Nuclear challenges and computing

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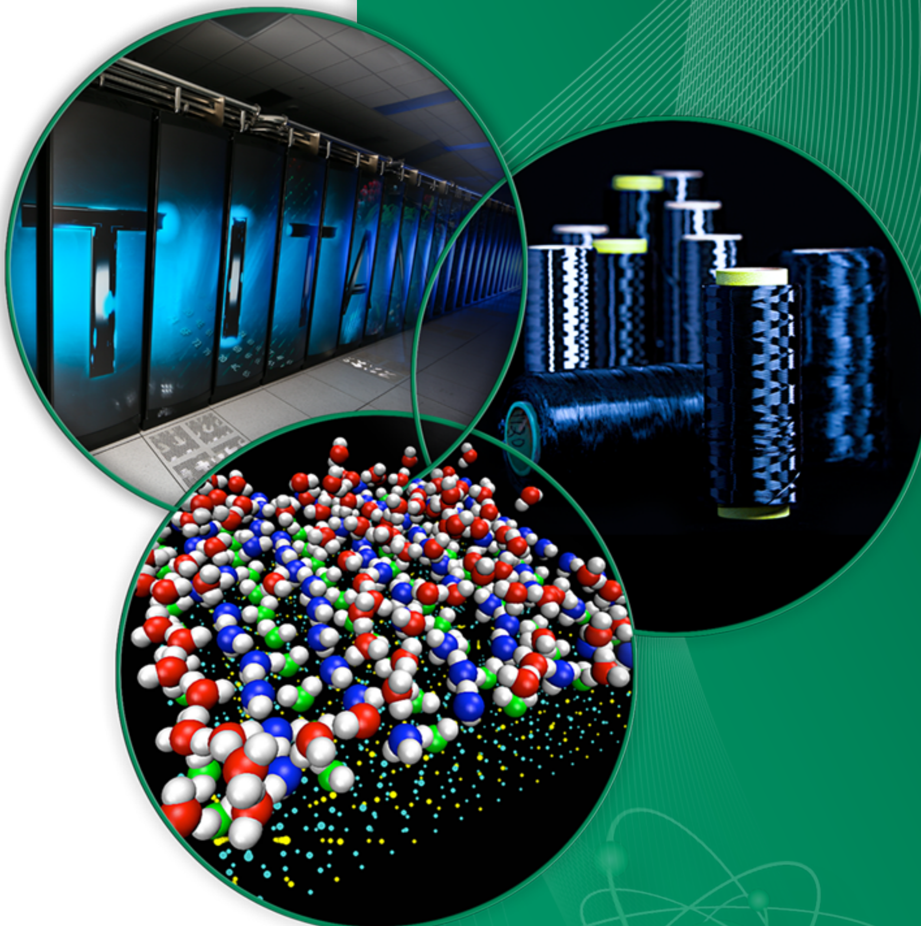


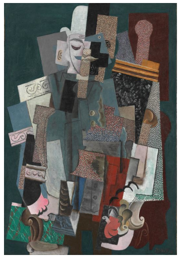
Nuclear Theory in the Supercomputing Era

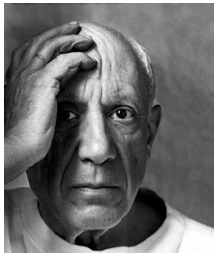
May 13, 2013

Nuclear Physics experiments

- Rare Isotopes
  - Pushing ‘ab initio’ further…
  - Thermal properties of a rotating nucleus
- Beyond Standard Model Physics
  - $0\nu\beta\beta$ decay; super allowed β-decay
- Nuclear Astrophysics Observations
  - Interplay between nuclear structure and astrophysics (r-process)
  - Core collapse mechanisms
- Quark Gluon liquids (early universe)
  - From flow to freeze out
- Nucleon structure
  - Parton distribution functions; the spin problem

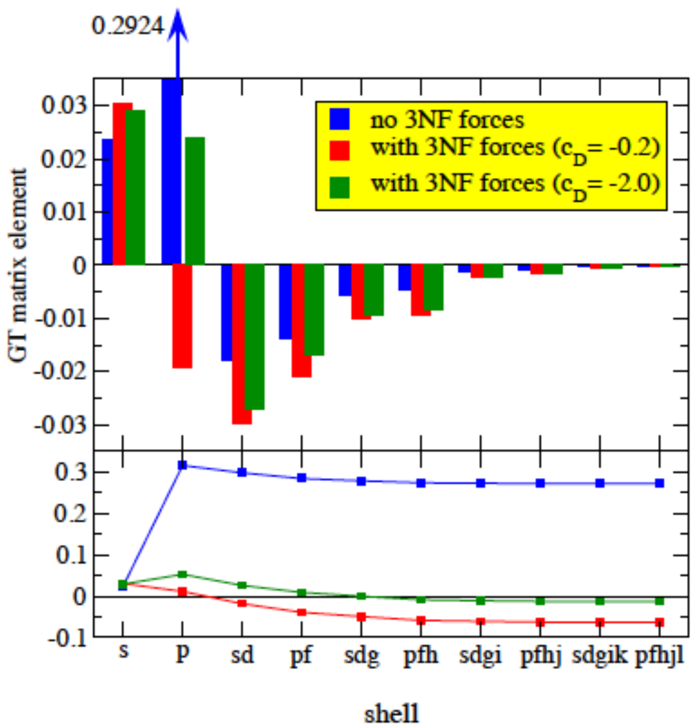
Computers are useless. They can only give you answers. – Pablo Picasso





Structure computing challenges

- It is still a question of the underlying nuclear interactions
  - See Gaute's talk – Pounding away at what should be a solvable problem
  - Interactions are not observables
  - What happens in light nuclei with the new interaction?

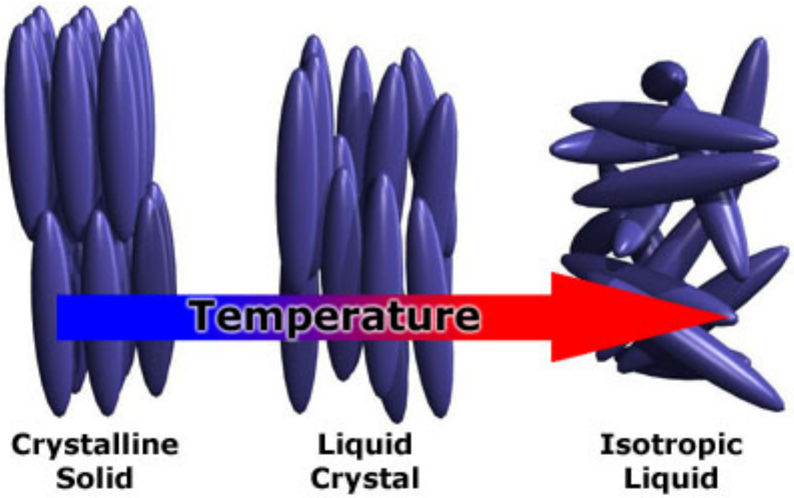


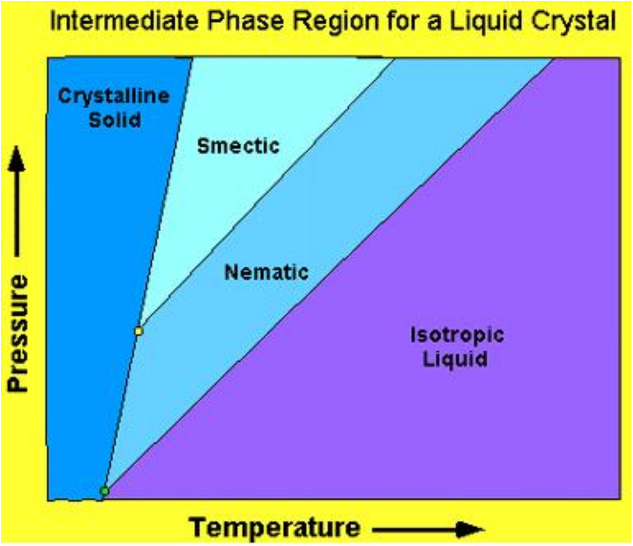
Maris, Vary, Navratil, Ormand, Nam, Dean, PRL 106, 202502 (2011)

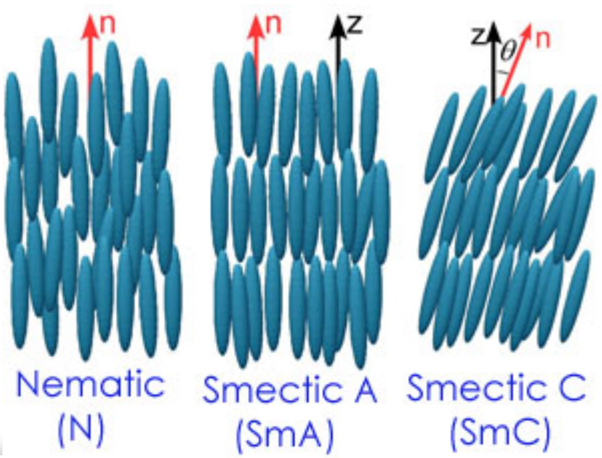
- We've been saying for a long time that 3NFs are important.
- "In conclusion, the chiral 3NF in ab initio nuclear physics produces a large amount of cancellation in the matrix element M_{GT} governing the beta decay of ^{14}C. This cancellation signals a major signature of 3NF effects in the spin-isopin content of the 0p orbitals in ^{14}C and ^{14}N."

- Such conclusions will need to be revisited…
- Stay tuned…

From another field: Liquid Crystal Phases



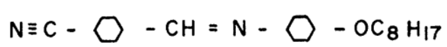




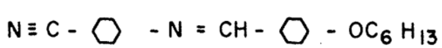
“Re-entrance” discovered for liquid crystals

New Liquid-Crystal Phase Diagram

P. E. Cladis
Bell Laboratories, Murray Hill, New Jersey
(Received 7 April 1975)



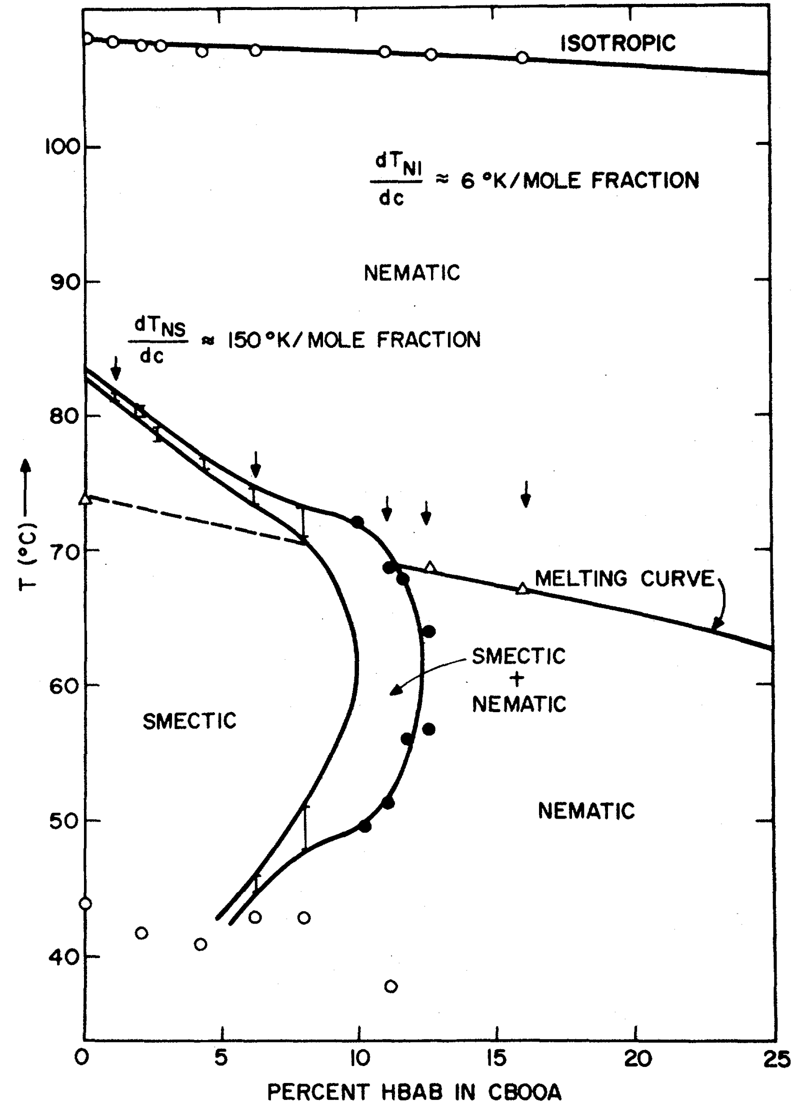
N - p - cyanobenzylidene - p - n - octyloxyaniline



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)

Early work on thermally assisted pairing

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

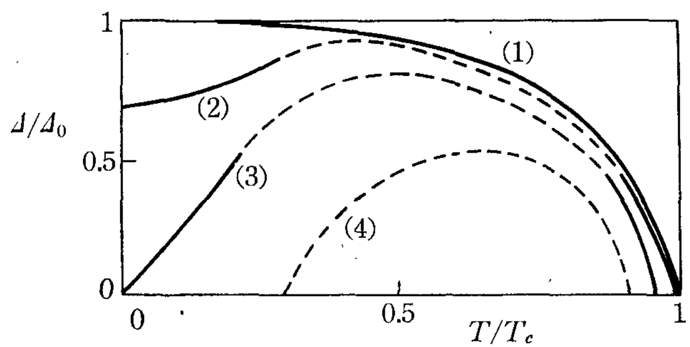


Fig. 2. Ratio of the energy gap to the gap at $T=0$ vs temperature for various values of spin projection M: (1) $M=0$, (2) $M=m$, (3) $M=2m$, (4) schematic plot for some higher M.

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

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

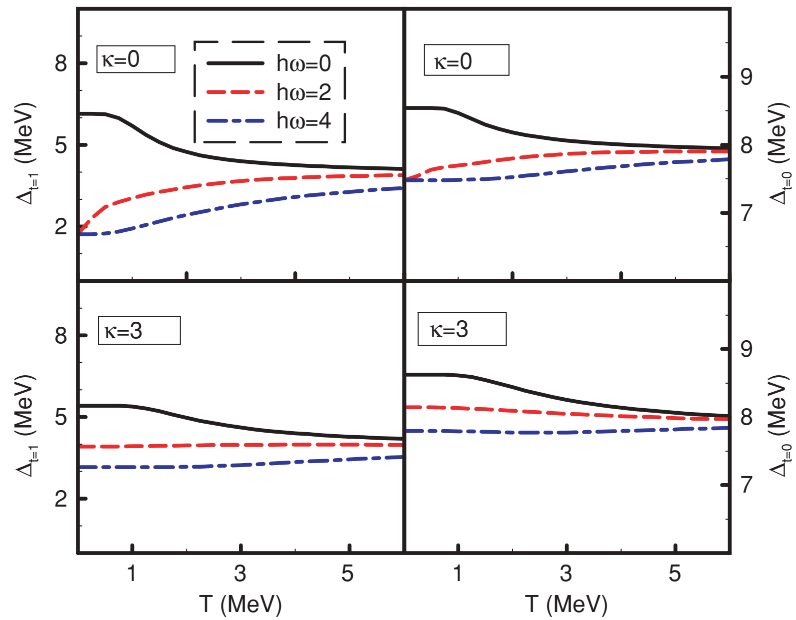


FIG. 2. (Color online) Results of the total isovector ($\Delta_{t=1}$) and isoscalar ($\Delta_{t=0}$) pair gaps are plotted as a function of temperature for three different rotational frequencies of $\hbar\omega = 0$, 2, and 4 MeV. The upper panel shown the results for $\kappa = 0$ and the lower panel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

Hamiltonian for this work

- Pairing+Quadrupole Hamiltonian

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

$0g_{7/2}$-1d-2s

0f-1p-$0g_{9/2}$

- Solve using Auxiliary Field Monte Carlo techniques

- Parameters:

One-body from W-S for ^{56}Ni

$$e_{0f_{7/2}} = 0.000 \quad e_{0f_{5/2}} = 6.42$$
$$e_{1p_{3/2}} = 4.350 \quad e_{1p_{1/2}} = 6.54$$
$$e_{0g_{9/2}} = 8.980 \quad e_{0g_{7/2}} = 17.59$$
$$e_{2d_{5/2}} = 12.95 \quad e_{2d_{3/2}} = 15.99$$
$$e_{2s_{1/2}} = 14.64$$

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

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

Reproduces collective Spectrum in ^{64}Ni and ^{64}Ge

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

For rotations:

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

Shell Model Monte Carlo Essentials

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

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

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

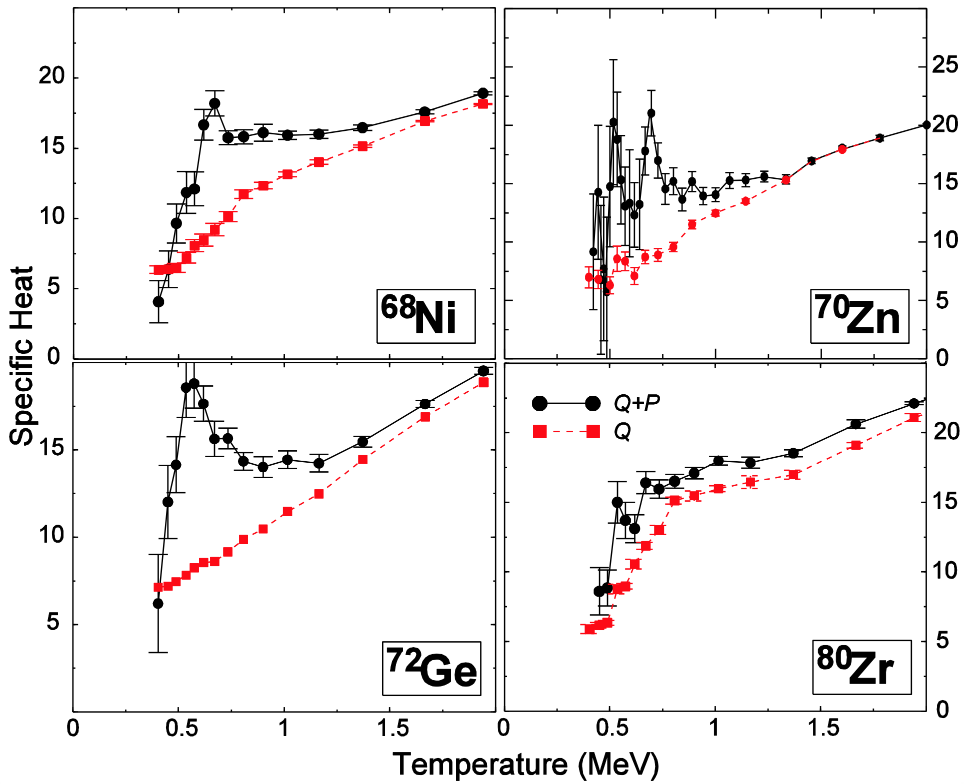
$$\hat{h} = \varepsilon \hat{\Omega} + sV\sigma\hat{\Omega}$$

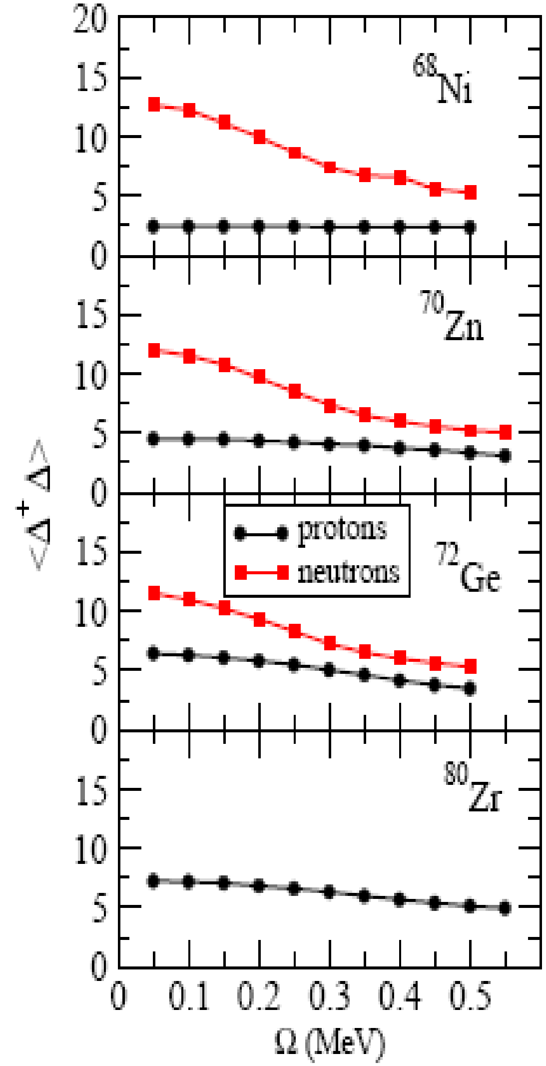
$$s = 1 \quad for \quad V < 0$$
$$s = i \quad for \quad V > 0$$

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

Competition between pairing and rotation in nuclei

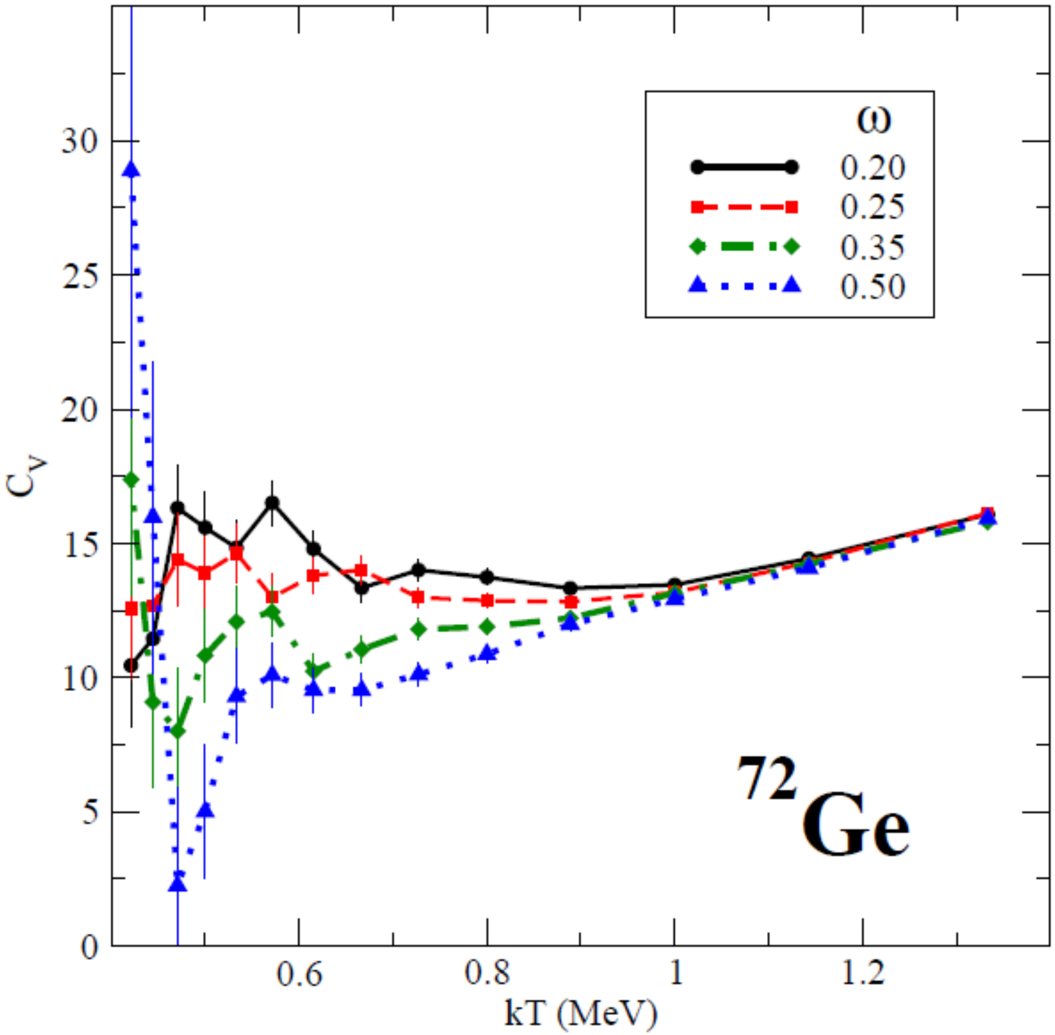
- Pairing phase transitions in nuclei; effects of rotation on pairing; effects of temperature on rotation and pairing
- SMMC calculations at finite temperature
  - Pairing+quadrupole Hamiltonian
  - fp-gsd model space





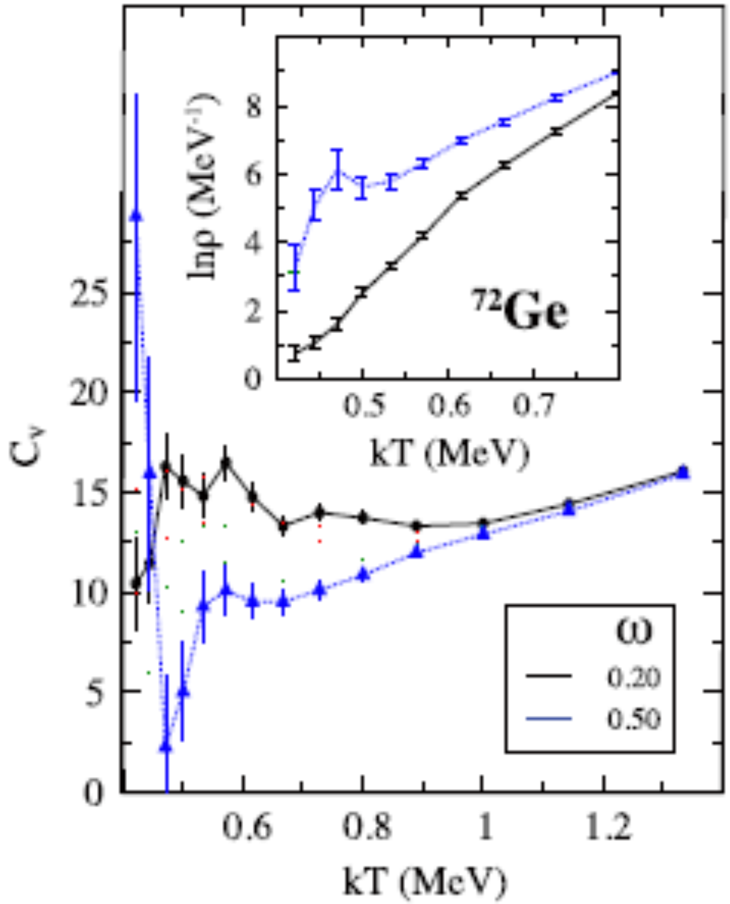
Langanke, Dean, Nazarewicz, NPA757, 360 (2005);

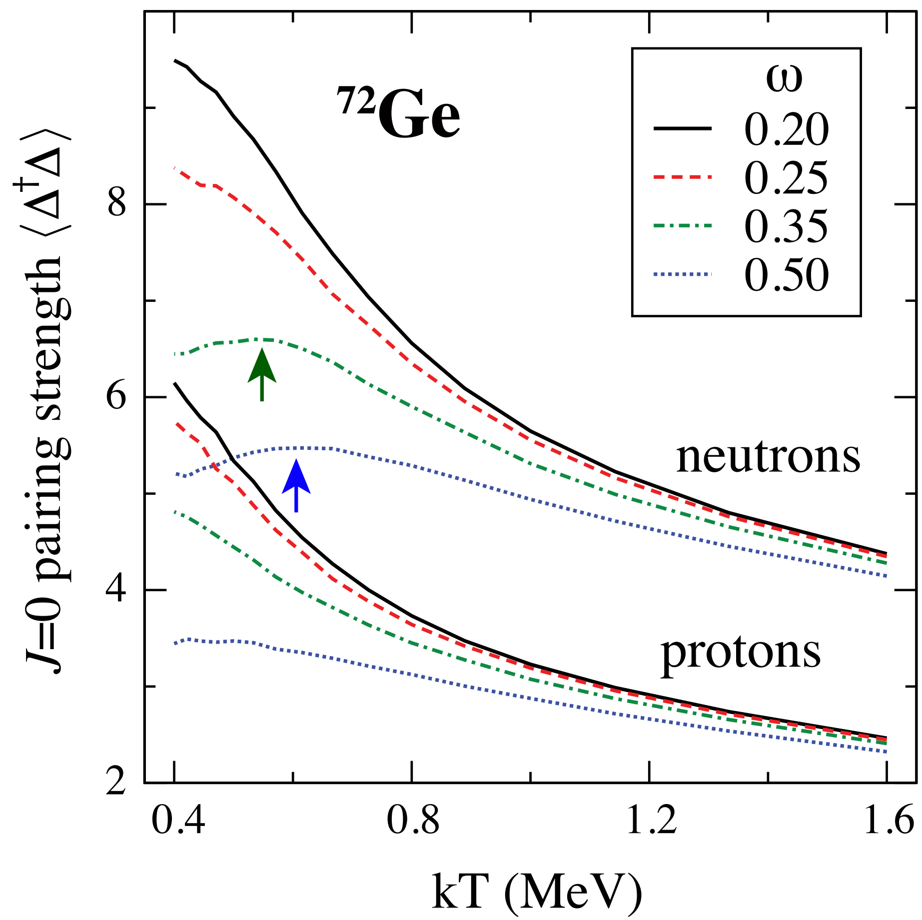
Nuclear Specific heat



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

Specific heat and pairing: reentrance

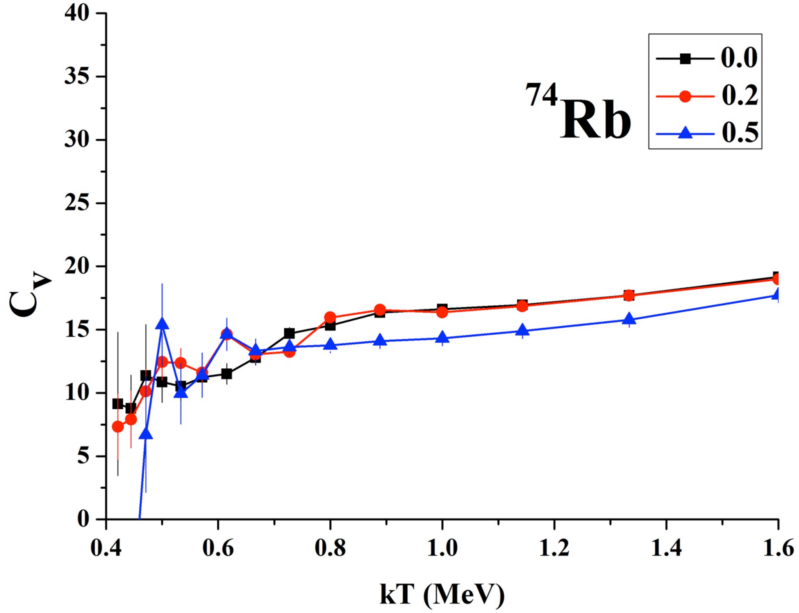


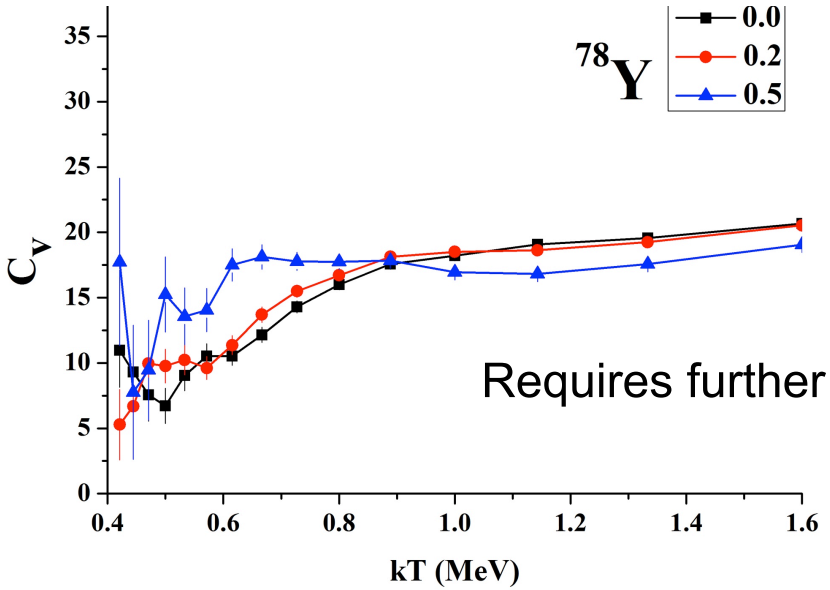


Dean, Langanke, Nam, Nazarewicz, Phys. Rev. Lett. 105, 212504 (2010)

Rotational effect on odd-odd N=Z

Nam et al, ongoing

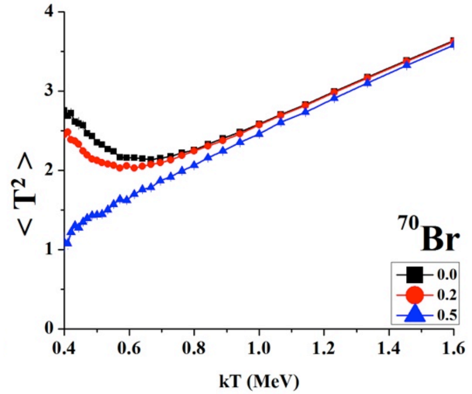


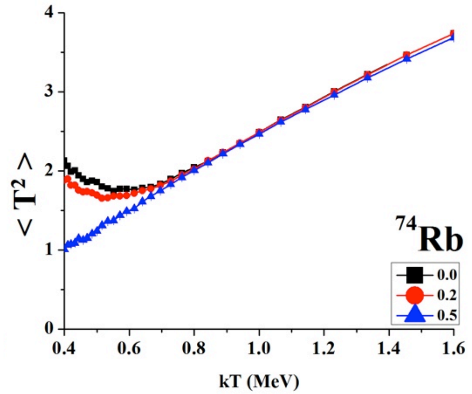


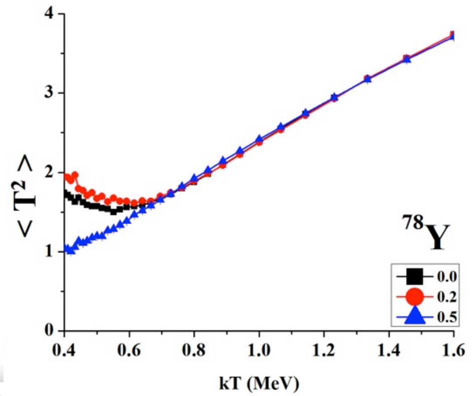
$$\left\langle T^2 \right\rangle$$

Exhibit
T(T+1)=2
Behavior at
Low frequency
And low temp

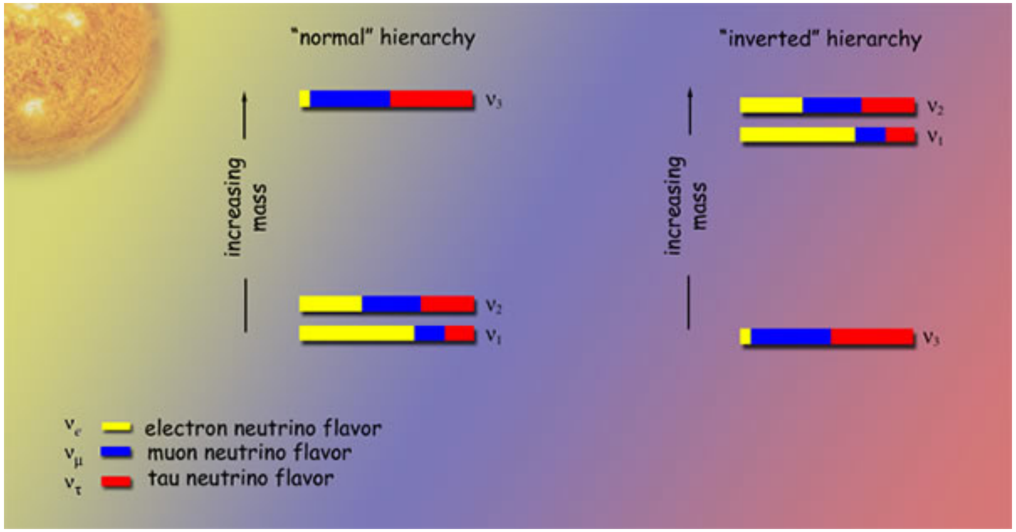
Requires further investigation

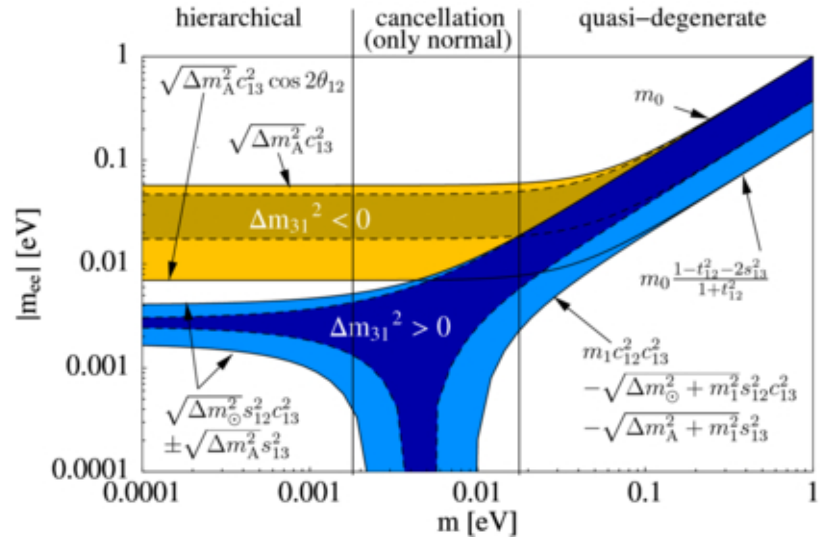






Fundamental Symmetries: 0νββ Decay





$$m_{12}^2 = (7.59 \pm 0.21) \times 10^{-5}\ \text{eV}^2$$

$$m_{32}^2 = (2.43 \pm 0.13) \times 10^{-3}\ \text{eV}^2$$

$$\langle m_\beta \rangle = \left(\sum_{i=1}^{3} m_i^2 |U_{li}|^2 \right)^{1/2} \qquad \beta\text{-decay}$$

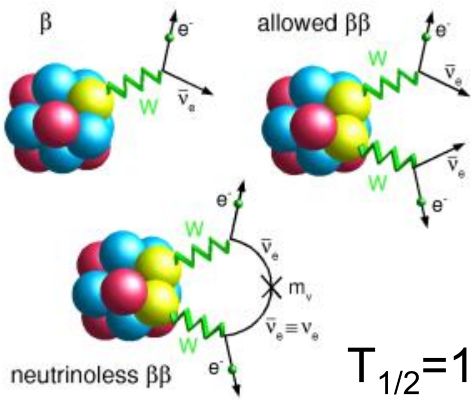
$$\langle m_{\beta\beta} \rangle = \left(\sum_{i=1}^{3} m_i^2 |U_{li}|^2 e^{i\alpha_i} \right)^{1/2} \qquad \alpha_i = \text{ Majorana Phases}$$

$$\Sigma = \sum_{i=1}^{3} m_i \qquad \text{Cosmology}$$

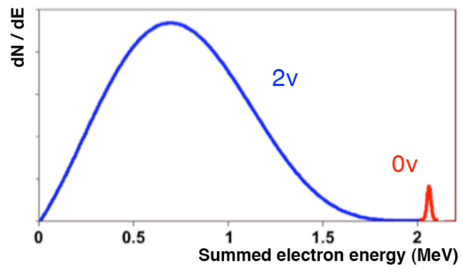
World wide, several experimental techniques under development…ORNL is the lead Lab for the Majorana Demonstrator (John Wilkerson, PM)

Why do it? Lepto-genesis

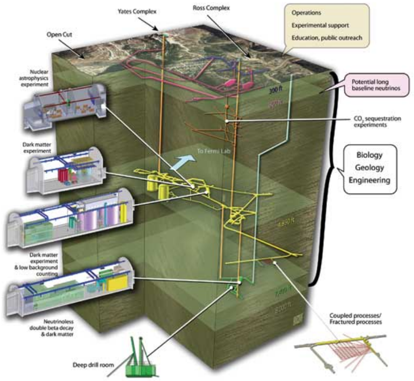
Majorana – Neutrinos



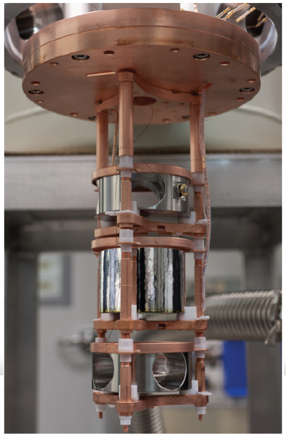
$T_{1/2}=10^{19}$ years



$T_{1/2}=10^{26}$ years



Physics Questions:
Are neutrinos their own antiparticles?
What is the neutrino hierarchy?



Majorana Demonstrator Project

- Demonstrate technology for tonne scale
- 30 kg enriched 76Ge crystals
- At 4850 feet in Sanford Underground Lab, SD

0νββ calculation status

$$\left(T_{1/2}^{0\nu}\right)^{-1} = G^{0\nu}(Q,Z)\left|M^{0\nu}\right|^2 \frac{\left|\langle m_{\beta\beta}\rangle\right|^2}{m_e^2}$$

$$M^{(0\nu)} = M_{GT}^{(0\nu)} - \left(\frac{g_V}{g_A}\right)^2 M_F^{(0\nu)} - M_T^{(0\nu)}$$

$$M_K^{(0\nu)} = \left\langle 0_f^+ \left| H_K\left(\vec{r}_1 - \vec{r}_2\right)\left(t_1^- t_2^-\right)\Omega_K \right| 0_i^+ \right\rangle$$

$$\Omega_F = 1,\ \Omega_{GT} = \vec{\sigma}_1\vec{\sigma}_2,\ \Omega_T = S_{12}$$

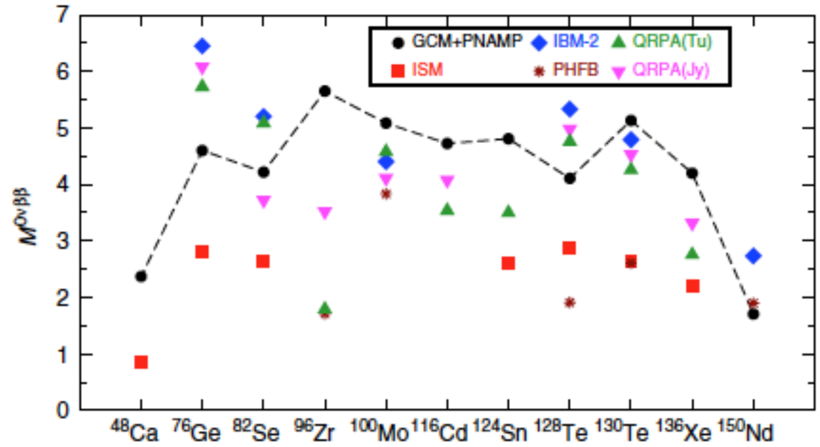
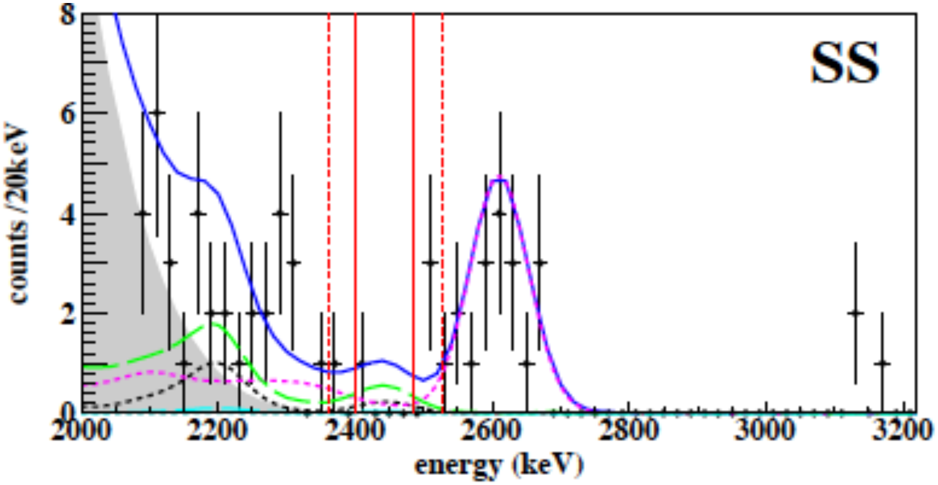


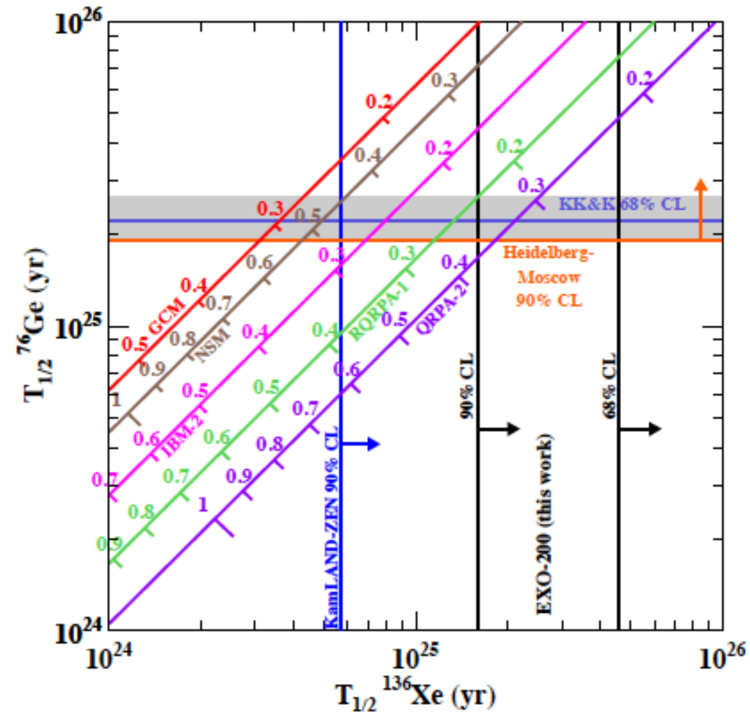
FIG. 3 (color online). Nuclear matrix elements calculated for different methods (ISM [5,22], QRPA(Jy) [8], QRPA(Tu) [7], IBM-2 [12], PHFB [10]) with UCOM short-range correlations. QRPA values are calculated with $g_A = 1.25$ and IBM-2 and PHFB results are multiplied by 1.18 to account for the difference between Jastrow and UCOM [29].

Experimentalists see a spread of a factor of 2-3 in the theory matrix element

$0\nu\beta\beta$: EXO 200 first results PRL 109, 032505 (2012)



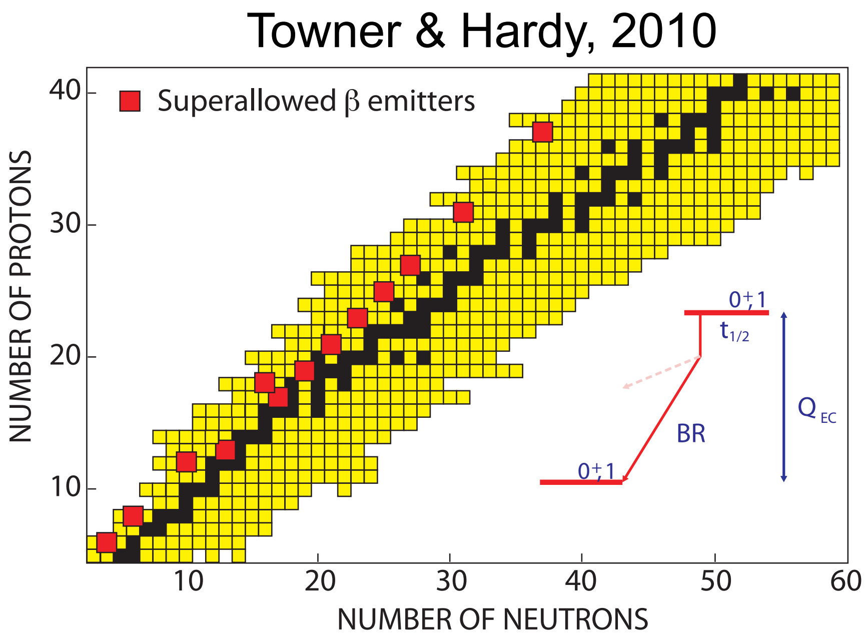
Xe-136 TPC



We report on a search for neutrinoless double-beta decay of ^{136}Xe with EXO-200. No signal is observed for an exposure of 32.5 kg-yr, with a background of $\sim 1.5 \times 10^{-3}\,\mathrm{kg^{-1}yr^{-1}keV^{-1}}$ in the $\pm 1\sigma$ region of interest. This sets a lower limit on the half-life of the neutrinoless double-beta decay $T_{1/2}^{0\nu\beta\beta}(^{136}\mathrm{Xe}) > 1.6 \times 10^{25}$ yr (90% CL), corresponding to effective Majorana masses of less than 140–380 meV, depending on the matrix element calculation.

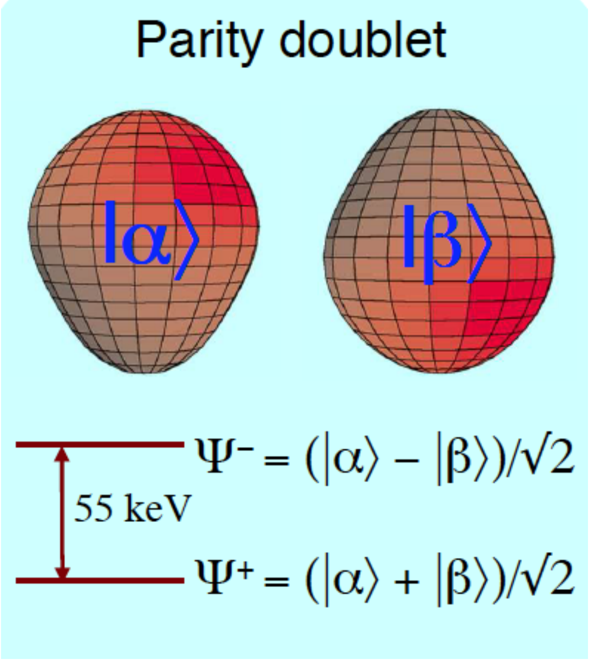
Mass derived from matrix elements. UQ? Quantitative would be good here.

Connections to Fundamental Symmetries



$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.99990(60)$$

- Super-allowed beta decay places stringent limits on physics beyond the standard model (CKM quark mixing matrix)
- Tremendous worldwide effort

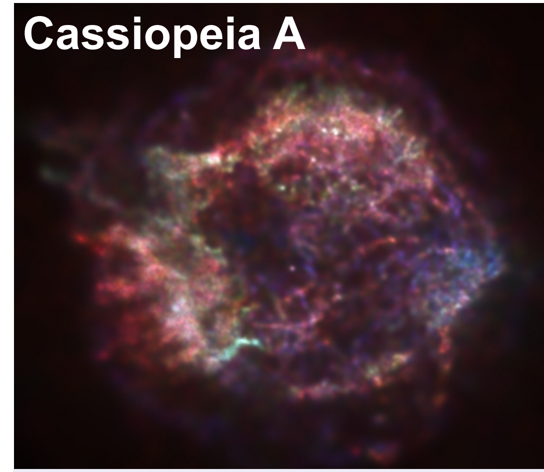


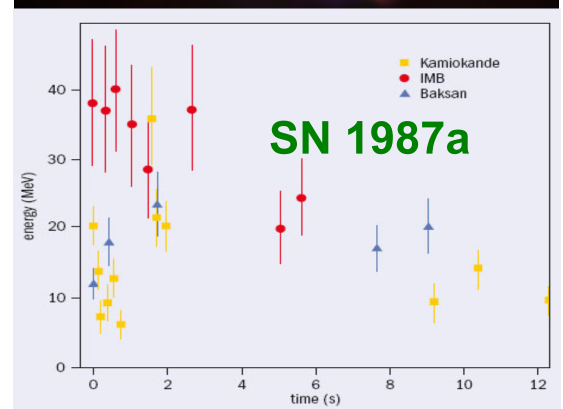
- Closely spaced parity doublet gives rise to enhanced EDM
- Large intrinsic Schiff moment
- Relativistic atomic structure

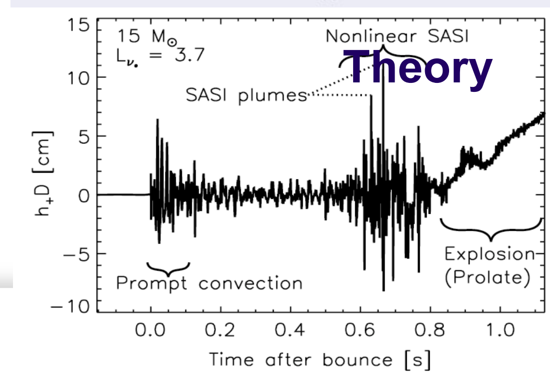
- ^{199}Hg (Seattle, 1980's – present)
- ^{225}Ra (Starting at ANL and KVI)
- Potential at FRIB (10^{12}/s w ISOL target (far future); 10^{10} initially

Core-Collapse Supernovae: making elements

- Mark the death of a massive star (> 10 solar mass) and the formation of a neutron star (or black hole)
- Dominant source of heavy elements, observable via optical, X-ray and γ-ray emission and terrestrial samples
- Also produce neutrino and gravitational wave signals

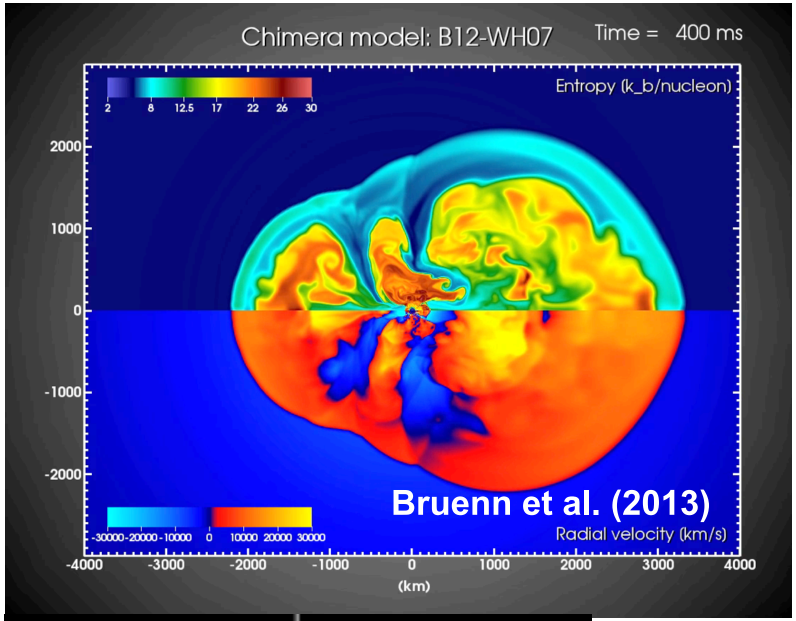


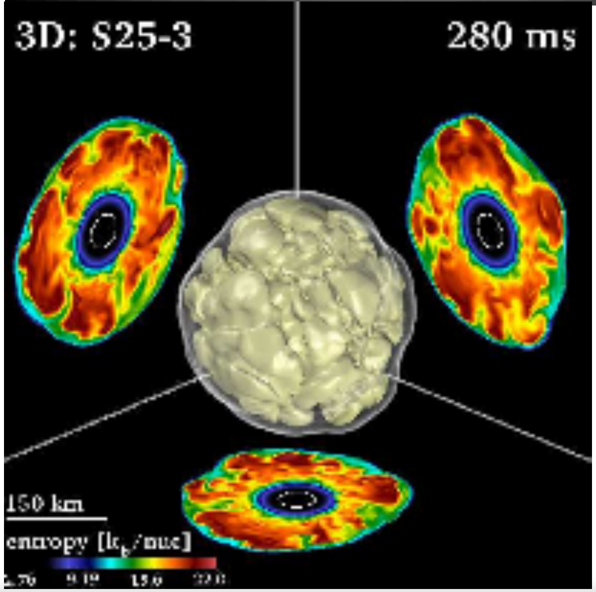




Modeling CCSN

- Simulations reveal that the explosion is powered by neutrinos carrying off the binding energy of the newly-formed neutron star.
- Spherically symmetric simulations fail because neutrino heating occurs only in a very restricted, stratified region.
- Axisymmetric (2D) simulations allow more efficient heating through buoyancy
- 3D is under investigation at various institutions (ORNL, Garching, Caltech…)



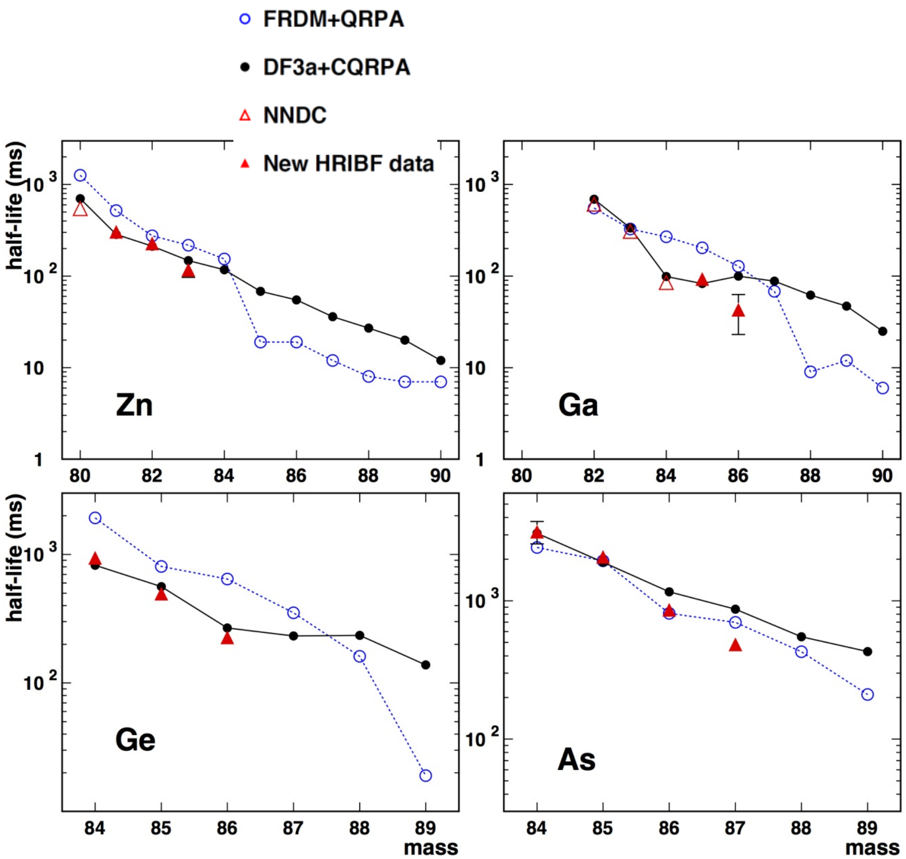


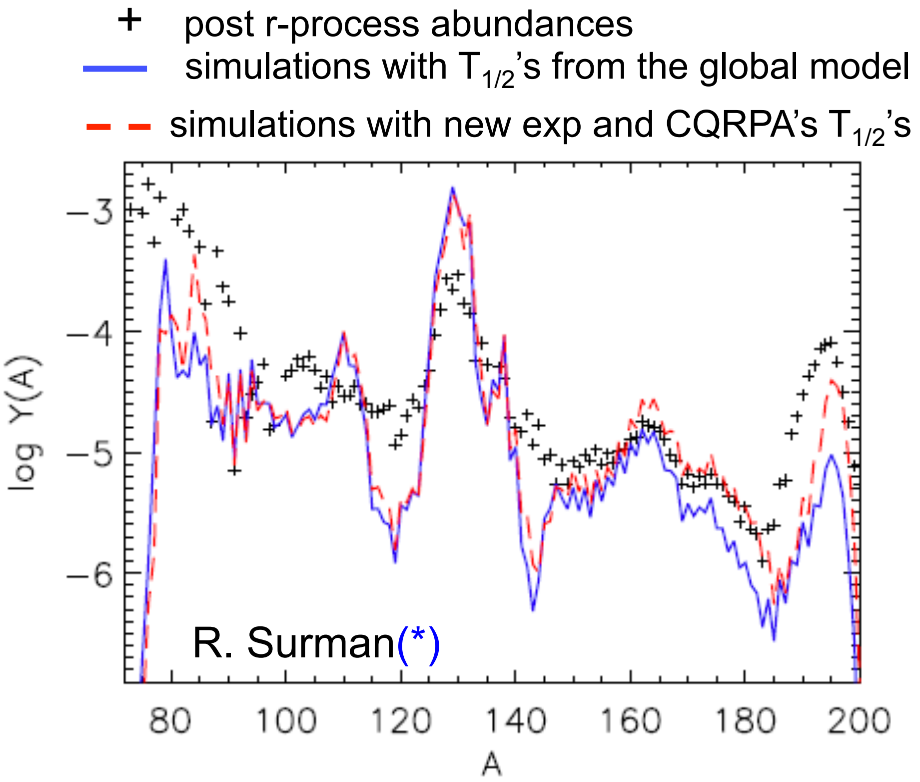
An example of a multi-physics problem

- 2D models with 1° resolution in latitude each cost 0.4 M core-hours
- 3D models at 1° resolution in latitude & longitude would cost at least 100 M core-hours

Large beta decay probabilities for neutron rich nuclei

Phys. Rev. Letters 109, 112501, 2012 and Phys. Rev. C 87, 034315, 2013





- Experimental beta half-lives are shorter than global model predictions
- Further from ^{78}Ni, improved calculations also depart from experiment, see ^{86}Ga and ^{87}As.

r-process sensitivity study

- Experiment: shorter half-lives near ^{78}Ni.
- Fast decays: faster flow towards higher mass nuclei A > 140

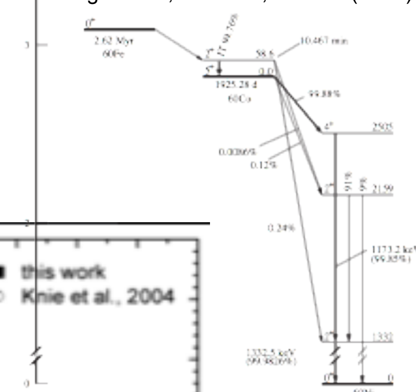
(*) R. Surman and J. Engel, PR C **64**, 035801, 2001.
R. Surman et al., Astrophys. J. **679,** L117, 2008.

Supernovae and the Earth

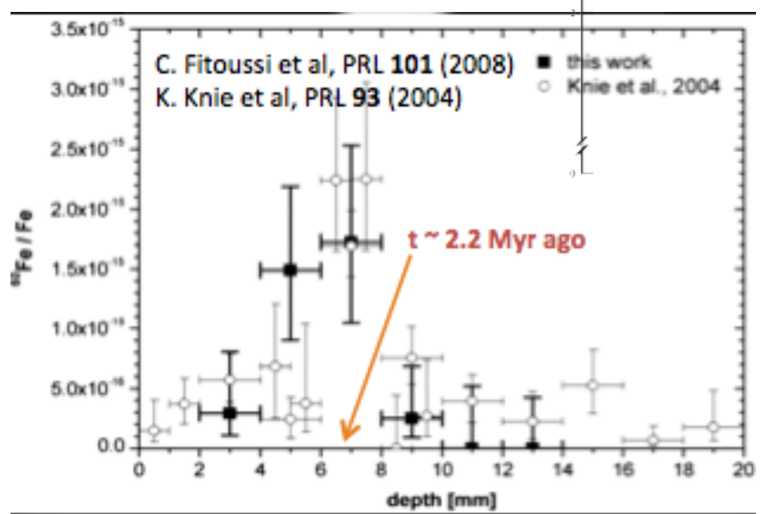
While the solar system was built from the products of supernova nucleosynthesis, we also find evidence of ongoing contributions to the solar system.

Any ^{60}Fe, half-life of 2.6 Myr, found on Earth must have been created deposited on Earth by recent supernovae.

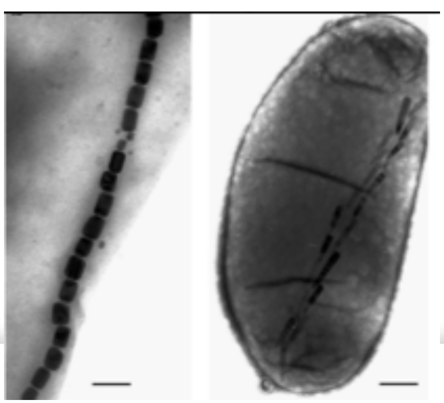
Rugel et al., PRL **103**, 072502 (2009)



Ferro-Manganese Crust samples raised from the seafloor show evidence for these recent contributions



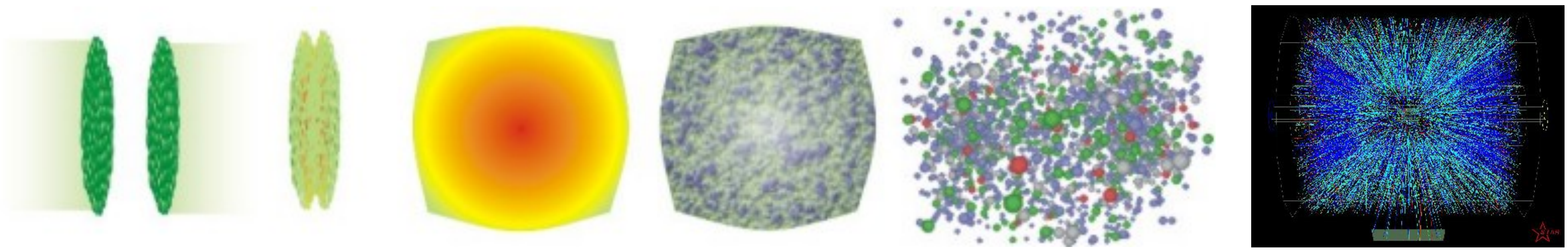
S. Bishop, APS meeting, (2013)

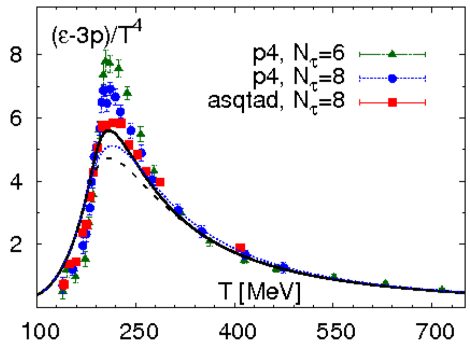


Magnetotactic Bacteria also contain ^{60}Fe!

Early Universe computing challenges

- Process is not reversible
- QCD is the underlying theory
- Do we understand hadronization?
- Over what scales does Hydrodynamics apply?
- Error propagation from initial to final state?





(Bazavov et al PRD80, 014504 (2009))

$$\partial_\mu T^{\mu\nu} = 0$$

UrQMD

Experiment

Represents a classic multiscale physics problem
- QCD gives EOS
- Hydro runs to 'freeze out'
- QMD to the detectors
- Geant-4 simulates detector response

Conclusions

- Big investments are being or may be made on experiments
  - FRIB
  - 1-tonne neutrinoless double beta decay
  - nEDM (more theoretical);
  - From HEP: Dark matter detection (WIMPS + nuclei as detectors – didn't talk about)
  - Upgrades at RHIC/LHC; upgrade of Jlab
- Theory should inform the investments: implies computational effort
- Thanks to efforts of people like James Vary, theory is making significant advances in lock step with computing in order to resolve interesting science questions…