected level density of $^{56}$Fe

$\rho \text{[MeV}^{-1}]$

$E_x \text{[MeV]}$

$⇒$ strong parity-dependence!

— not well considered so far

sensitive to shell structure

$→ (Z- &) \text{ } N$-dep.
Systematics for (β-stable) even-even nuclei in the $50 \leq A \leq 70$ region

SMMC → fit to BBF

Nuclei: $^{54–58}\text{Fe}$, $^{58–64}\text{Ni}$, $^{64–70}\text{Zn}$, $^{70,72}\text{Ge}$

Single-particle level density parameters $a$:

Backshift parameters $\Delta$:
Total level densities of $A = 55$ isobars

Many empirical formulae predict equal $\rho(E_x)$ among odd-$A$ isobars — not true! (← exp. & micro. cal.)

Exp.: W. Dilg et al., Nucl. Phys. A217, 269 ('73)
$T, \pi$-projected level densities of $^{58}\text{Cu}$

$\rho_{tot}(E) = \sum_{T \geq |T_z|, \pi = \pm} \rho_{T,\pi}(E)$

($E \leftarrow$ correction of $E_T - E_{T=0}$)

---

Total level densities of $^{58}\text{Cu}$

With $T$-projection

Without $T$-projection

With perturbative correction

perturbative corr. — not so good

$T$-projection is important for $Z = N$ (& $Z = N \pm 1$?) nuclei
Extension to higher energy

higher energy (i.e. higher $T$) … size of model space is more important,
2-body correlation becomes less important

→ connection to Hartree-Fock approach (without space truncation)

free energy:

\[
F(\beta) = F_{\text{SM, trunc}}(\beta) + [F_{\text{HF, full}}(\beta) - F_{\text{HF, trunc}}(\beta)]
\]

1st term ↔ 2-body corr. at low $E_x$
2nd term ↔ full d.o.f. at high $E_x$
    (& subtract d.o.f.
    included in 1st term)

Note: in agreement with SMMC result
at $E_x \lesssim 25 \text{ MeV}$

Total level densities of $^{56}\text{Fe}$

Ref.: Y. Alhassid et al., P. R. C 68, 044322 ('03)
IV. Deformed nuclei — rare-earth region

quadrupole deformation $\rightarrow$ influence level density $\cdots$ how?

- deformation itself?
- collective rotation?
- influence of non-coll. d.o.f.?

— all of them should be taken into account $\rightarrow$ shell model in large model space

Note: ‘collective enhancement’?

Sm isotopes:
(exp. data)

```
\begin{align*}
\text{Ex [MeV]} & \quad 90 \quad 88 \quad 86 \\
\text{N} & \\
0^+ & \quad 2^+ & \quad 4^+ \\
\end{align*}
```

```
\begin{align*}
\text{B(E2;0^+\rightarrow2^+)} [e^2 b^2] & \quad 90 \quad 88 \quad 86 \\
\text{N} & \\
0 & \quad 2 \quad 4 \\
\end{align*}
```

```
\begin{align*}
\text{a [MeV]} & \quad 90 \quad 88 \quad 86 \\
\text{N} & \\
15 & \quad 16 \quad 17 \\
\end{align*}
```

quadrupole collectivity $\leftrightarrow$ enhancement of $\rho$
What is important?

- at high $E_x (E_x \gtrsim 5 \text{MeV})$ · · · non-coll. (i.e. s.p.) d.o.f. dominant
  $\leftrightarrow$ degree of quadrupole deformation $\leftrightarrow$ strength of $Q \cdot Q$-int.
  $\leftarrow$ checked by MF approx.

- at low $E_x (E_x \lesssim 2 \text{MeV})$ · · · $\rho(E) \propto (\text{mom. of inertia } I)$
  $\leftrightarrow$ single rotational band
  $\leftrightarrow$ strength of pairing int.  $\leftarrow$ checked from $\langle J^2 \rangle_T (\approx 2I \cdot T)$ for small $T$
  (or Thouless-Valatin estimate?)

$\Rightarrow$ preliminary result for $^{162}\text{Dy}$ (in collaboration with L. Fang & Y. Alhassid)
model space $\approx 1.5 \hbar \omega$, WS s.p.e. + pairing int. + multipole int.
Total level density of $^{162}\text{Dy} — \ln \rho(E_x)$

(preliminary)
V. Summary

1. SMMC approaches to nuclear structure at finite temperature
   → accurate microscopic calculations of nuclear level densities
     (for spherical & nearly spherical nuclei)
     ⇒ application to astrophysics?  Ref.: D. Mocelj et al., N.P.A 758, 154c

2. Extensions
   higher energy ← connection to HF · · · works well
   deformed nuclei — promising (work in progress)

3. Problems
   int. parameters for deformed nuclei — systematics?  (↔ predictability)
   connection between spherical & deformed region
Crude overview of ‘shell model world’ at present (or in near future)
Collaborators:

Y. Alhassid, S. Liu, L. Fang (Yale Univ., U.S.A.)
G. F. Bertsch (Univ. of Washington, U.S.A.)

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