Pairing correlations af finite temperature

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Pairing correlations around the drip-line of finite system, and beyond

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Outline

Motivation

Pairing correlations and thermal effects

Theoretical Models

Particle number conserving approaches, Projected-BCS at Finite Temperature

Applications and Results

- The Pairing (Richardson) Model, testing the Projected-BCS at Finite-T [a]
- Finite Nuclei, Preliminary results for ^{161,162}Dy and ^{171,172}Yb [b]

[a] DG and D.Lacroix, PRC 85, 044321 (2012)
[b] DG, D. Lacroix and N. Sandulescu, in preparation

Thermodynamics description of pairing effects

Pairing in Nuclei

- Pairing effects in atomic nuclei are well established:
  Energy Gap in even-even-nuclei spectra, Binding energy and odd-even effects,..
- Thermal signatures of the pairing interaction are less known

Thermodynamics properties of nuclei

- One of the key quantity is the statistical nuclear level density:
  Specific Heat, Entropy, Temperature, Compound nuclei properties,...
- Astrophysics
  reaction rates, supernovae, s- and r- processes,hot neutron stars, ..

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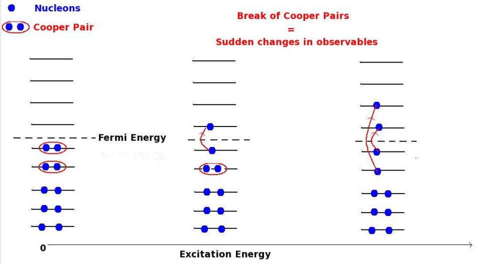
Theoretical description is a quite complicated task

- Critical behaviour and Phase Transitions
- Interplay between single particle and collective d.o.f.
- Continuum coupling

Pairing correlations and interplay with thermal effects

A Simplistic View

- Pairing correlations are expected to be more important at low energy
- Paired correlated particles, Cooper pairs



- As the energy increases the pair will break up
- Pair break ⇒ drastic changes (level density,specific heat, backbending,..)
- Excitation energy reduces pairing correlations

Pairing correlations and finite-size effects

Pairing correlations in Mesoscopic Systems

- Mesoscopic Systems (*atomic nuclei,quantum dots, ultra-small grains*)
- Thermodynamical properties deviate from infinite systems

The Pairing GAP thermal evolution in finite systems

- In infinite systems it decreases to zero as a function of the temperature
- In finite nuclei the BCS/HFB predict the same behaviour, i.e. a sharp phase transition at $T_c \approx 0.5\Delta_0$
- Experimentally a much more smoothed behaviour is observed
- A S-shape in the specific heat instead of a sharp phase transition
- **Theories able to describe both quantal and statistical fluctuations are needed**

Quantal Fluctuations

The BCS Case T=0

- BCS case

$$| BCS\rangle = \prod_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger) \mid 0\rangle$$

  where $a_i^\dagger$ creates a particle in φ_i,$a_{\bar{i}}$ time reversed state, $\mid 0\rangle$ is the vacuum.
- $\hat{N} \mid BCS\rangle \neq N \mid BCS\rangle$,not eigenstate of $\hat{N}$, $\mid BCS\rangle = \sum_N c_n \mid \Psi_N\rangle$
- BCS *breaks* U(1) Symmetry, Particle Number non Conserved

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Quantal Fluctuations: BCS case

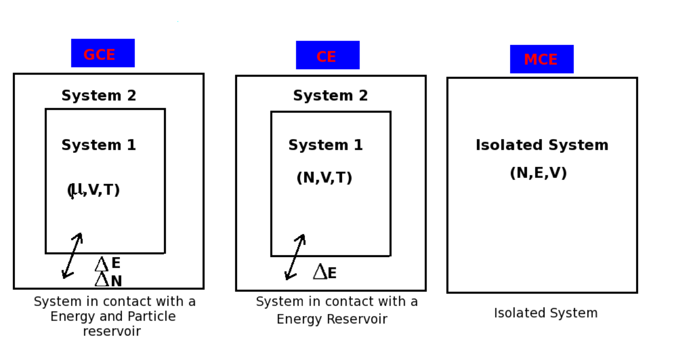
$$\langle (\hat{N} - \langle \hat{N}\rangle)^2 \rangle = \langle \hat{N}^2\rangle - \langle \hat{N}\rangle^2 \neq 0$$

How to solve that?
Project onto Good Particle Number$\Rightarrow$ $\langle \hat{N}^2\rangle = \langle \hat{N}\rangle^2$

Thermodynamics Description

Statistical Ensembles

- Grand-Canonical Ensemble (GCE), $\Rightarrow \langle \hat{N}^2 \rangle \neq \langle \hat{N} \rangle^2$
- Canonical Ensemble (CE), $\Rightarrow \langle \hat{N}^2 \rangle = \langle \hat{N} \rangle^2$
- Microcanonical Ensemble (MCE)



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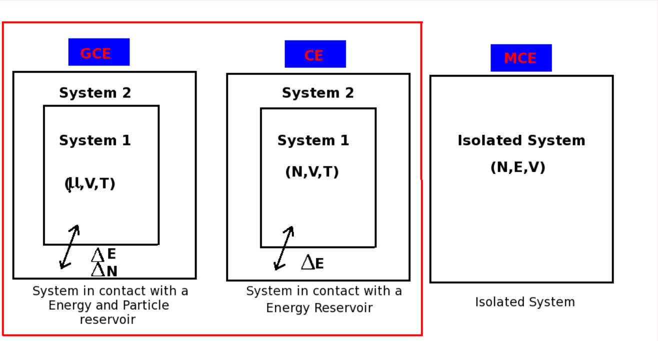


Statistical Fluctuations

From a Grand-Canonical to a Canonical Description

- The **BCS at finite-T** (FT-BCS) amounts to work in the **GC** Ensemble
- We apply a **Variation after Projection** at finite-T (**FT-VAP**) method which allows to give a **Canonical** description within a mean-field level
- Proposed by C. Esebbag and E. Egido, NPA 552,205 (1993)
- but applied only to a degenerate model because of its complexity

BCS at Finite-T, (Grand-Canonical)

- $H \simeq h = \sum_i E_i \alpha_i^\dagger \alpha_i, \quad \alpha_i^\dagger = U_i a_i^\dagger - V_i a_{\bar{i}}$
- Statistical density operator D

$$D = e^{-\beta h} / Tr\{e^{-\beta h}\}, \qquad \beta = 1/K_B T$$

- The FT-BCS equations are obtained by minimizing the Free Energy

$$F = < H > - TS - \mu N$$

$$< H > = Tr\{DH\}, \qquad , S = -K_B Tr\{D log D\}$$

- Usual (T=0) BCS equations with Gap Temperature dependent, i.e

$$\Delta_i = \sum_j \frac{\Delta_j G_{ij}}{2E_j}(1 - 2f_j); \qquad f_j = (1 + e^{\beta E_j})^{-1}$$

Projected BCS at Finite-T, (Canonical)

Projected BCS at Finite-Temperature

- $H \approx h = \sum_i E_i \alpha_i^\dagger \alpha_i, \quad \alpha_i^\dagger = U_i a_i^\dagger - V_i a_{\bar{i}}$
- We define the Projected density operator D_N

$$D_N = P_N e^{-\beta h} P_N / Tr\{P_N e^{-\beta h} P_N\}, \quad \beta = 1/K_B T$$

and P_N is the Particle Number Projector,

$$P_N = \frac{1}{2\pi} \int_0^{2\pi} e^{i\phi(\hat{N}-N)} d\phi$$

- The Free Energy is minimized

$$F =< H >_N - TS, \quad < H >_N = Tr\{D_N H\}, \quad S = -K_B Tr\{D_N log D_N\}$$

Application: Pairing Pickt-Fence Model

Pairing Model (Richardson)

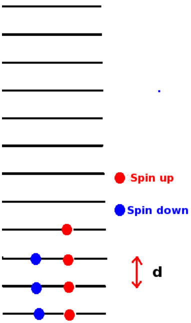
- N particles distributed over Ω doubly-folded equidistant levels of energy ϵ_i

$$H = \sum_{i,\sigma} \epsilon_i a^\dagger_{i,\sigma} a_{i,\sigma} - G \sum_{i,j} a^\dagger_{i,+} a^\dagger_{i,-} a_{j,-} a_{j,+}$$

- Exact Canonical Solution

$$Z(T) = \sum_n e^{-\beta E_n} ; < E(T) >= \sum_n E_n e^{-\beta E_n} / Z(T)$$

all the eigenvalues are needed.

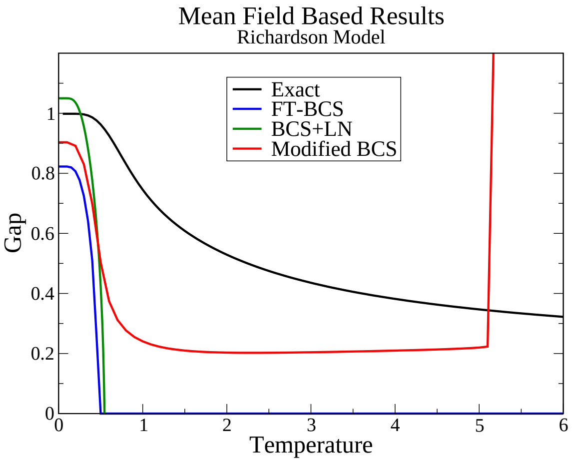


Mean Field Description

Mean Field (BCS or HFB based) approaches at finite T

- Finite Temperature BCS, minimizes F= $\langle H - \lambda \hat{N} \rangle$ -TS
- BCS plus Lipkin Nogami at Finite-T, minimizes F= $\langle H - \lambda \hat{N} - \lambda_2 \hat{N}^2 \rangle$ -TS
- Modified BCS
  (statistical fluctuations are incorporated in a *second* quasi-particle transformation)
  N. Dinh Dang and A. Arima PRC 68, 014318 (2003).

Applications to the Pairing Model (Richardson), N=Ω=10, G=0.4d



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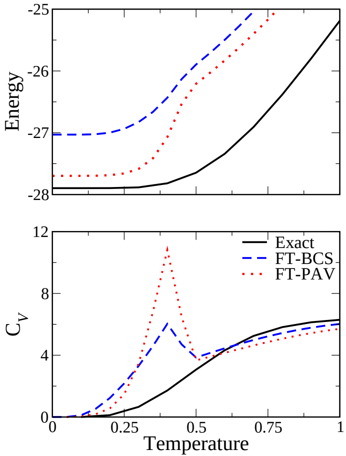
Approximated Scheme

- Projected after Variation (PAV):
  We solve FT-BCS equation and the we calculate $< H >= Tr\{D_N H\}$
- Commonly used in the T=0 case.

Results: FT-BCS and FT-PAV Vs Exact, N=Ω=10, G=0.4d



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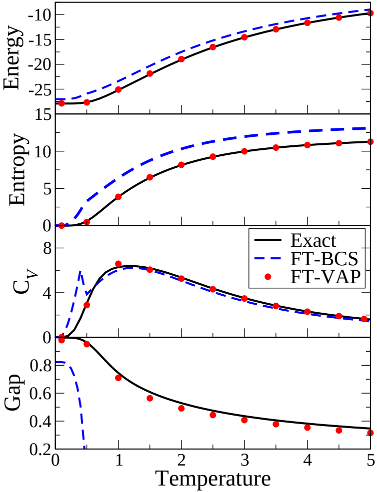
- Not easy...h and D_N **do not commute**

Variation After Projection (VAP)

- Direct (Numerical) Minimization, E_i and V_i variational parameters whose $< H >_N$ and S depend on
- We perform a full Finite-Temperature Variation After Projection (FT-VAP)
- For more details see DG and D.Lacroix, PRC 85, 044321 (2012)

Results: **FT-VAP Vs Exact**, N=Ω=10, G=0.4d



Results: **FT-VAP Vs Exact**,N=10,11 and Ω=10, G=0.4d

Odd-Even Effects

- Pairing Gaps
- Spin Susceptibility $\chi(T) = -\frac{1}{T}\left(\langle\hat{M}^2\rangle - \langle\hat{M}\rangle^2\right), \quad \hat{M} = -\mu_B \sum_{\sigma,i} \sigma a^{\dagger}_{i,\sigma} a_{i,\sigma}$

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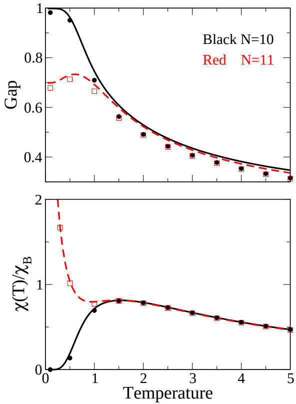

We test the FT-VAP approach in the Richardson Model

- The FT-VAP is able to reproduce low- and high-T thermodynamics properties
- It works both for odd and even systems

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Part II

Applications to atomic nuclei

Specific Heat in ^{161,162}Dy and ^{171,172}Yb

Oslo Group measurements

- Level density extracted from γ-ray spectra
- Using $(^{3}He, \alpha\gamma)$ on ^{162,163}Dy and ^{172,173}Yb targets [a]

[a] A. Schiller *et al.* PRC63,021306(R)

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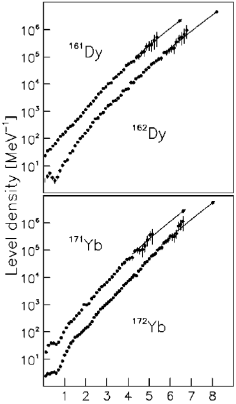

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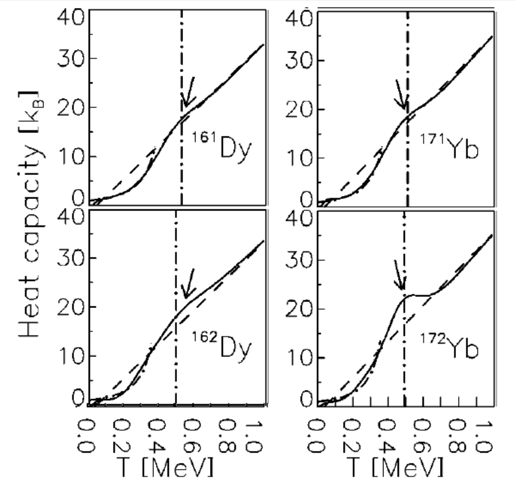
Specific Heat



Calculation Details

Basic input for CE and FT-VAP calculations

- Single particle (sp) basis form Relativistic Mean Field (RMF,PK1) and Hartee-Fock (HF,SLY4) axially deformed calculations
- Truncation in sp basis is needed, i.e. active window
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Hamiltonian and Pairing Strengths

- $$H = \sum_{q,i,\sigma} \epsilon_i^q a^\dagger_{iq,\sigma} a_{iq,\sigma} - G^q \sum_{q,i,j} a^\dagger_{iq,+} a^\dagger_{iq,-} a_{jq,-} a_{jq,+}$$

  $q = \nu$ neutron or π proton
- G^q is fixed at BCS (T=0) level to have reasonable gaps

Some Pairing properties in the Active window

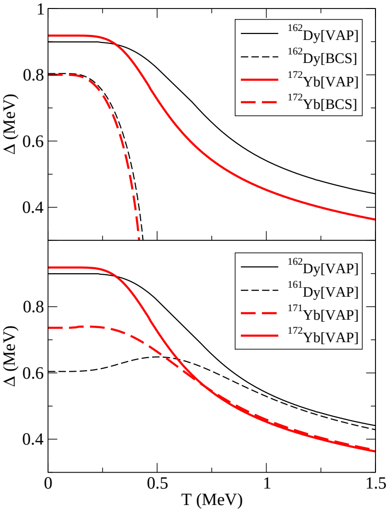
Pairing Gap properties and Condensate Fraction

- The pairing plays a role only in the active window
- Some pairing properties in the reduce space (i.e. 3 MeV around Fermi Energy)

Thermal Evolution of

- Pairing Gap
- Condensate Fraction

Neutron Pairing Gaps: VAP vs BCS and odd-even features



Condensate Fraction

Superconducting phenomena

- Cooper pairs, strongly correlated pair via the pairing interaction
- Bosonic-like properties and they can (eventually) condensate
- The quantitative description of these features is not easy

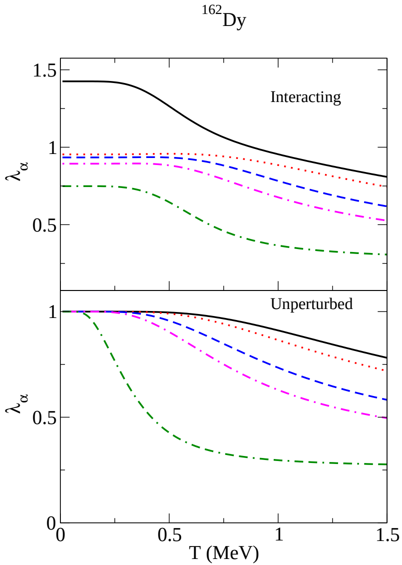
Off-diagonal long-range order (ODLRO)

- Connection with the ODLRO[a] in the density matrix ρ_n where n is the number of particles forming a condensate unit
- Appearance of eigenvalues of ρ_n much larger than the others connected to the appearance of (pseudo)-condensate
- Eigenvalues of the two-body matrix

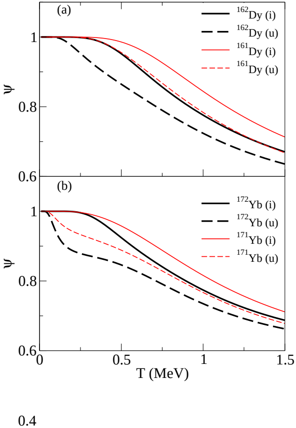
$$C_{ij} = \langle P_i^\dagger P_j \rangle_T, \quad P_i^\dagger = a_i^\dagger a_{\bar{i}}^\dagger$$

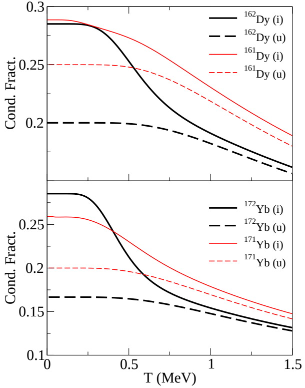
[a] C.N. Yang, Rev. Mod. Phys. 1962

Two-Body matrix eigenvalues, (five biggest ones)



Order Parameter and Condensate Fraction





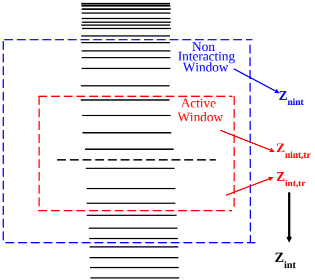
$\sum_\alpha \lambda_\alpha = \mathrm{N}_{pair} - \langle s \rangle$;
$\psi = (\mathrm{N}_{pair} - \langle s \rangle)/\mathrm{N}_{pair}$

Cond. Fract. $\lambda_{max}/\mathrm{N}_{pair}$

Full Results

Full interacting partition function

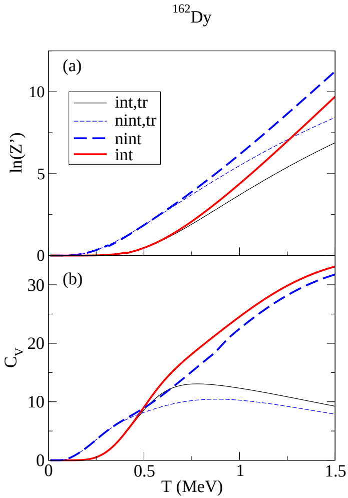
Active Window: 3 MeV around the Fermi Energy
Non Interacting Window: 7 MeV around the Fermi Energy



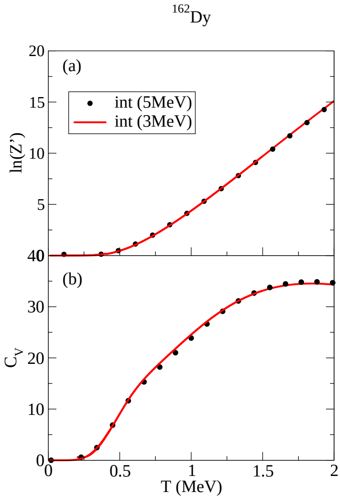
$$\ln Z_{int} = \ln Z_{int,tr} - \ln Z_{nint,tr} + \ln Z_{nint}$$

A. Alhassid *et al.* PRC68, 2003

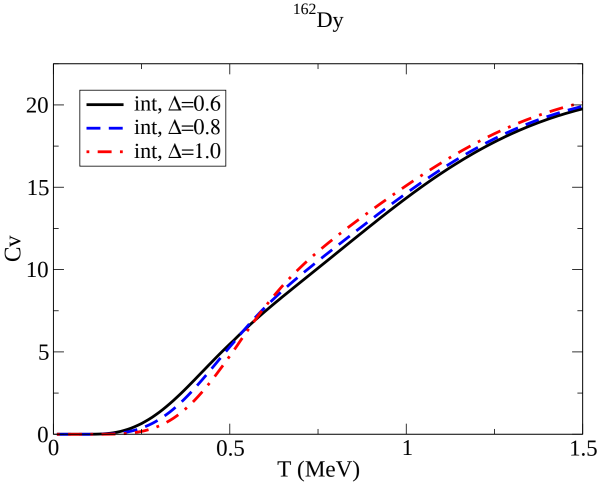
Partition Function and Specific Heat



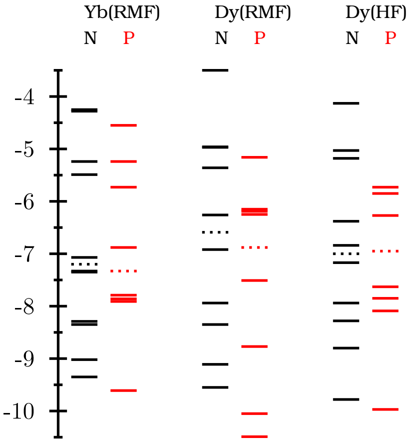
Results Stability...increasing the active window: from 3 to 5 MeV



Dependence on the pairing strength



Dependence on the mean field input



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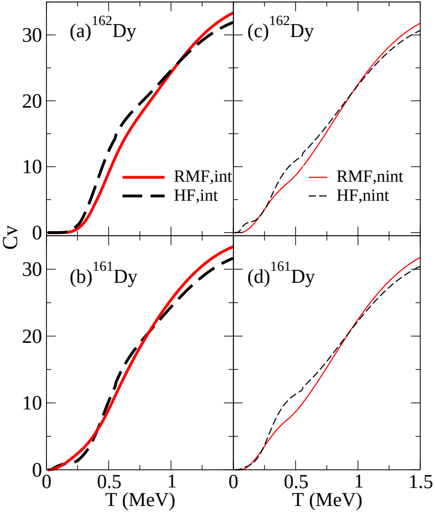
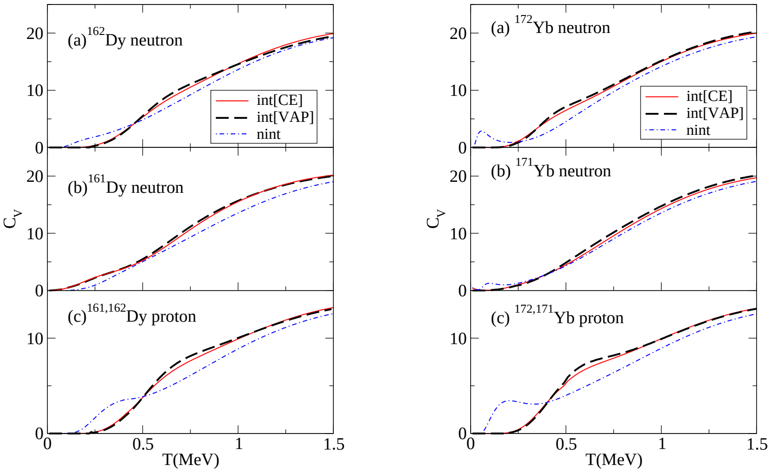
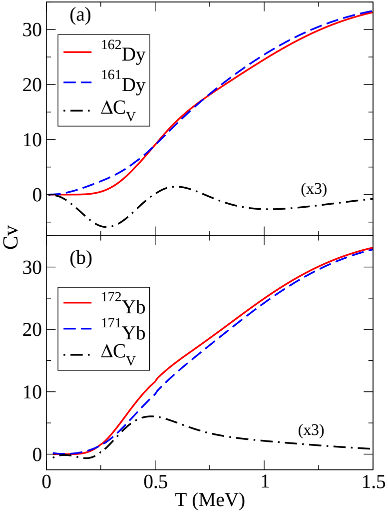


CE versus VAP description



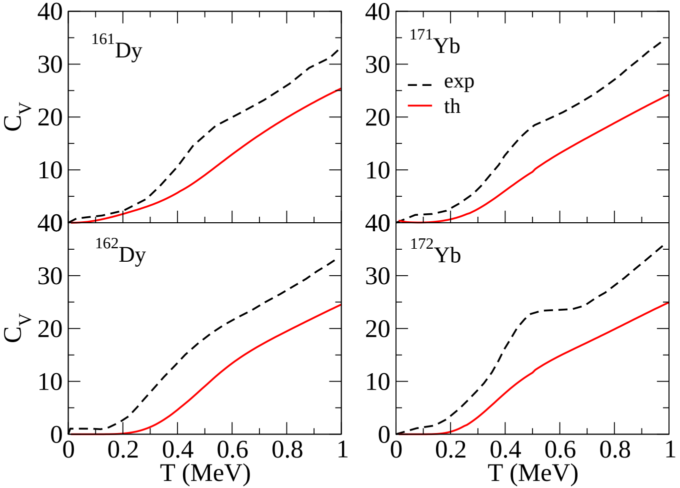
Odd-Even comparison



Part III

Comparison with experimental specific heat

Specific Heat in ^{161,162}Dy and ^{171,172}Yb



Comparison with Experimental data

(Semi)experimental Specific Heat

- Level densities (from γ-ray spectra) up to 6 MeV (odd) and 8 MeV (even) systems
- For the high energy part (up to 40 MeV) they use the Back Shifted Fermi GAS (BSFG)

$$\rho_{BSFG}(U) = f \frac{exp(2\sqrt{aU})}{12\sqrt{0.1776a}U^{\frac{3}{2}}A^{\frac{1}{3}}}$$

- $U = E - E_1, \quad E_1 = C_1 + \Delta, f$ parameter fixed to match neutron resonance

Full interacting partition function

$$ln\ Z_{int} = ln\ Z_{int,tr} - ln\ Z_{nint,tr} + ln\ Z_{nint} \Rightarrow$$

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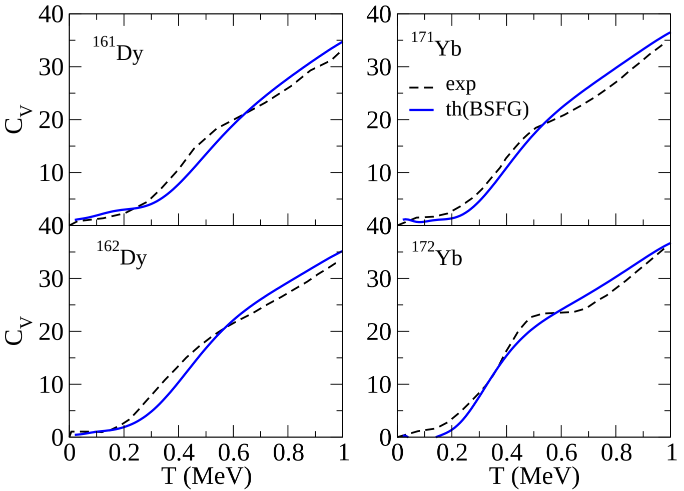

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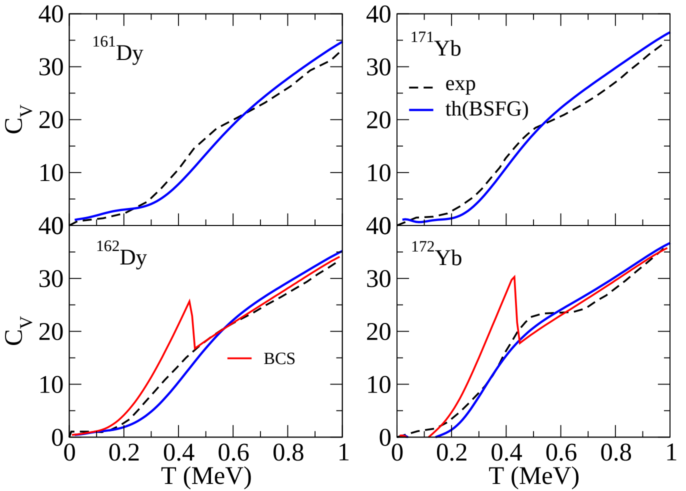


Conclusions and Outlook

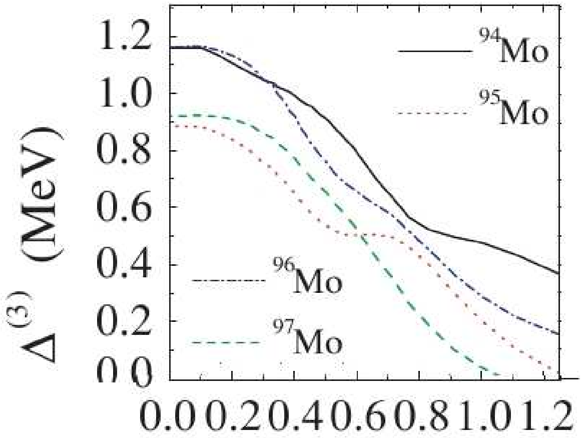
Conclusions

- Thermodynamics Pairing Properties in Finite Systems
- Both CE and FT-VAP solutions
- Thermal evolution of Pairing Gap and Condensate Fraction indicate smooth phase transition
- Specific Heat in ^{161,162}Dy and ^{171,172}Yb
- S-Shape related both to pairing interaction and s.p. states around Fermi Energy

Outlook

- Phenomenological Single Particle basis (i.e. Wood-Saxon)
- More general Hamiltonian (quadrupole part,..)
- Including continuum coupling (Exotic Systems)
- From a Canonical to the Microcanonical description

Experimental GAP in Mo isotopes



K. kaneko et al., PRC 74, 024325

Odd-Even Entropy Effects

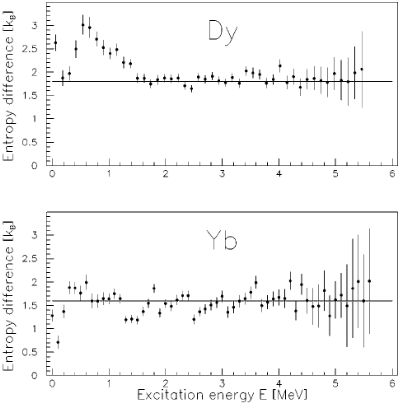
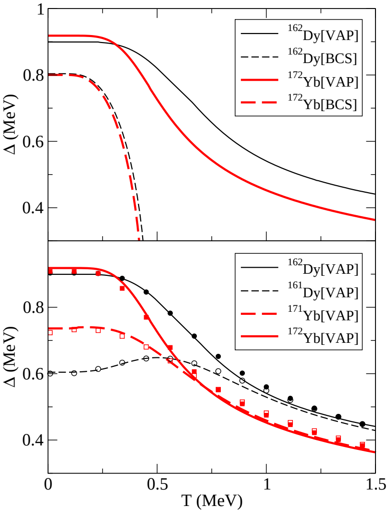


FIG. 9. Entropy difference in ^{161}Dy compared to ^{162}Dy (upper panel) and in ^{171}Yb compared to ^{172}Yb (lower panel). The lines through the data points indicate the average values found.

M Guttormsen et al., PRC 62, 024306

Pairing Gaps: VAP vs BCS and odd-even features



The Entropy...

The calculation of the Entropy is the most difficult task..

- We need the eigenvalues of D^N in the many-body Fock space with N particles
- Each state is characterized by η pairs and I unpaired particles, such as $2\eta + I = N$
- diagonalization of block matrices for each allowed seniority I

Required computational cost

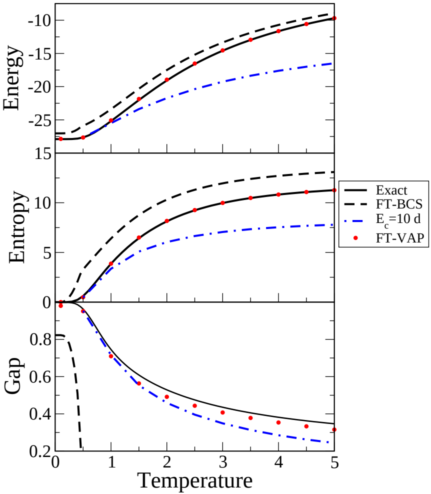
- 1) calculation of the matrix elements (ME) of D^N
  bit representation of the states, ME are obtained by using logical operations (much faster)
- 2) diagonalization
  standard QR algorithm is used

The Entropy...A more direct and simple approach

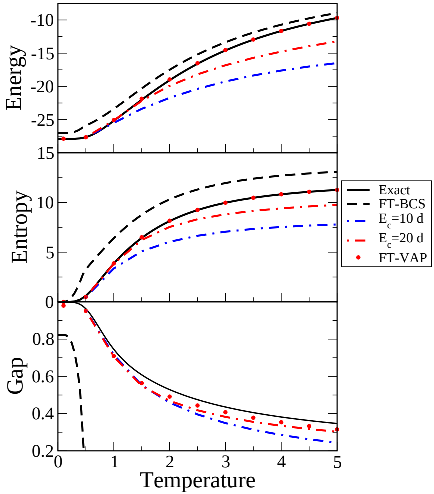
The calculation of the Entropy is the most difficult task..

- We need the eigenvalues of D_N in the many-body Fock space with N particles $|N, i\rangle$
- $\langle N, i|e^{-\beta h}|N, j\rangle$
- High energy configurations are expected to be less important
- We consider only the states $|N, i\rangle$ whose energy is less than E_c
- We increase E_c to study the reliability of the solution

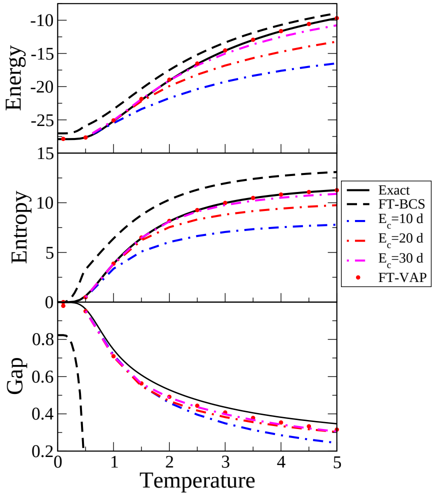
N=Ω=10, G=0.4d


Energy
-10
-15
-20
-25
Entropy
15
10
5
0
Gap
0.8
0.6
0.4
0.2
0
1
2
3
4
5
Temperature
Exact
FT-BCS
E_c=10 d
FT-VAP

N=Ω=10, G=0.4d

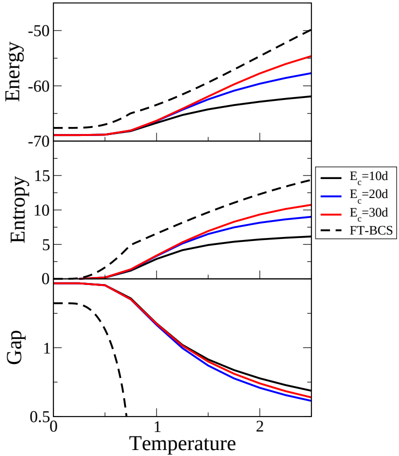

Energy
-10
-15
-20
-25
Entropy
15
10
5
0
Gap
0.8
0.6
0.4
0.2
0
1
2
3
4
5
Temperature
Exact
FT-BCS
E_c=10 d
E_c=20 d
FT-VAP

$N=\Omega=10$, $G=0.4d$



Applications to the Pairing Model (Richardson),

N=Ω=16, G=0.4d



No Exact Solution