

# Reentrance in nuclei

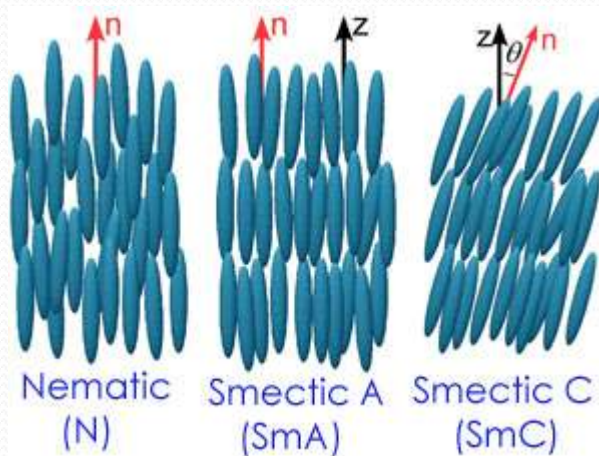
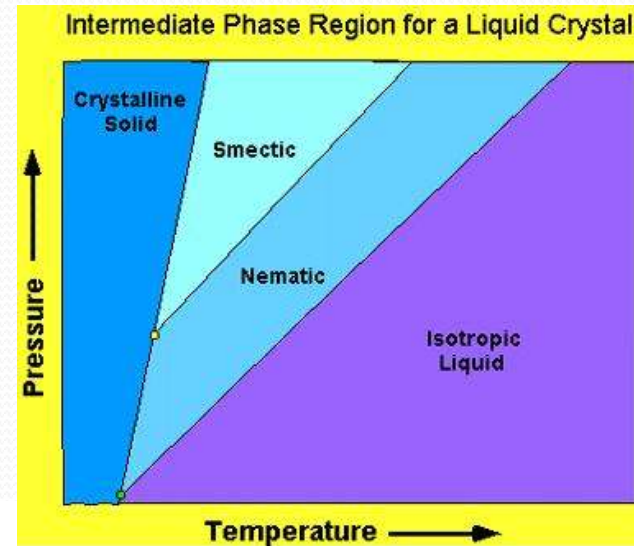
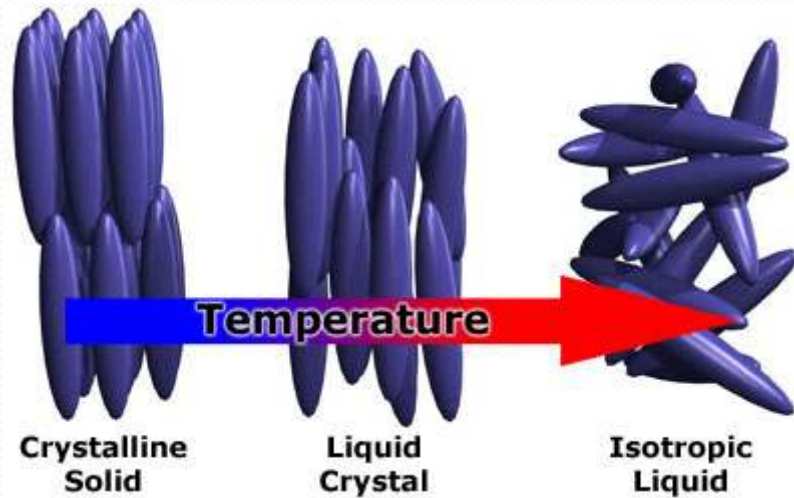
Competitive phenomena

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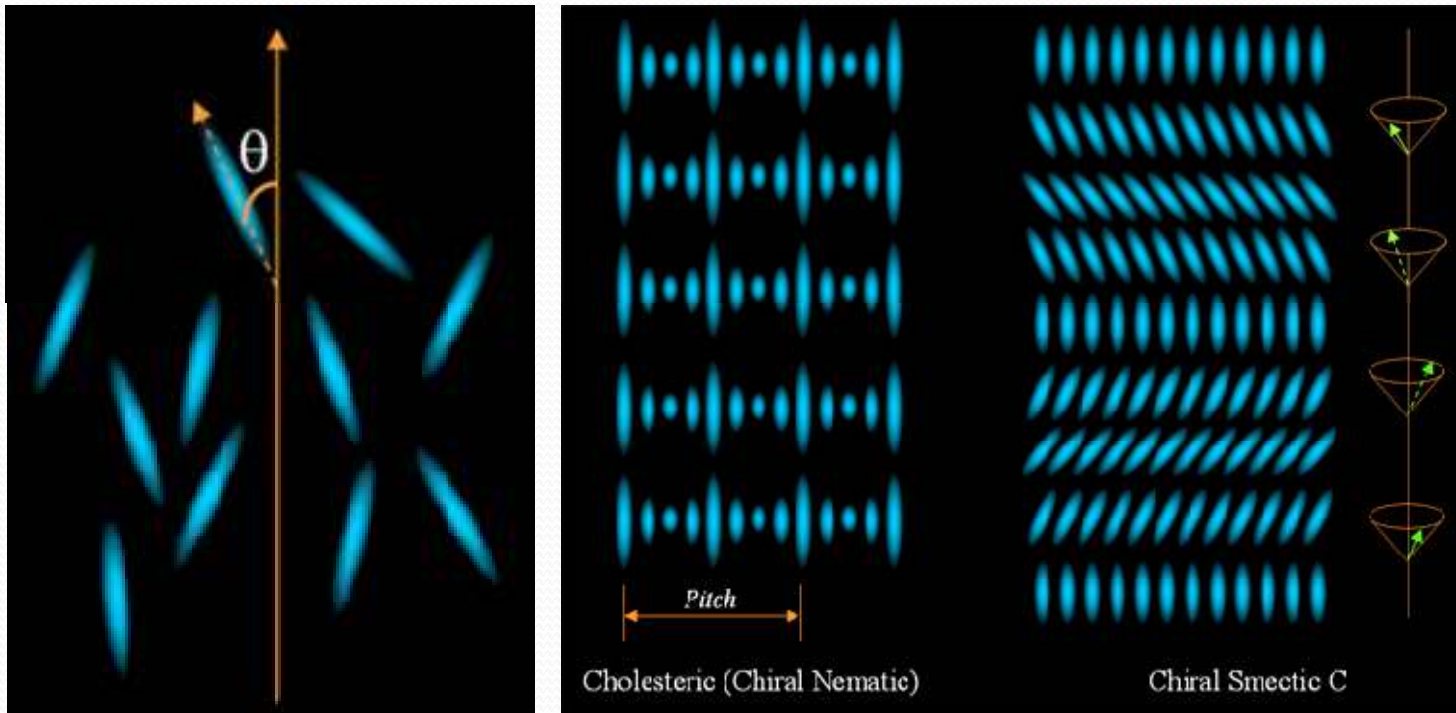
# Outline

- A brief survey of *reentrance*
- Nuclear “phases” (this is not Italy)
- The competition between deformation and temperature
- The competition between rotation, deformation and temperature
- A few words on simulations and computing mixed in

# Liquid Crystal Phases



# Liquid crystal alignment



$$S = \langle P_2(\cos \theta) \rangle = \left\langle \frac{3 \cos^2 \theta - 1}{2} \right\rangle$$

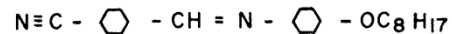
# “Re-entrance” discovered for liquid crystals

## New Liquid-Crystal Phase Diagram

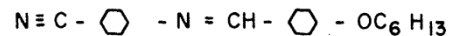
P. E. Cladis

*Bell Laboratories, Murray Hill, New Jersey*

(Received 7 April 1975)



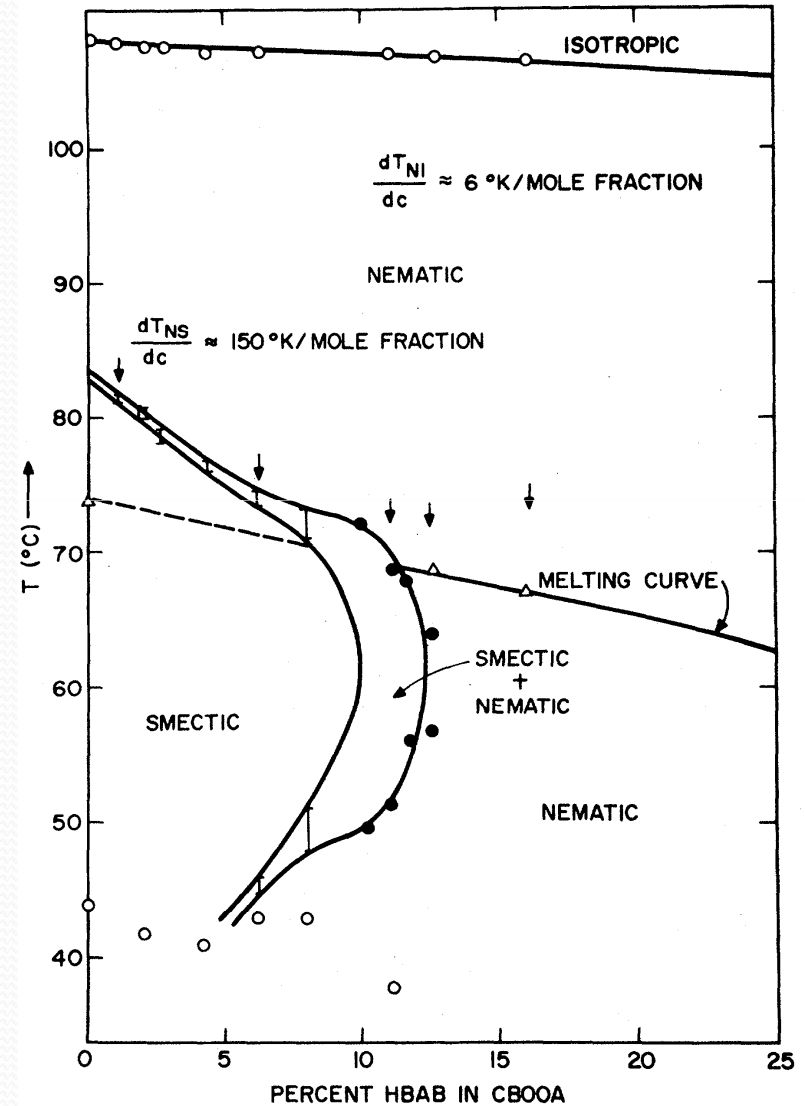
N - p - cyanobenzylidene - p - n - octyloxyaniline



p - [(p - hexyloxybenzylidene) - amino] benzonitrile

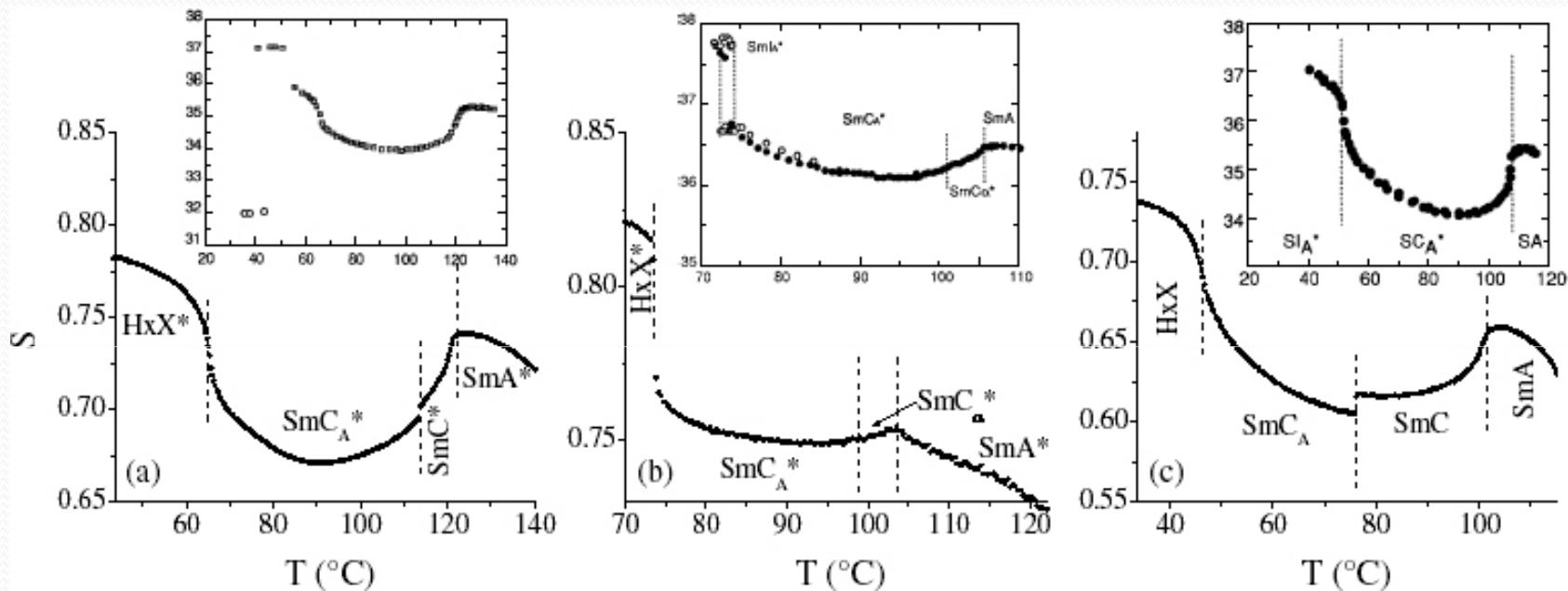
FIG. 1. CBOOA (top) and HBAB.

“By mixing HBAB in CBOOA, I have found that a smectic phase may be formed which reverts to the nematic phase at still lower temperatures. As far as I can ascertain, this is the first time such an effect has been observed.”

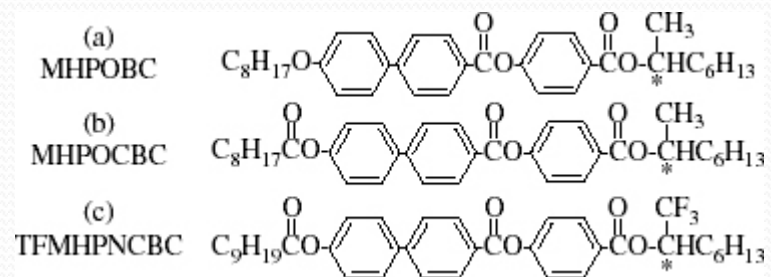


PRL 35, 48 (1975)

# Liquid crystal phases

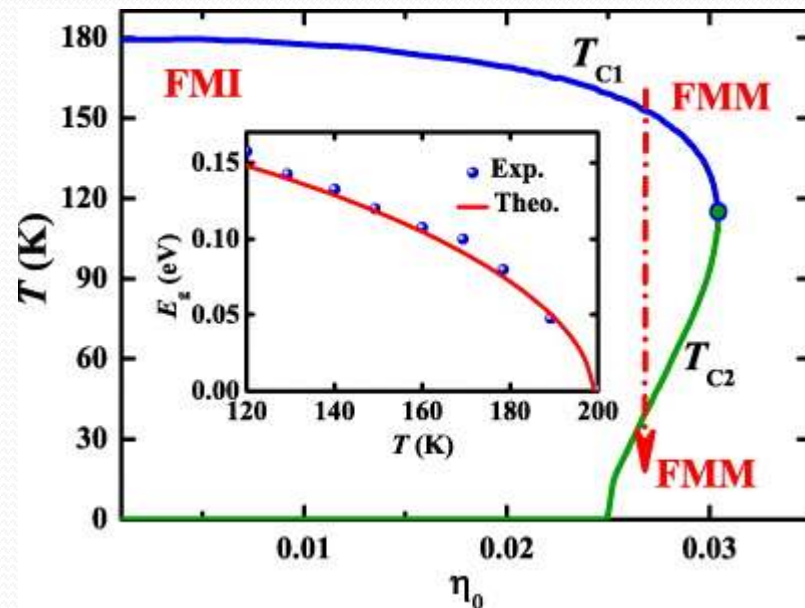


R. Korlacki et al., 2007 *EPL* 77 36004



# Quantum phase reentrance

Ferromagnetic Insulator



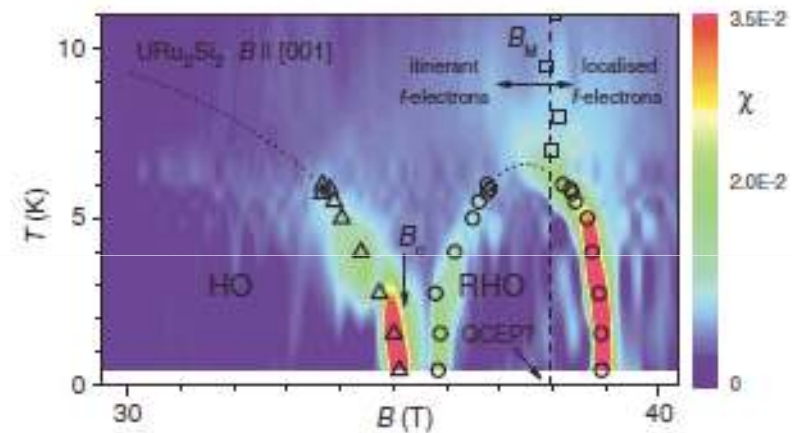
**Figure 2.** Two critical temperatures of metal–insulator transitions ( $T_{c1}$  and  $T_{c2}$ ) as a function of interchain coupling strength  $\eta_0$ . The large dots are the coincident points of  $T_{c1}$  and  $T_{c2}$ . The re-entrance of the ferromagnetic metal state is shown by the big arrow.

Wei et al., N. J. Phys. 12, 053201 (2010)

FMM=Ferromagnetic metal state

FMI=Ferromagnetic insulator state

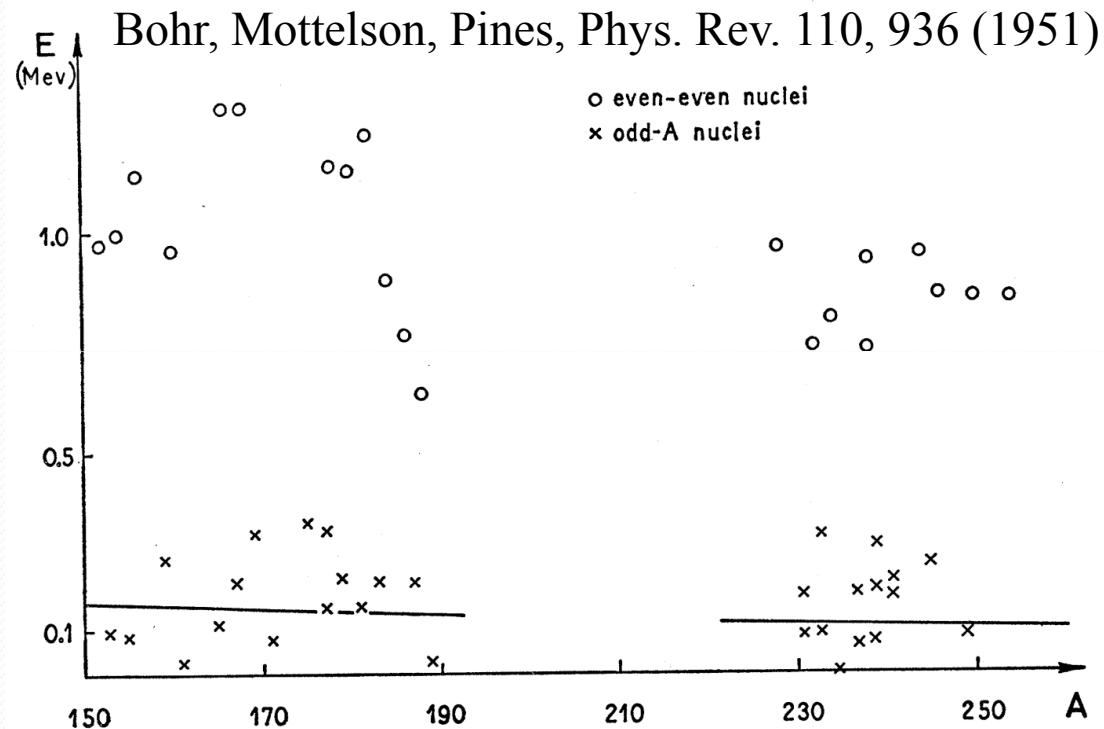
Hidden Order States –  
orbital antiferromagnetism



**FIG. 1 (color).** The  $B > 30$  T versus  $T$  phase diagram of  $URu_2Si_2$  combined with a color intensity plot of  $\chi$  measured at many different temperatures. Square, triangle, and circle symbols mark  $B_M$  and transitions into and out of the HO and RHO hidden order (RHO) phases, respectively. The curved dotted lines depict the continuation of the phase boundaries revealed by specific heat and transport studies [4].

Harrison et al., PRL 90 96402 (2003)

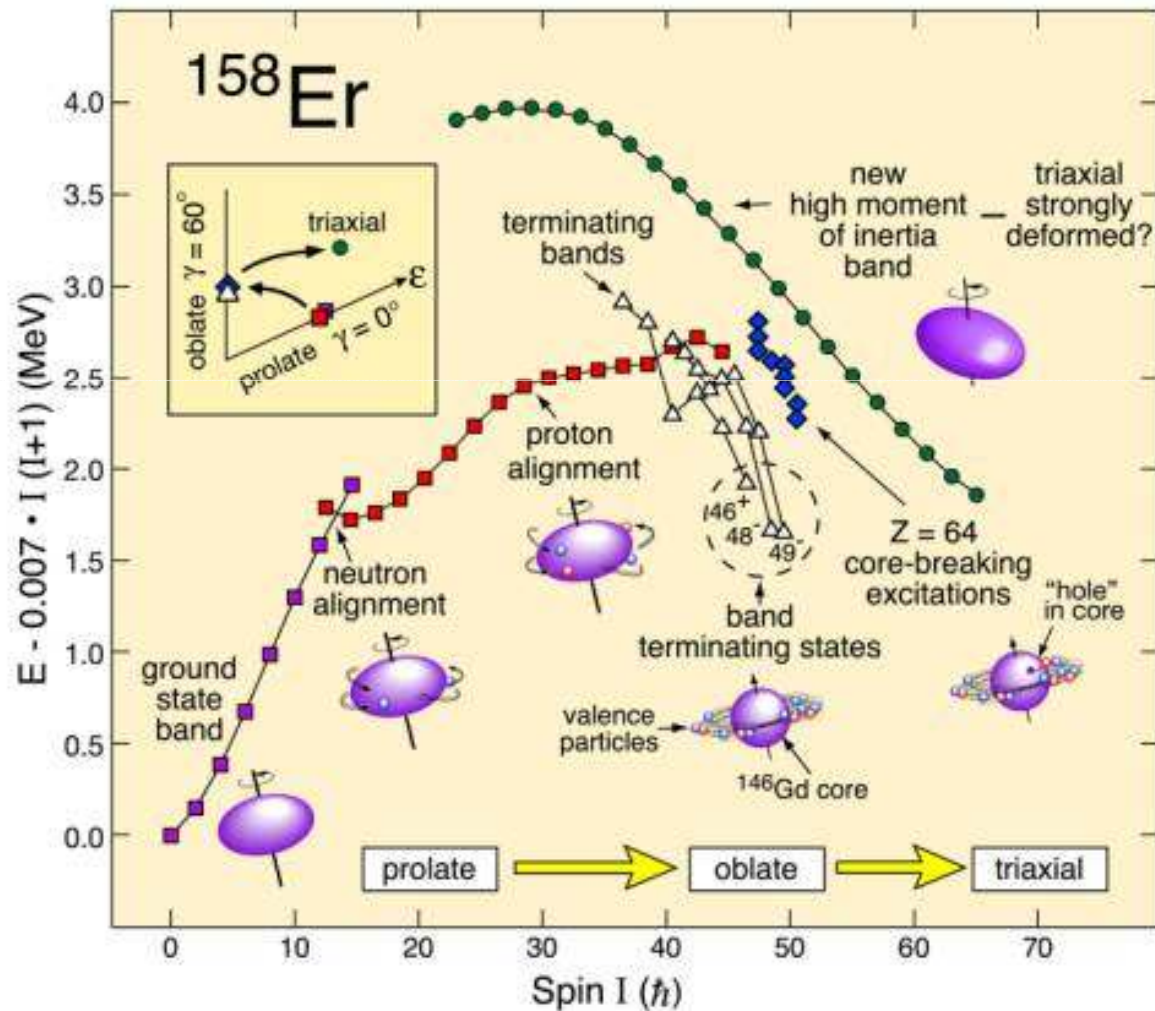
# Nuclear Pairing: one phase of nuclei



- Pairing effects cause the gap
- Collective behavior and emergent phenomena
- Points to superconductivity



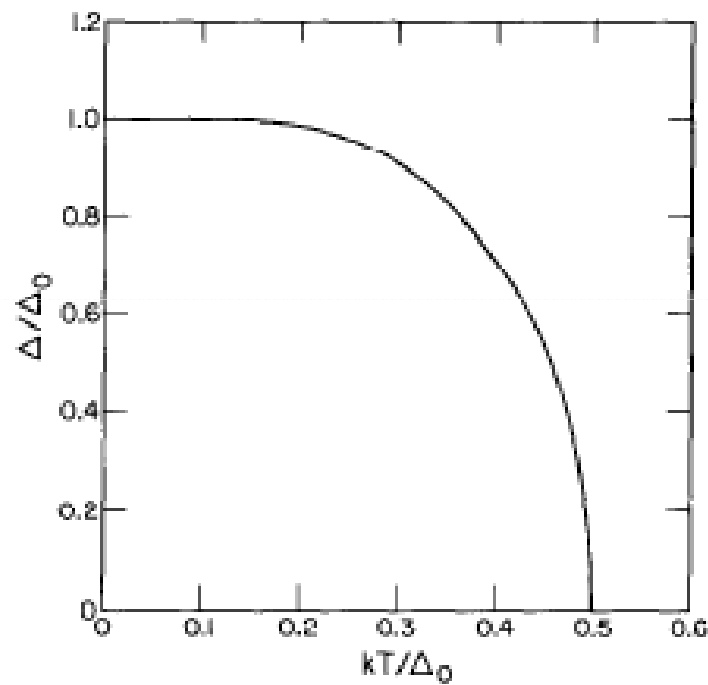
# Nuclear Deformation: collective behavior phases



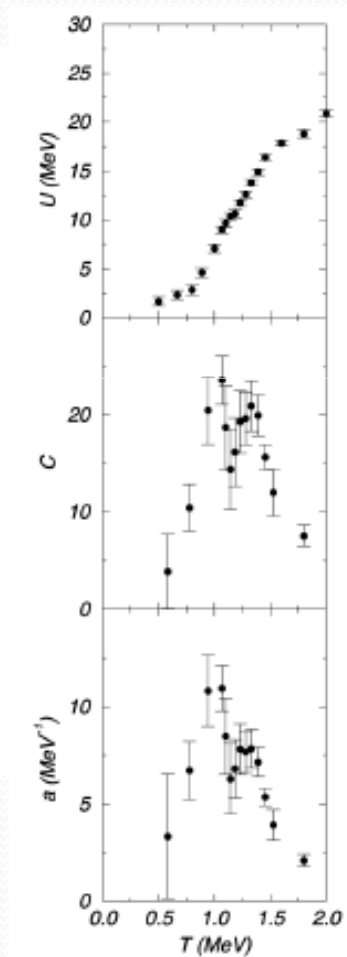
# Pairs can be thermally broken

Goodman, NPA 352, 30 (1981)

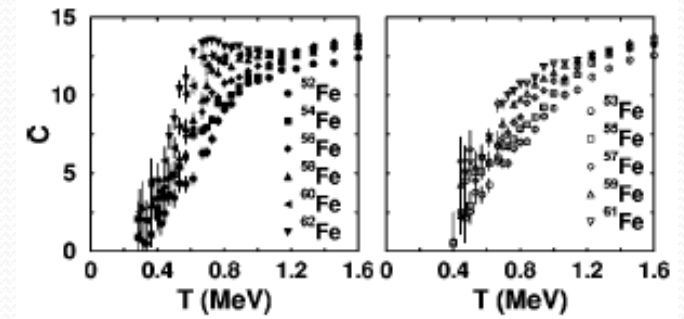
FT-HFB



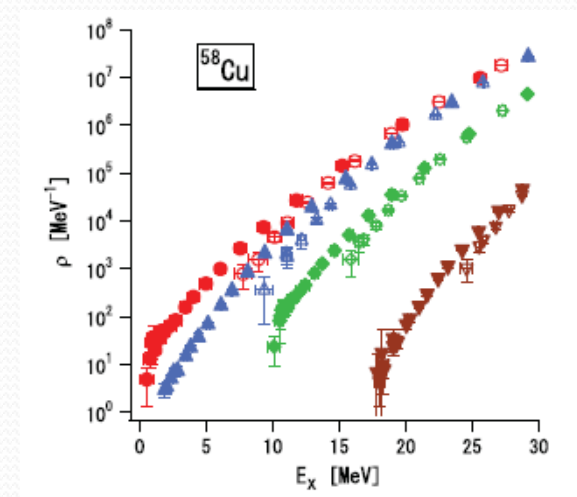
Thermal transition to unpaired state occurs around 0.5-1.0 MeV



Dean et al., PRL 1994



Liu, Alhassid, PRL 2001



Nakada, Alhassid, PRC, 2008

# Early work on thermally assisted pairing

Tamura, Prog. Theor. Phys. 31, 595 (1964)

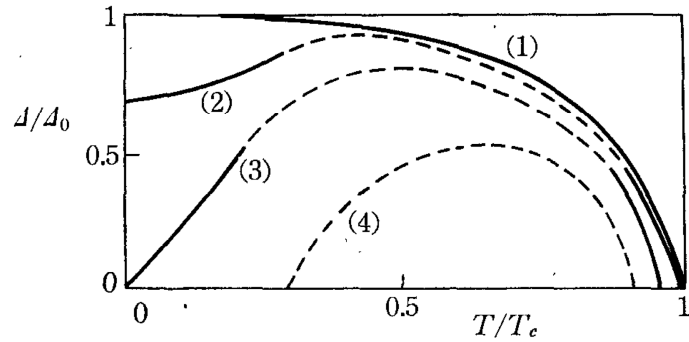


Fig. 2. Ratio of the energy gap to the gap at  $T=0$  vs temperature for various values of spin projection  $M$ : (1)  $M=0$ , (2)  $M=m$ , (3)  $M=2m$ , (4) schematic plot for some higher  $M$ .

$$H = \sum_{s, \rho} (e_s - \lambda) a_{s\rho}^* a_{s\rho} - G \sum_{s, s'} a_{s-}^* a_{s+}^* a_{s'+} a_{s'-} - \omega J_z$$

Exact model shows a pairing-deformation relation  
 Sheikh et al, PRC 72, 041301 (2005)

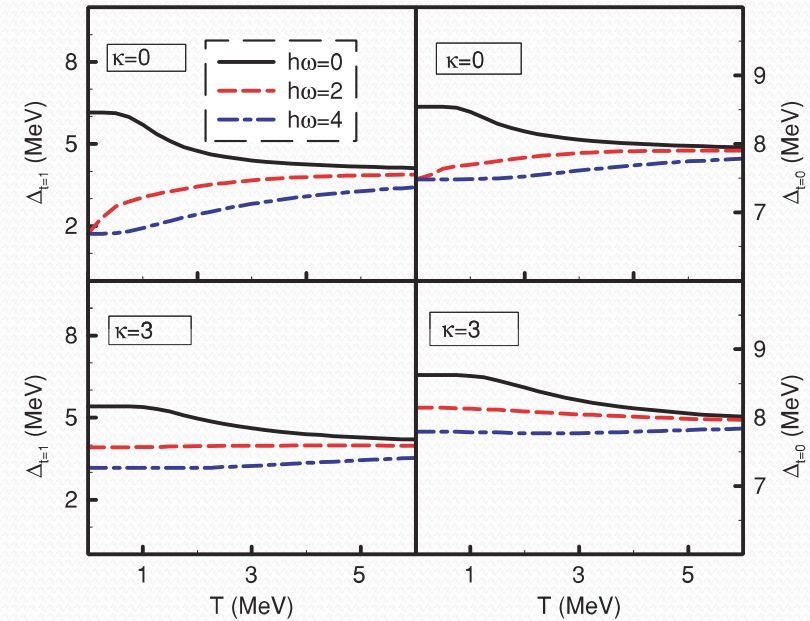


FIG. 2. (Color online) Results of the total isovector ( $\Delta_{T=1}$ ) and isoscalar ( $\Delta_{T=0}$ ) pair gaps are plotted as a function of temperature for three different rotational frequencies of  $\hbar\omega = 0, 2,$  and  $4$  MeV. The upper panel shown the results for  $\kappa = 0$  and the lower panel depicts the results for  $\kappa = 3$  MeV.

# Hamiltonian for this work

- Pairing+Quadrupole Hamiltonian

$$H = \sum_{j m_t z} e(j) a_{j m_t z}^+ a_{j m_t z} - \frac{G}{4} \sum_{\alpha \alpha' t_z} P_{JT=01, t_z}^+(\alpha) P_{JT=01, t_z}(\alpha') - \chi \sum_{\mu} (-1)^{\mu} Q_{2\mu} Q_{2-\mu}$$

0g<sub>7/2</sub>-1d-2s  
0f-1p-0g<sub>9/2</sub>

- Solve using Auxiliary Field Monte Carlo techniques

- Parameters:

One-body from  
W-S for <sup>56</sup>Ni

$$e_{0 f_{7/2}} = 0.000 \quad e_{0 f_{5/2}} = 6.42$$

$$e_{1 p_{3/2}} = 4.350 \quad e_{1 p_{1/2}} = 6.54$$

$$e_{0 g_{9/2}} = 8.980 \quad e_{0 g_{7/2}} = 17.59$$

$$e_{2 d_{5/2}} = 12.95 \quad e_{2 d_{3/2}} = 15.99$$

$$e_{2 s_{1/2}} = 14.64$$

$$\chi = 0.0104 \text{ MeV}^{-1}$$

$$G = 0.106 \text{ MeV}$$

Reproduces collective  
Spectrum in <sup>64</sup>Ni and <sup>64</sup>Ge

For rotations:

$$H^{\omega} = H - \omega J_z$$

Langanke, Dean, Nazarewicz, NPA757, 360 (2005);  
Dean, Langanke, Nam, Nazarewicz, PRL105, 212504 (2010)

# Shell Model Monte Carlo Essentials

$$\hat{H} = \varepsilon \hat{\Omega} + \frac{V}{2} \hat{\Omega}^2$$

$$Z = \text{Tr}[\exp(-\beta \hat{H})] \quad \rightarrow \quad \langle \hat{H} \rangle = \frac{\text{Tr}[\exp(-\beta \hat{H}) \hat{H}]}{Z}$$

$$\exp(-\beta \hat{H}) = \sqrt{\frac{\beta |V|}{2\pi}} \int_{-\infty}^{\infty} d\sigma \exp(-\beta |V| \sigma^2 / 2) \exp(-\beta \hat{h})$$

$$\hat{h} = \varepsilon \hat{\Omega} + sV \sigma \hat{\Omega}$$

$$s = 1 \quad \text{for} \quad V < 0$$

$$s = i \quad \text{for} \quad V > 0$$

Koonin et al., Phys. Repts. 287, 1 (1997)

# SMMC for a general interaction

$$\hat{H} = \sum_{\alpha} \left( \varepsilon_{\alpha} \hat{\Omega}_{\alpha} + \frac{V_{\alpha}}{2} \hat{\Omega}_{\alpha}^2 \right)$$

$$Z = \text{Tr}[\exp(-\beta\hat{H})] \rightarrow \text{Tr}[\exp(-\Delta\beta\hat{H})]^{N_t} \rightarrow$$
$$\int D[\sigma] G(\sigma) \text{Tr} \left\{ \prod_{n=1}^{N_t} \exp[-\Delta\beta\hat{h}(\sigma_n)] \right\} = \int D[\sigma] W(\sigma) \Phi(\sigma)$$

$$W(\sigma) = G(\sigma) |\text{Tr}[\ ]| \quad \Phi(\sigma) = \frac{\text{Tr}[\ ]}{|\text{Tr}[\ ]|}$$

Particle number projection

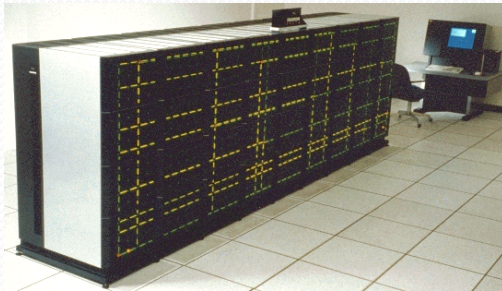
$$\text{Tr}[\hat{\Omega}] \equiv \text{Tr}_N[\hat{\Omega}] = \sum_i \langle i | \hat{P}_N \hat{\Omega} | i \rangle$$

$$\hat{P}_N = \delta(\hat{N} - N) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \exp\{i\varphi(\hat{N} - N)\}$$

Thermal operator expectation

$$\langle \hat{\Lambda} \rangle = \frac{\text{Tr}[\exp(-\beta\hat{H}) \hat{\Lambda}]}{\text{Tr}[\exp(-\beta\hat{H})]}$$

# Simulations in science (Nortur2011 talk)



Intel Touchstone Delta  
 512 nodes  
 10 Gflops peak; 8 Gbytes total memory

1992-1995



ORNL Jaguar, Cray XT5  
 224,500 cores  
 2.3 Pflops peak; 289 Tbytes total memory

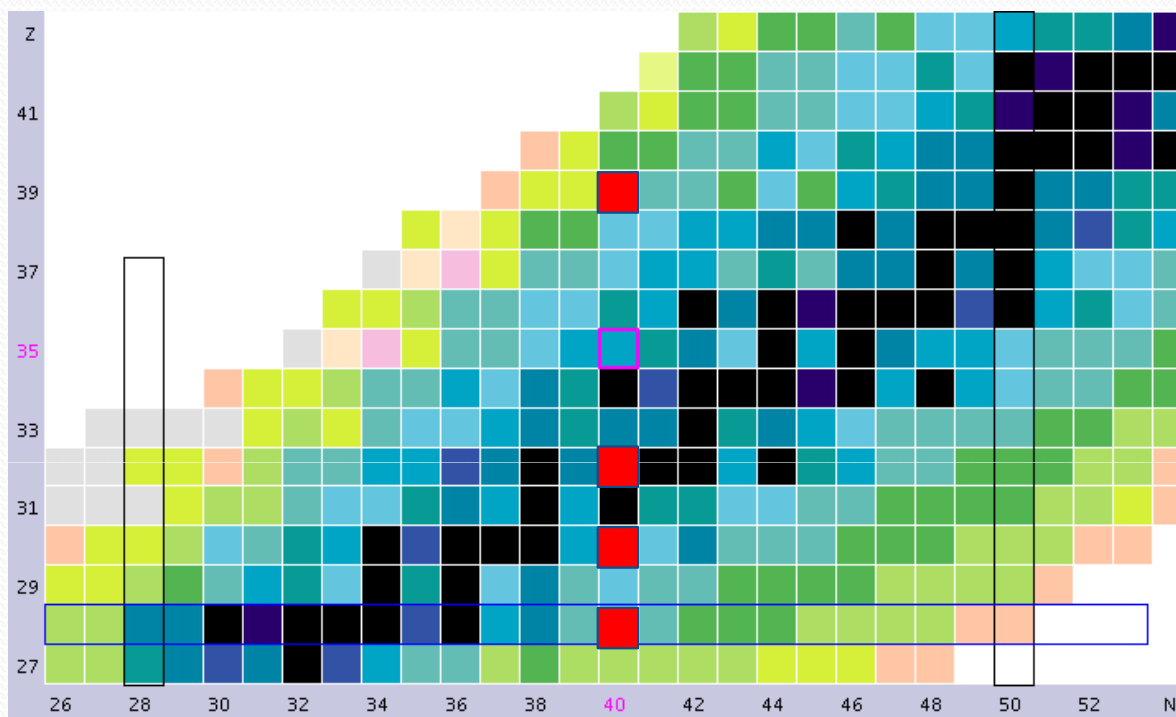
2011

- Flops are free
- Memory onto the chip (3-d)
- More cores/chip
- Exascale science by end of the decade

<b>ELECTRICITY</b>	<b>Today</b>	<b>Tomorrow (exa)</b>
Electricity Cost	\$0.1/kW-hr	\$0.1/kW-hr
Requirement	7MW	21MW
Cost/hour	\$700/hour	\$2100/hour
Cost/year	\$5.6M	\$16.8M

Power is a new constraint

## Nuclei in the fp-gds region

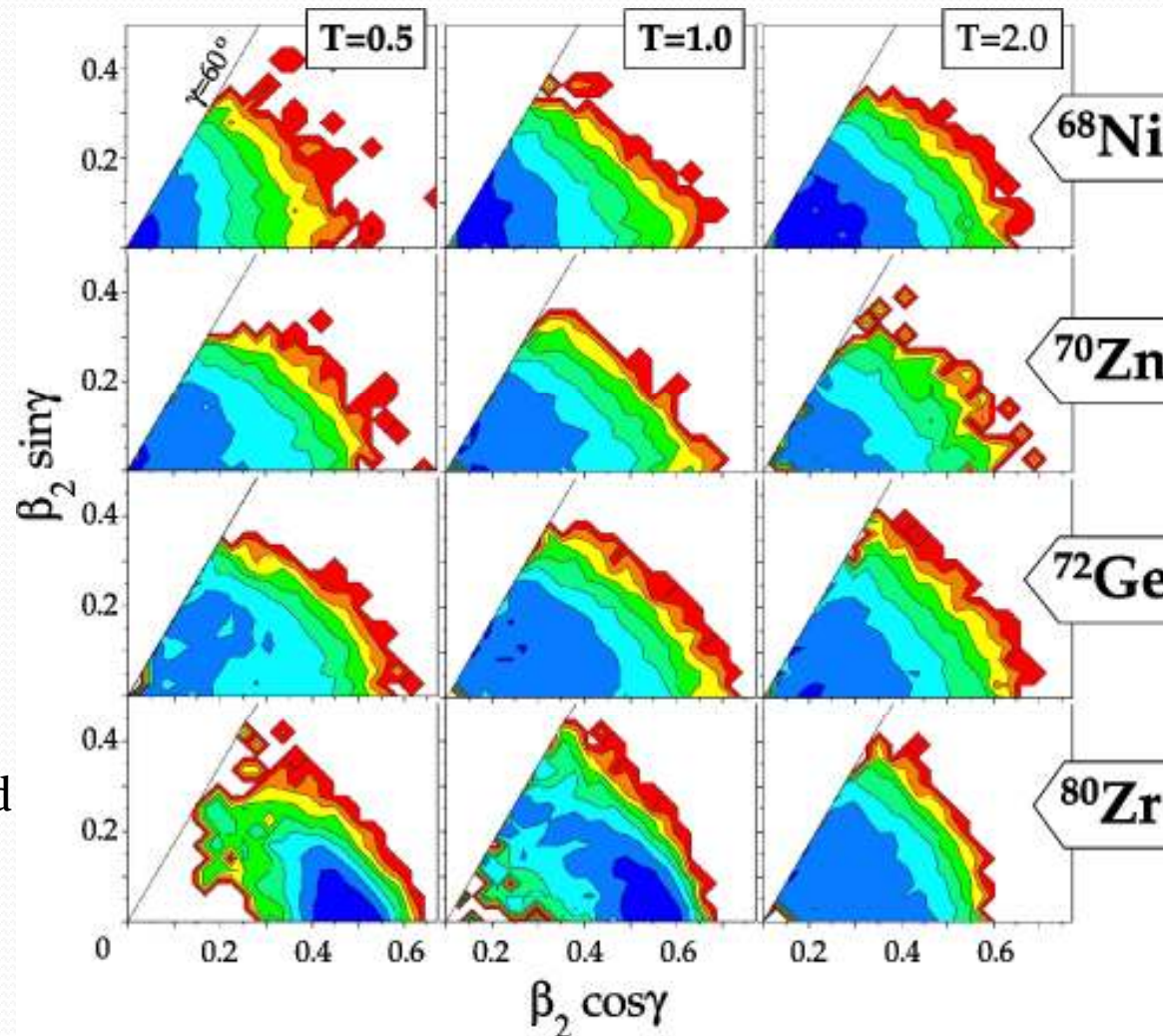


- $^{68}\text{Ni}$  Spherical ground state; weak  $N=40$  shell closure
- $^{70}\text{Zn}$  Stronger proton pairing correlations;  
Some quadrupole collectivity; erosion of  $N=40$  shell gap
- $^{72}\text{Ge}$  Shape coexistence phenomena; static proton and neutron pairing
- $^{80}\text{Zr}$  Very deformed; large  $N=40$  shell effects, weakened pairing



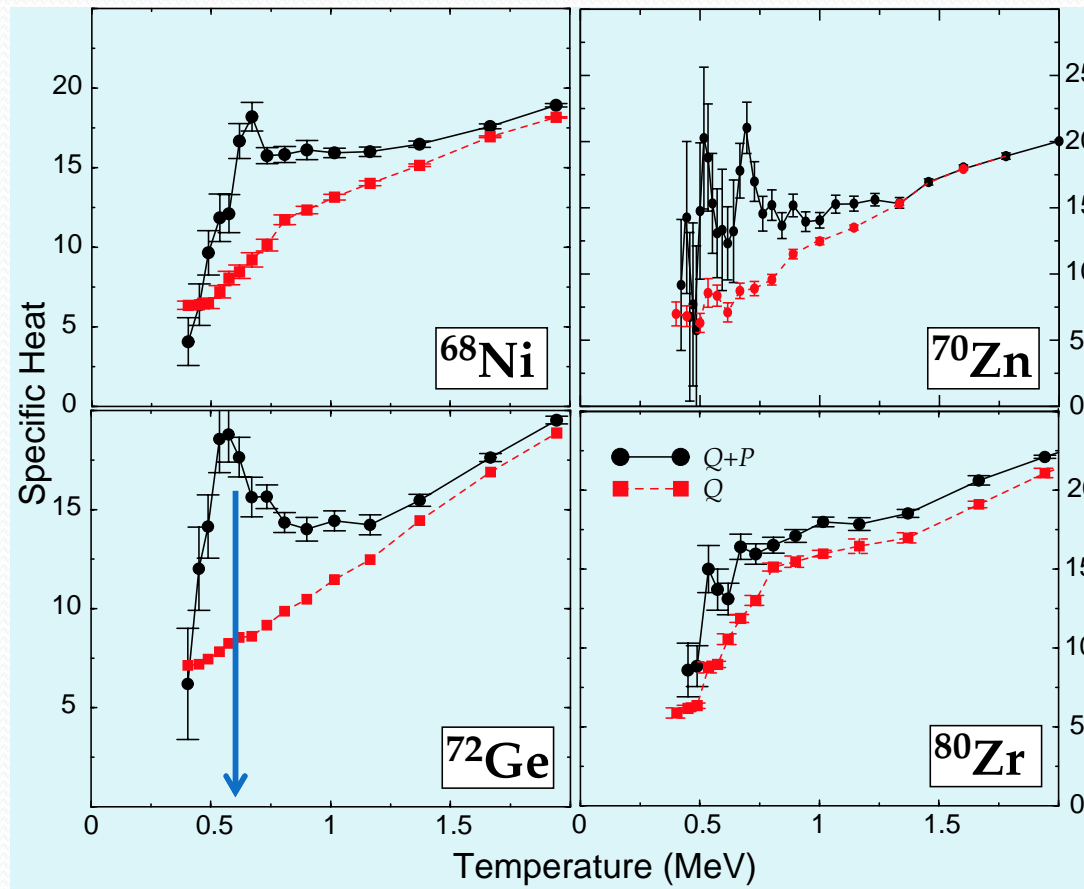
# Calculated free energy surfaces

Spherical



Deformed

# Pairing, deformation and the specific heat



$T_c \sim 0.6 \text{ MeV}$

Red: quadrupole only

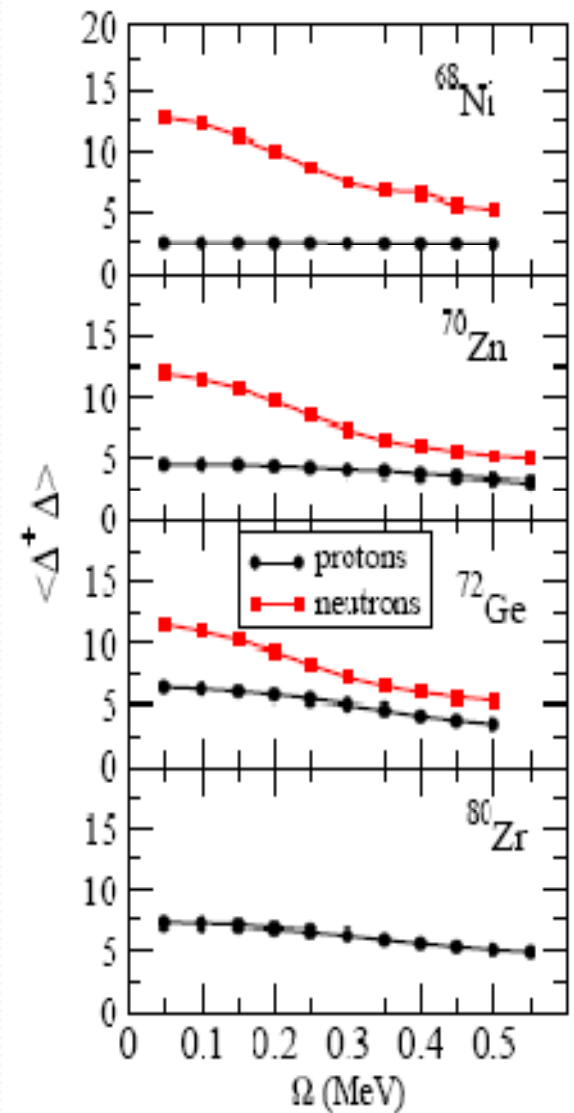
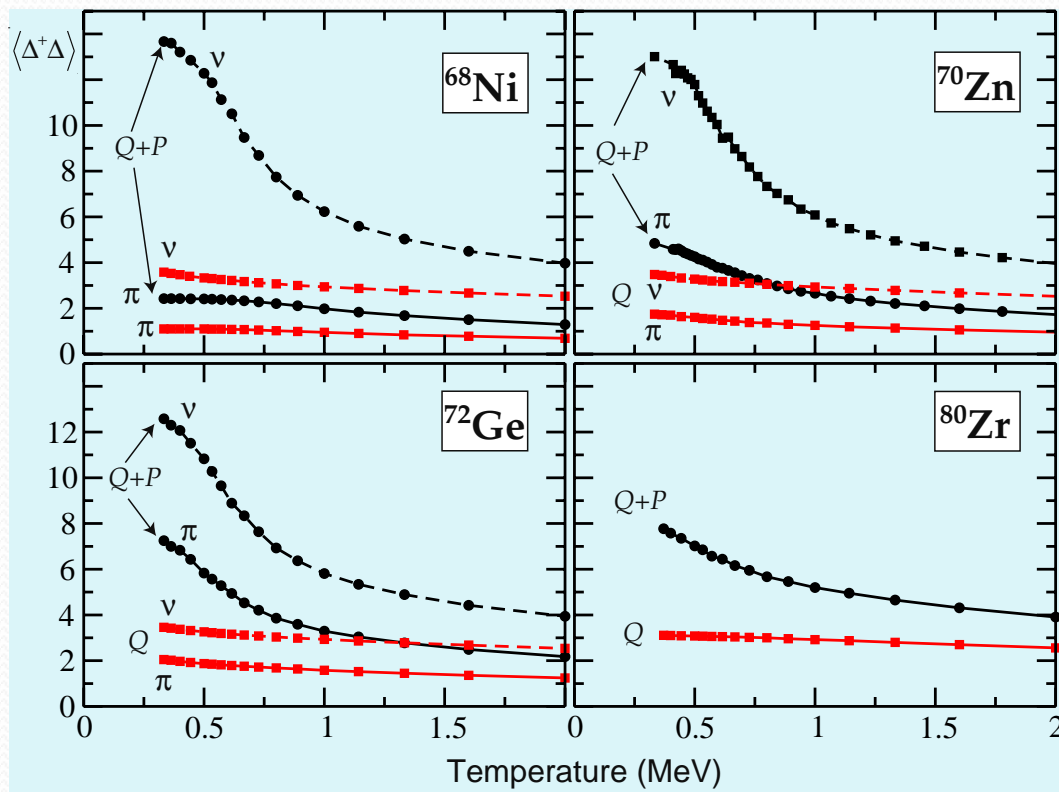
Black: pairing+quadrupole

$$E(\beta) = \frac{\text{Tr}[\exp(-\beta H)H]}{\text{Tr}[\exp(-\beta H)]}$$

$$C_v = -\beta^2 \frac{dE}{d\beta}$$

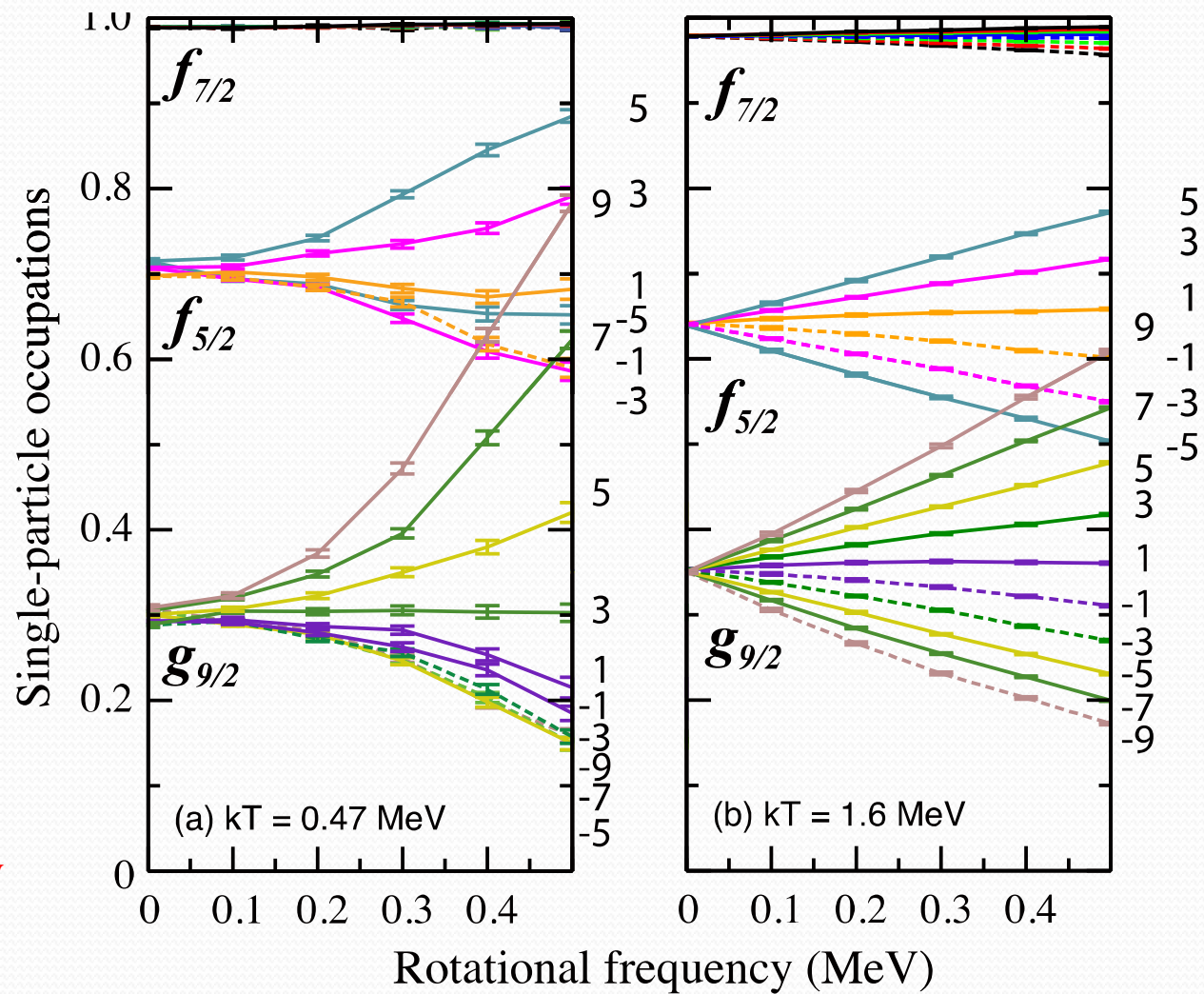
# How does rotation affect pairing?

No rotation – thermal effect only



Rotation low-temp

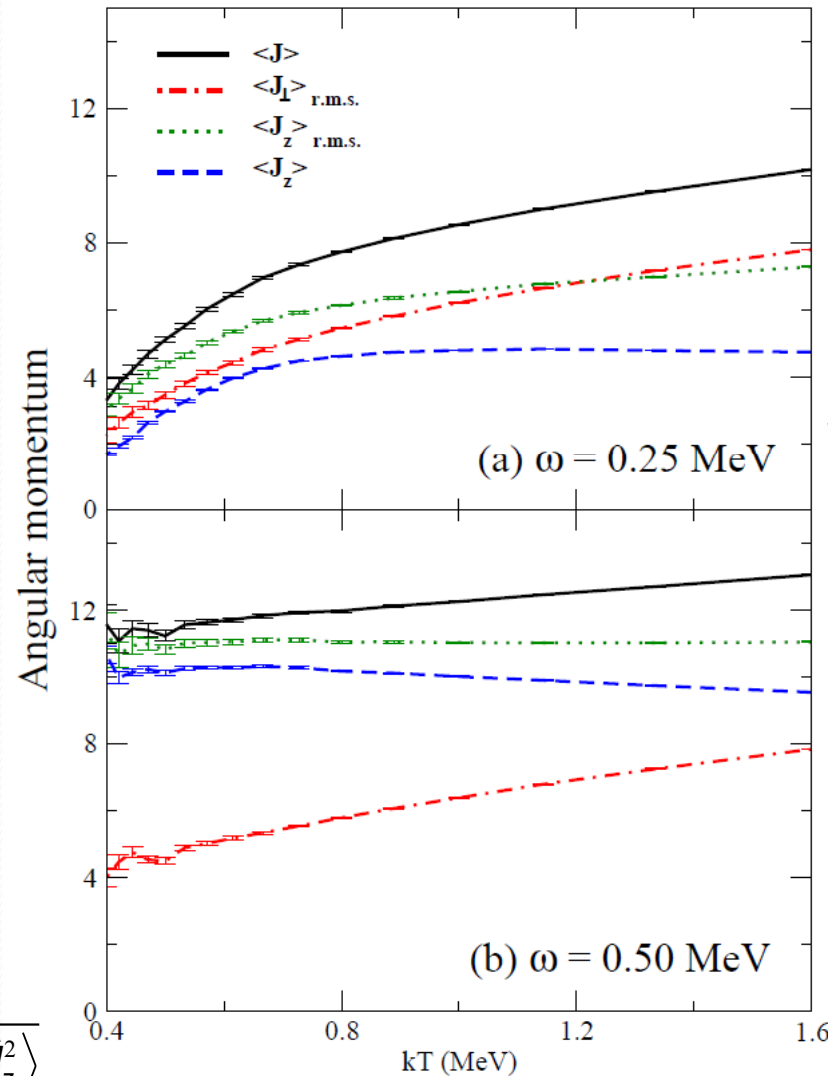
# $^{72}\text{Ge}$ occupations with rotation



Below  
 $T_c$

Above  
 $T_c$

# Temperature and rotation



At low  $\omega$ ,  $\langle J \rangle$  increase due to increased thermal fluctuations both parallel and perpendicular to rotation

$$\langle J_z \rangle \approx 4.5\hbar$$

At high  $\omega$ ,  $\langle J \rangle$  increase due to increased quantum fluctuations perpendicular to rotation

$$\langle J_z \rangle = 2.5\hbar$$

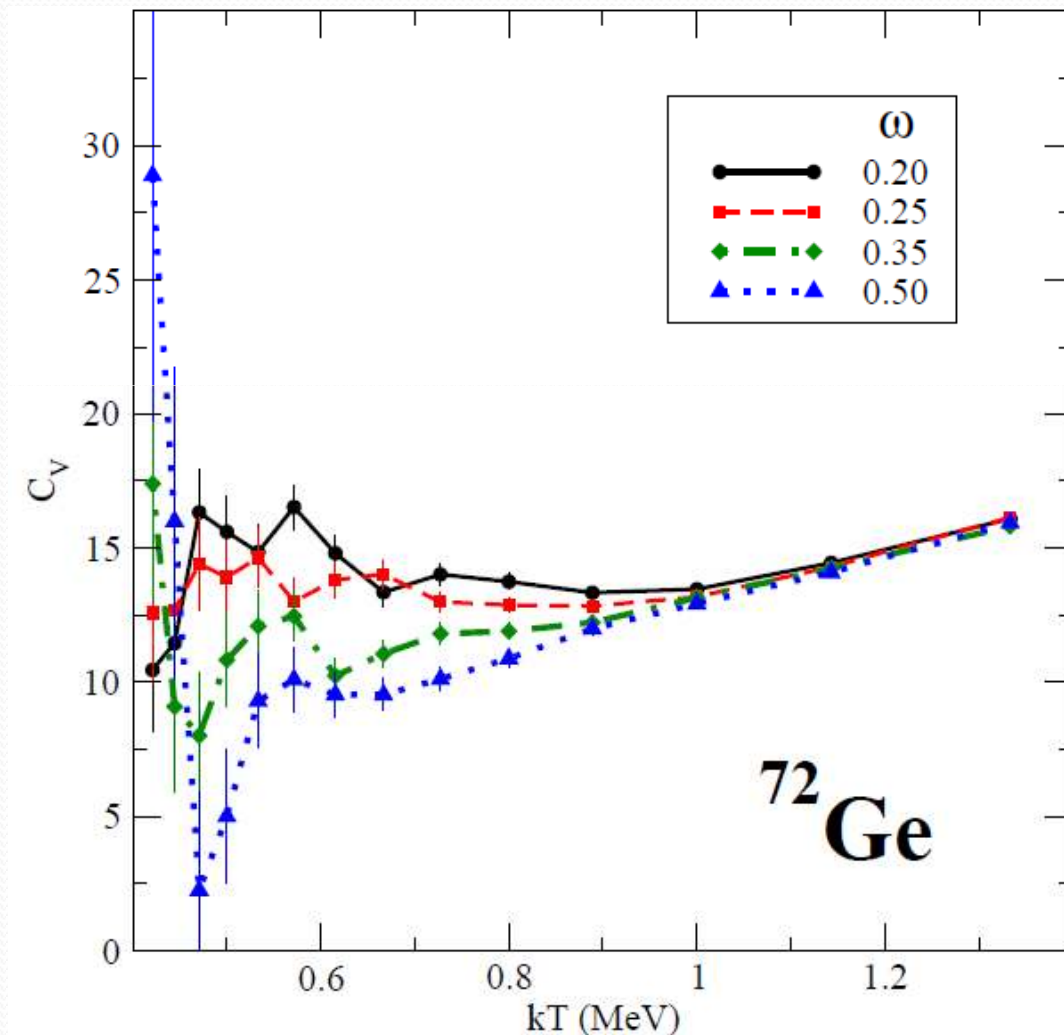
$$\langle J_z \rangle \sim 10.5\hbar$$

$$\langle \hat{J}^2 \rangle = \langle J \rangle (\langle J \rangle + 1)$$

$$\langle J_z \rangle_{r.m.s.} = \langle \hat{J}_z^2 \rangle$$

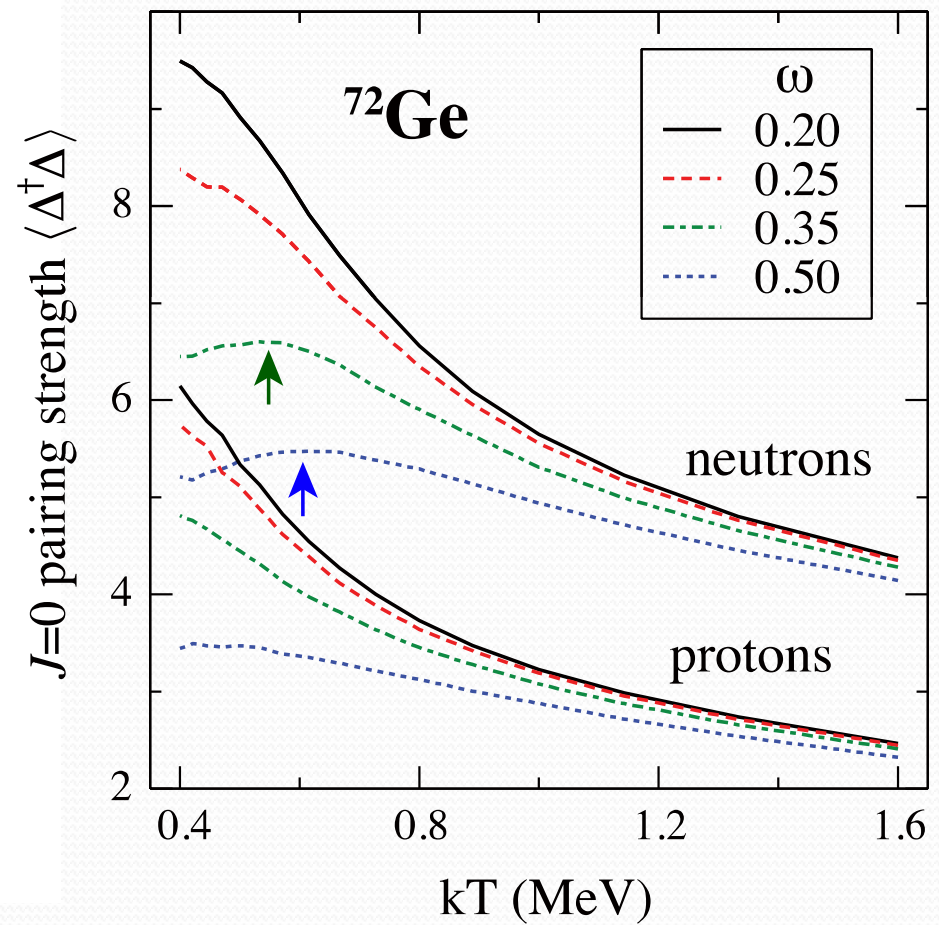
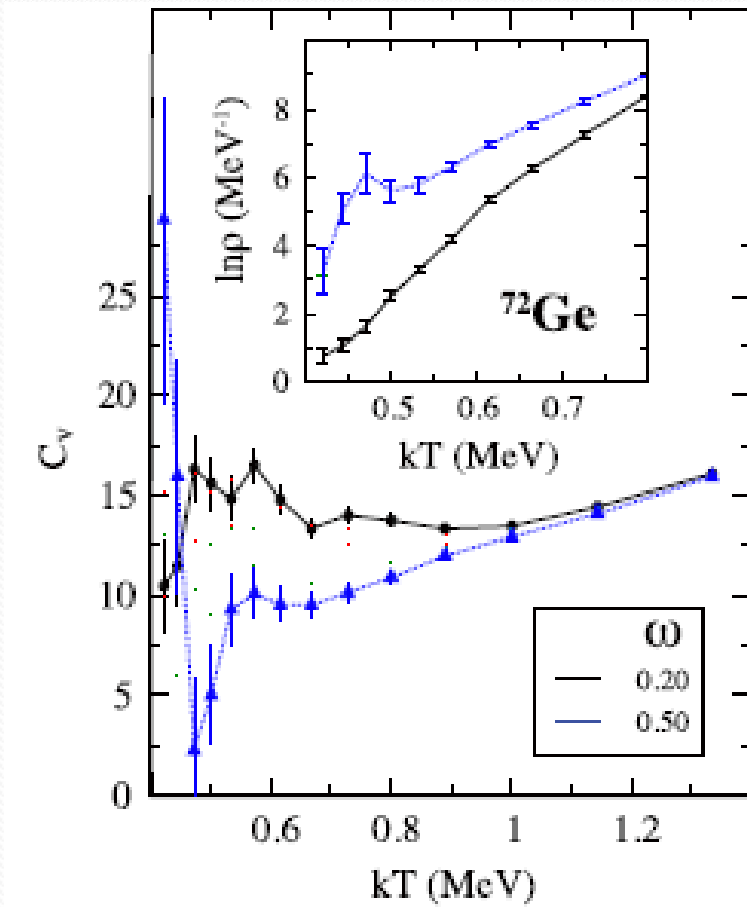
$$\langle J_{\perp} \rangle_{r.m.s.} = \sqrt{\langle \hat{J}^2 - \hat{J}_z^2 \rangle}$$

# Nuclear Specific heat

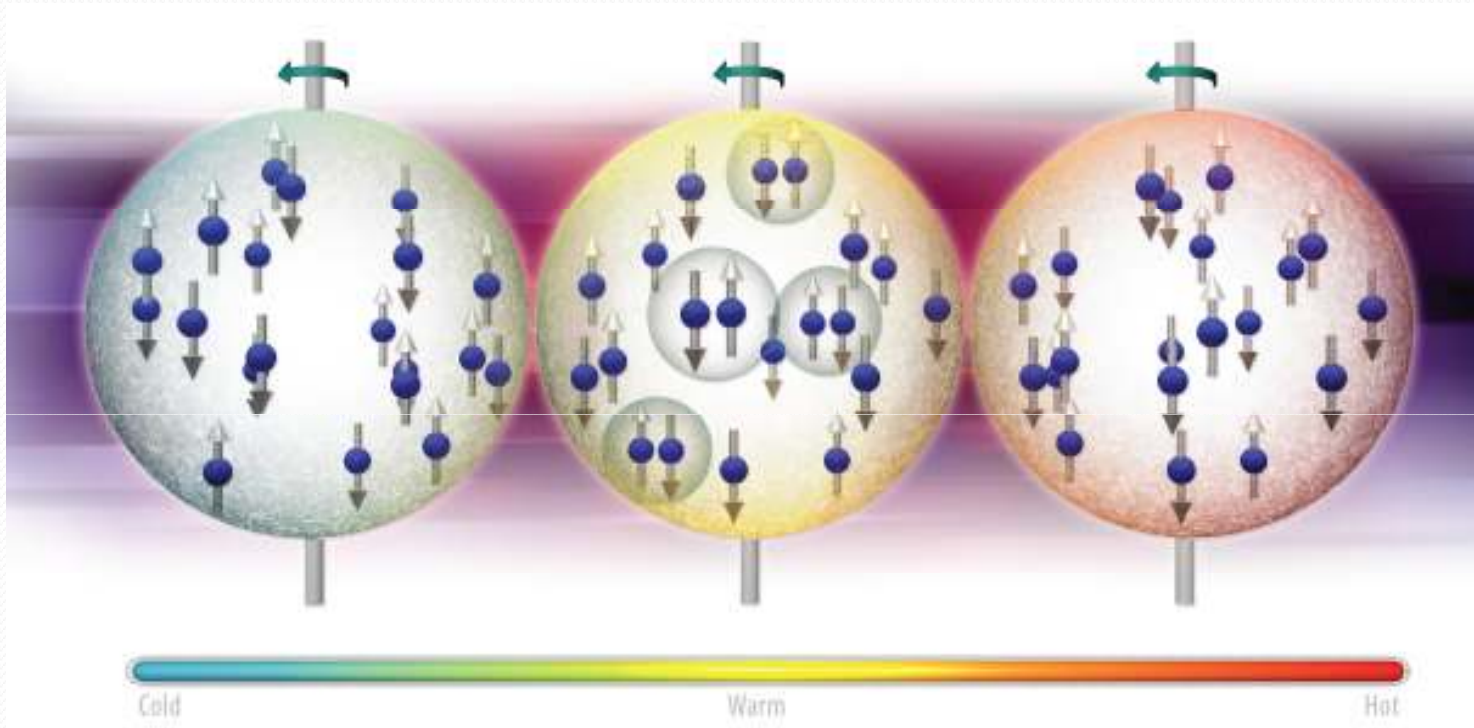


- Gradual entrance of the dip with increasing  $\omega$
- Statistical errors are large at large  $\omega$
- Dip definitely influences level density
- Due to pairing reentrance

# Specific heat and pairing: reentrance



# Conclusions



- In many electron systems magnetic fields produce reentrance effects
- In nuclei, rotation acts as the 'magnetic' field
- Reentrance should be visible in level density data at a given value of rotation
- HPC enables physics insights