Modeling excess heat and related issues

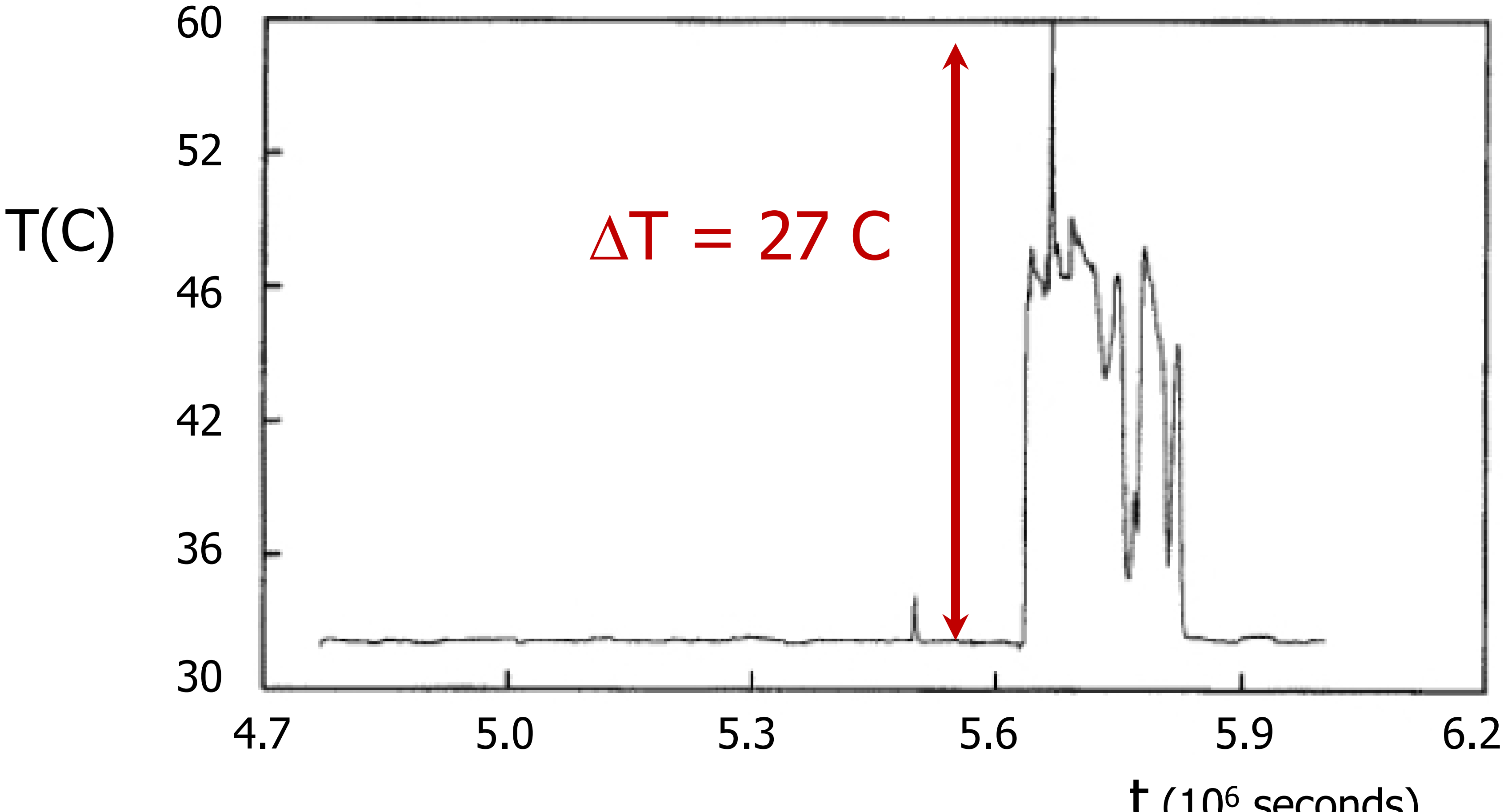
Peter Hagelstein

Research Laboratory of Electronics

MIT

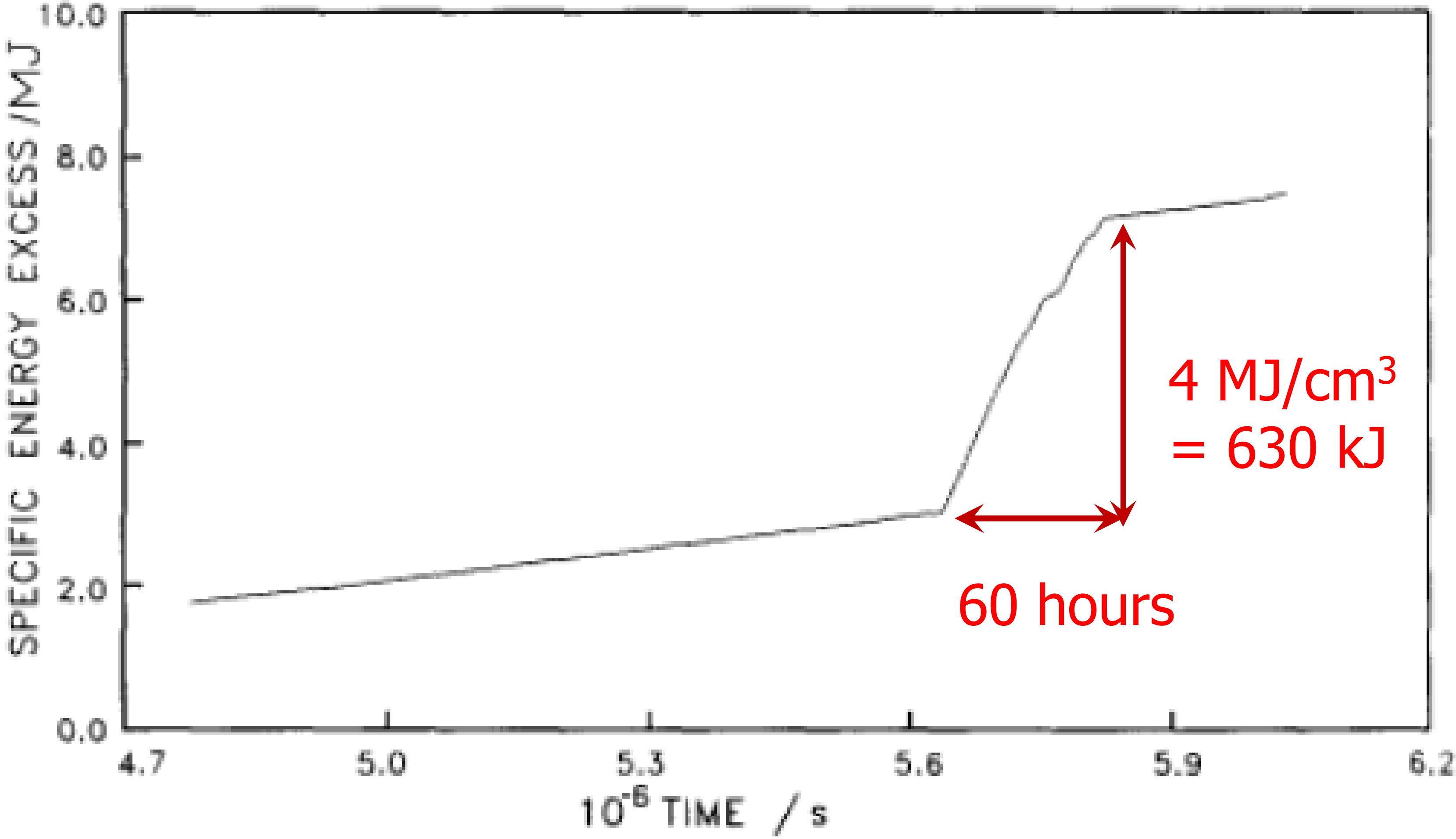
ILENRS-12, July 2, 2012

Observation of a heat burst



Fleischman, Pons, et al, *J Electroanal Chem* **287**, 293 (1990)

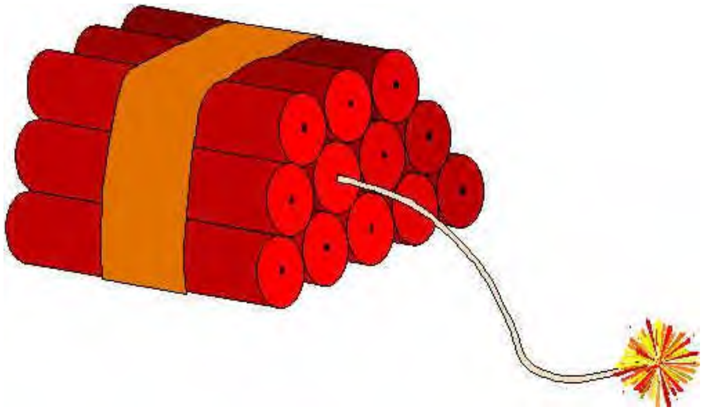
Integrated energy



Thinking about the energy

$$\frac{0.63\ \text{MJ}}{60\ \text{hr}} = 2.9\ \text{Watts}$$

We would only get 1.2 kJ from detonating an equivalent volume (0.157 cc) as the Pd cathode of TNT



Effect not chemical

No commensurate chemical reaction products observed:

In the cell are

Electrolyte: D_2O + 0.1 M LiOD

Cathode: Pd

Anode: Pt

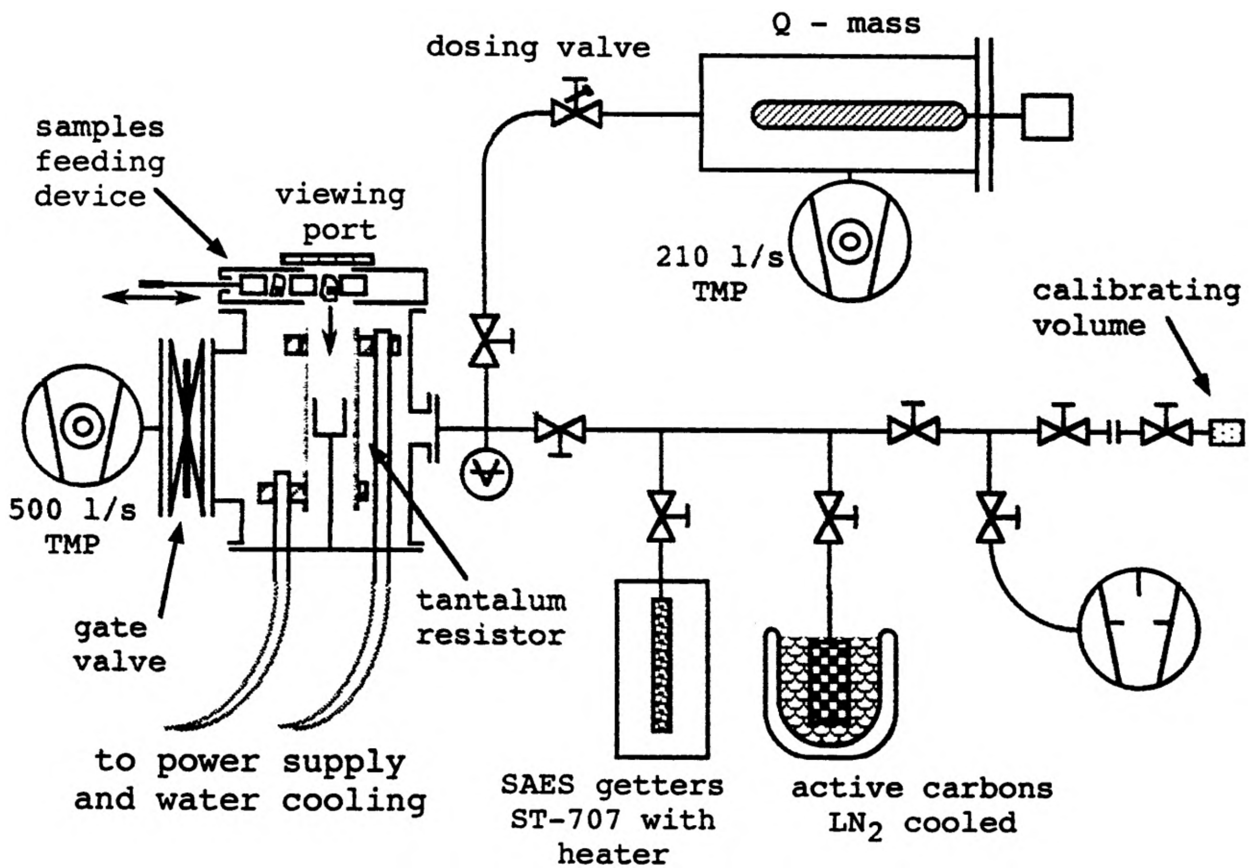
Reference electrode: Pd

Fleischmann conjecture:

Energy produced is of nuclear origin.

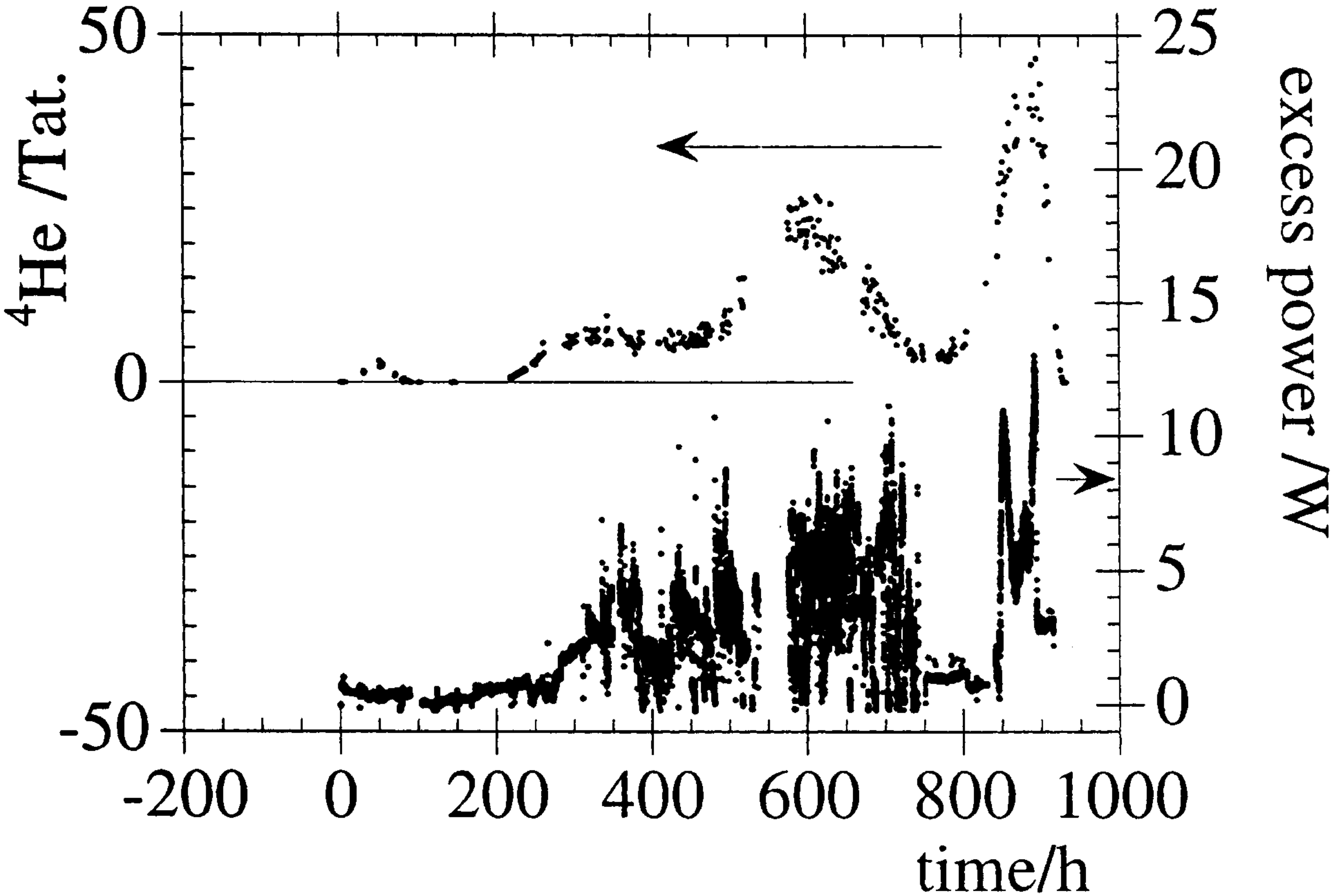
Perhaps deuteron-deuteron fusion reactions of some new kind.

La Sapienza (Rome) exp't



D. Gozzi, F. Cellucci, P.L. Cignini, G. Gigli, M. Tomellini, E. Cisbani, S. Frullani, G.M. Urciuoli, *J. Electroanalyt. Chem.* **452** 254 (1998).

t-correlation of P_{xs} and ^4He

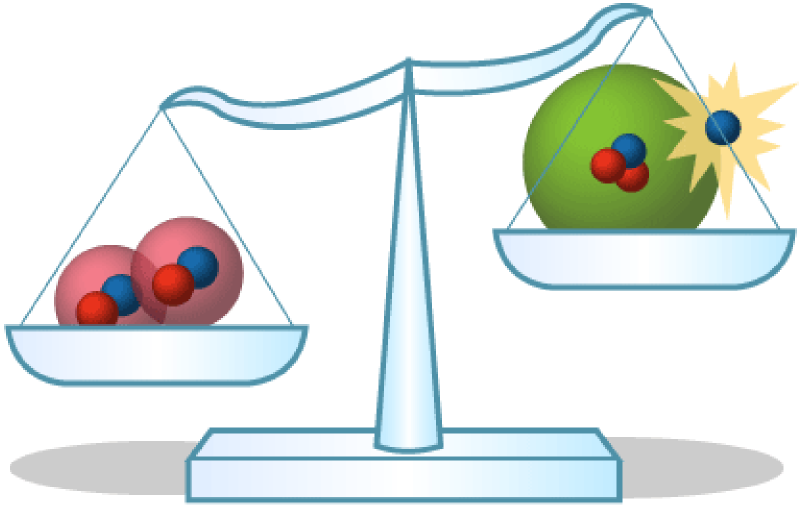


Excess energy per ^{4}He

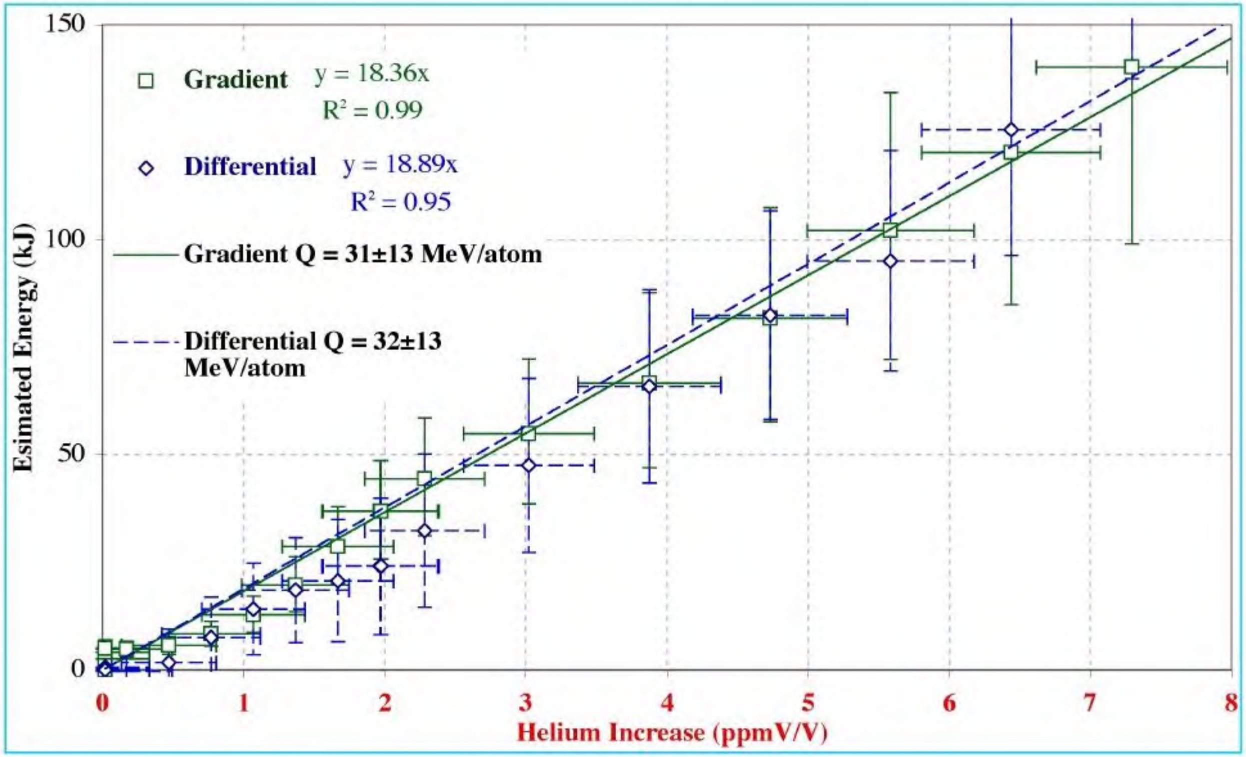
The mass difference between d+d and ^{4}He is

$$2M_d c^2 - M_{4He} c^2 \ = \ 23.85 \text{ MeV}$$

Is this consistent with experiment?



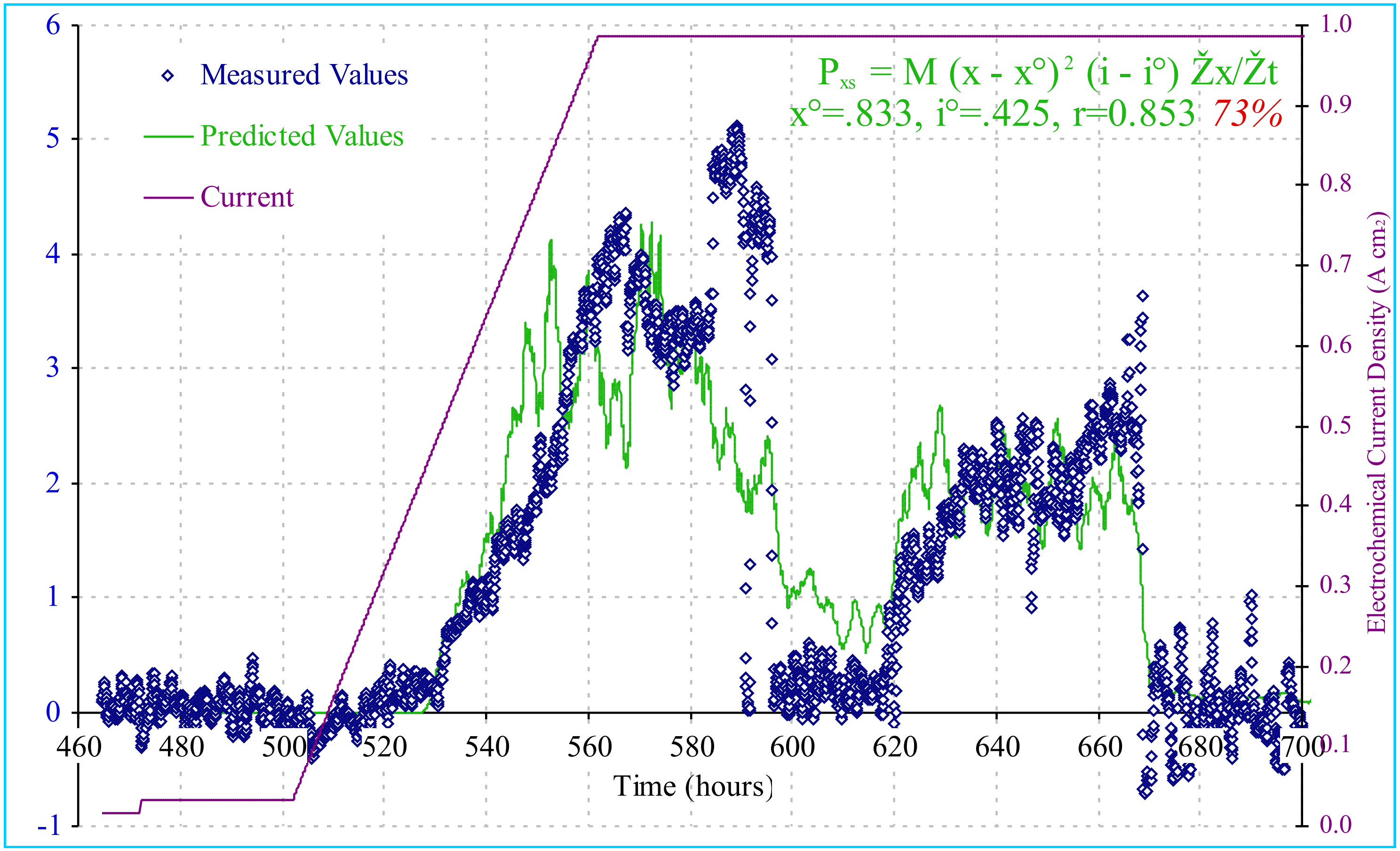
Energy as a function of ^{4}He



M. C. H. McKubre, *ICCF10 Short Course slides* (2003).

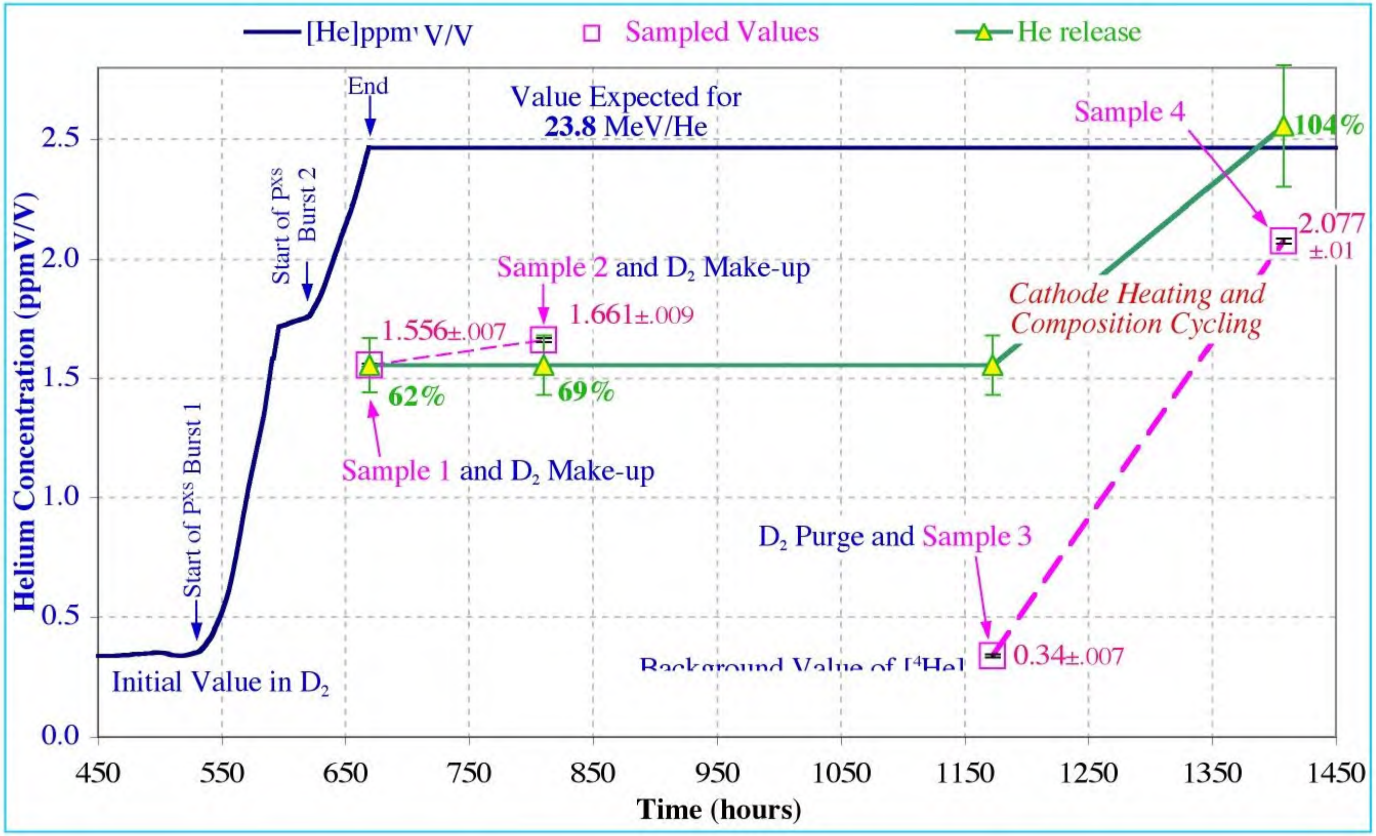
M4: Excess Power Correlation at SRI

[Closed, He-leak tight, Mass-Flow Calorimeter, Accuracy ±0.35%]



M. C. H. McKubre, *ICCF10 Short Course slides* (2003).

^{4}He measurements



M. C. H. McKubre, *ICCF10 Short Course slides* (2003).

Take away message

- If d+d → ^4He, would expect 24 MeV for Q-value
- But experiments need to weigh in (might be other reactants)
- ^4He retention problem
- Results from (2) experiments with scrubbing give 24 MeV
- Consistent with d+d → ^4He (but not proof of)
- Need more experiments (prevented by lack of support)
- Theoretical issues loom large since no 24 MeV γ

Energy and momentum conservation

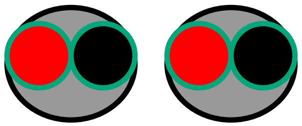
In nonrelativistic limit, can determine final state energies and momenta from conservation

$$\left(\mathbf{p}_1 + \mathbf{p}_2\right)_f = \left(\mathbf{p}_1 + \mathbf{p}_2\right)_i$$

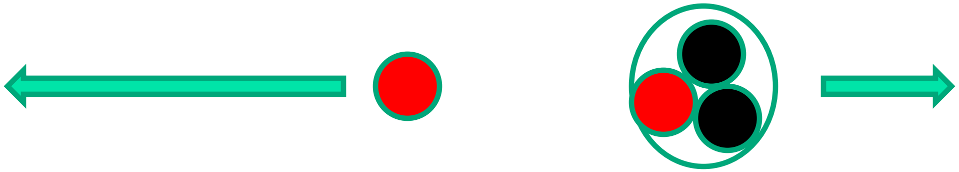
$$\left(\frac{1}{2} m_1 \left|\mathbf{v}_1\right|^2 + \frac{1}{2} m_1 \left|\mathbf{v}_2\right|^2\right)_f = \left(\frac{1}{2} m_1 \left|\mathbf{v}_1\right|^2 + \frac{1}{2} m_1 \left|\mathbf{v}_2\right|^2\right)_i + Q$$

Energy and momentum conservation

Initial state:



Final state:



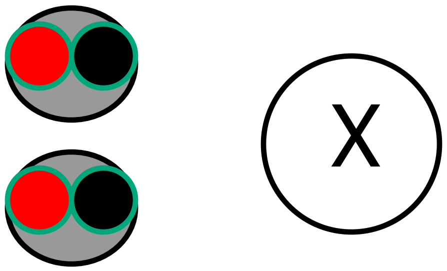
$$\frac{1}{2}M_1\left|\mathbf{v}_1\right|^2 = \left(\frac{M_2}{M_1+M_2}\right)Q = \frac{3}{4}Q$$

$$\frac{1}{2}M_2\left|\mathbf{v}_2\right|^2 = \left(\frac{M_1}{M_1+M_2}\right)Q = \frac{1}{4}Q$$

Can learn about the reaction if we knew ^{4}He energy

A proposed reaction scheme:

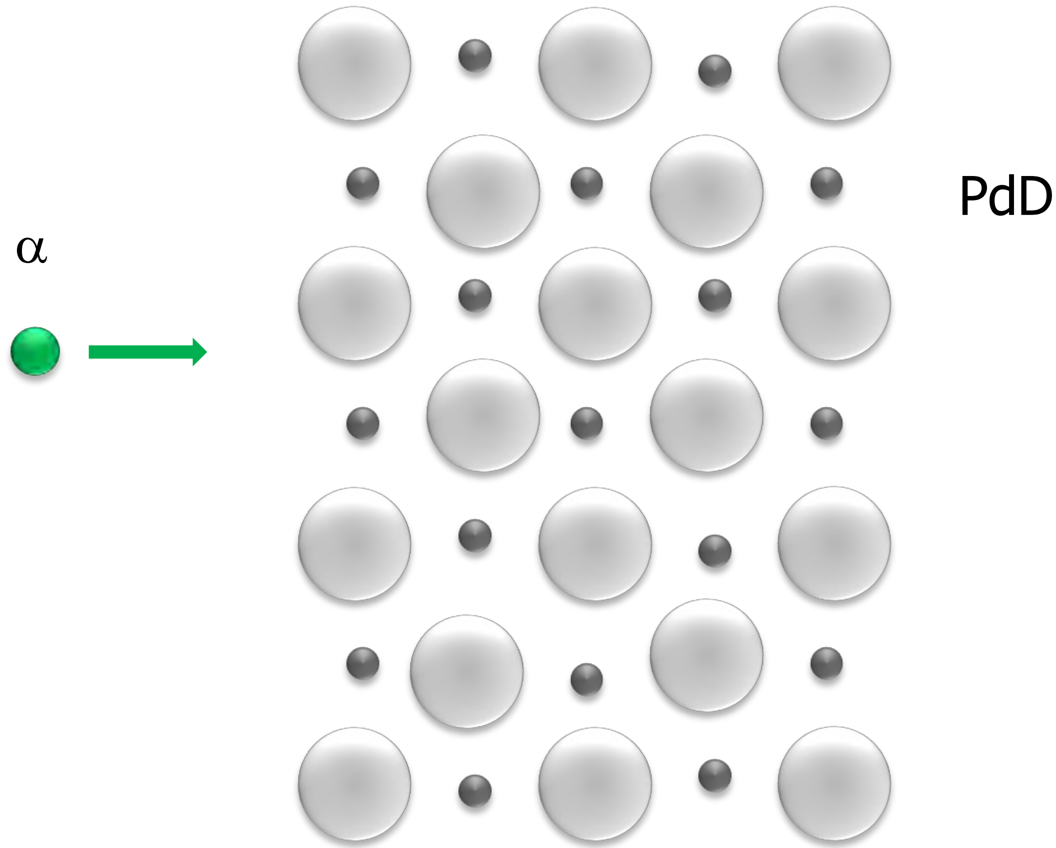
$$d + d + X \rightarrow$$
$$^4\mathrm{He} + X + 23.85\ \mathrm{MeV}$$



$$\frac{1}{2} M_{4He} \left| \mathbf{v}_{4He} \right|^2 = \left(\frac{M_X}{M_{4He} + M_X} \right) 24\ \mathrm{MeV}$$

$$\frac{1}{2} M_X \left| \mathbf{v}_X \right|^2 = \left(\frac{M_{4He}}{M_{4He} + M_X} \right) 24\ \mathrm{MeV}$$

Propose using PdD as detector



Stopping power from SRIM

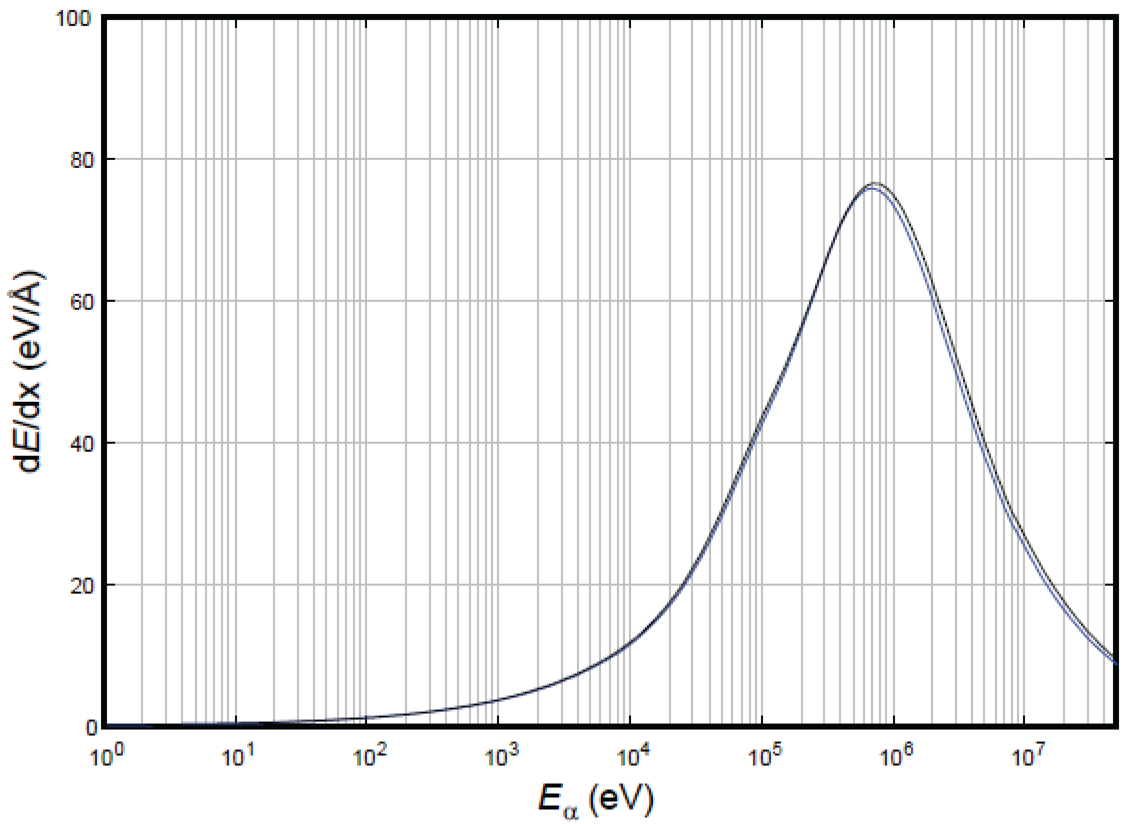
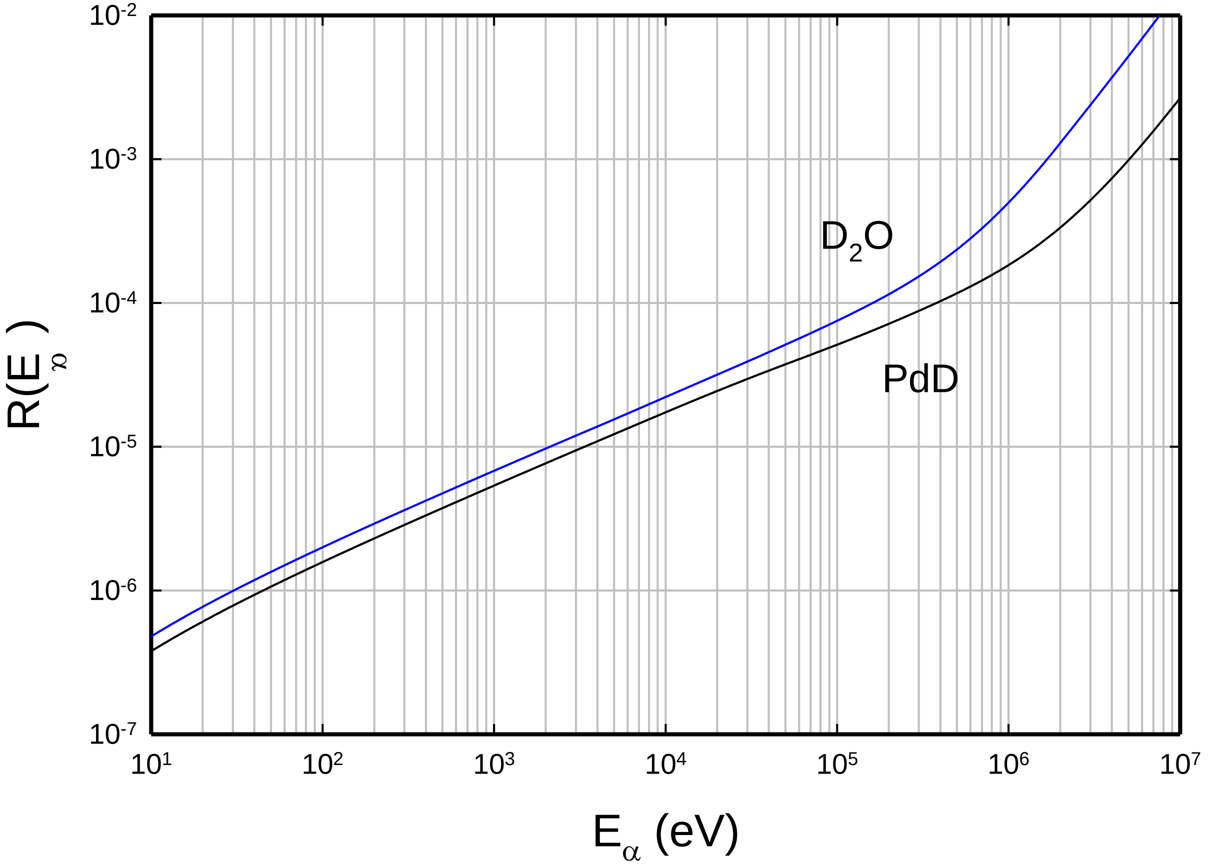


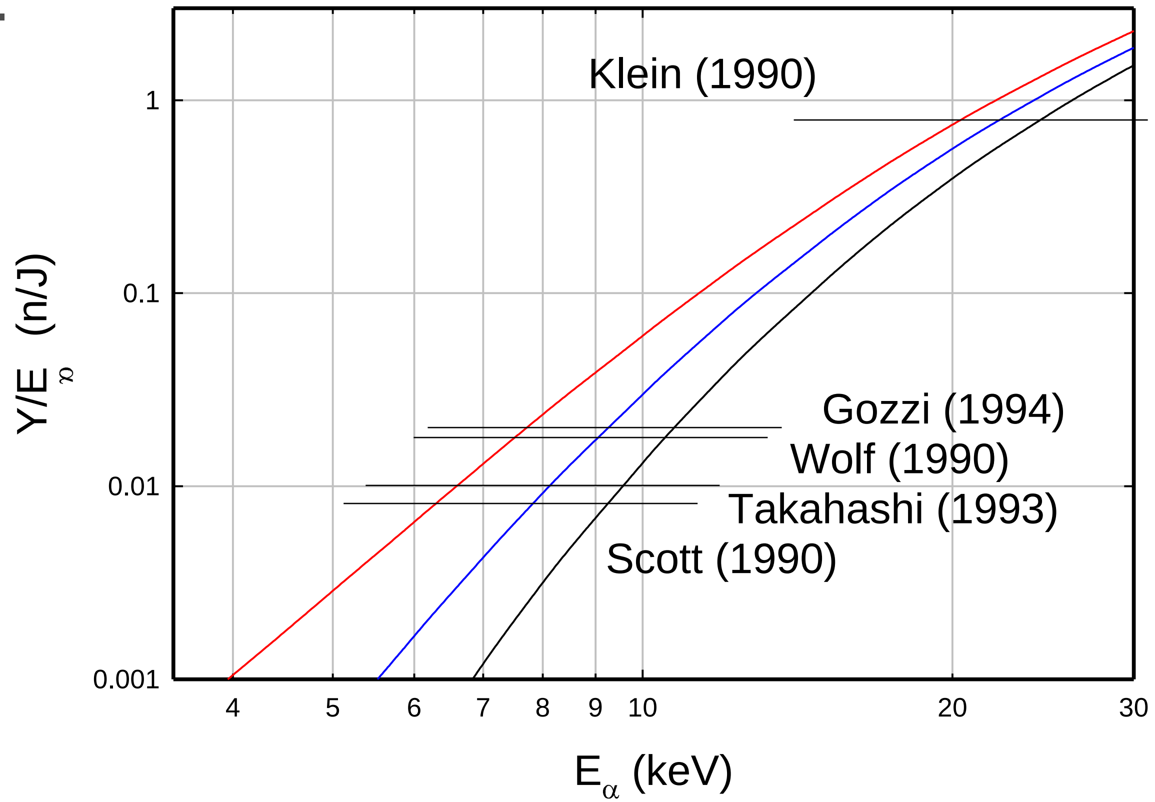
Figure 2. Stopping power for alpha particles in in Pd (black) and in PdD (blue) from SRIM2008.

Range



10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
$R(E_\alpha)$
D_2O
PdD
10^1
10^2
10^3
10^4
10^5
10^6
10^7
E_α (eV)

Yield/energy for secondary neutrons



P. L. Hagelstein, *Naturwissenschaften* (2010)

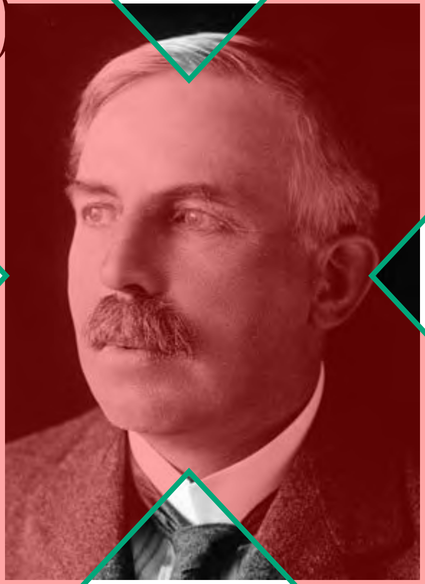
Examine d+d+X candidates

$$d + d + \mathrm{Pd} \rightarrow {}^{4}\mathrm{He}\left(23.0\ \mathrm{MeV}\right) + \mathrm{Pd}\left(0.85\ \mathrm{MeV}\right)$$

$$d + d + d \rightarrow {}^{4}\mathrm{He}\left(7.95\ \mathrm{MeV}\right) + d\left(15.9\ \mathrm{MeV}\right)$$

$$d + d + e^{-} \rightarrow \mathrm{He}\left(76\ \mathrm{keV}\right) + e^{-}\left(23.77\ \mathrm{MeV}\right)$$

We can rule out all Rutherford picture d+d+X reactions as inconsistent with experiment



What is going on?

- Lots of energy seen in F&P experiments
- Commensurate ^4He observed correlated with P_{xs}
- Q-value consistent with $d+d \rightarrow {}^4He$
- But no commensurate nuclear radiation
- And ^4He born essentially at rest
- And no plausible Rutherford reaction consistent with experiment

- So, where does the energy go?

Letts 2-laser experiment

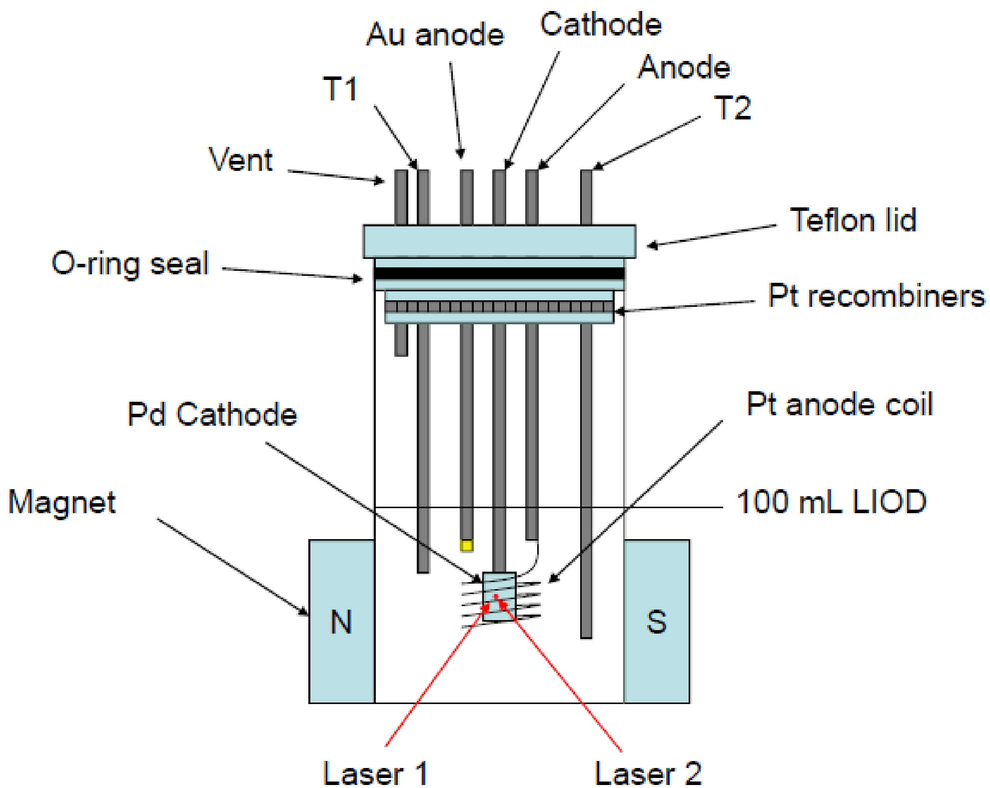
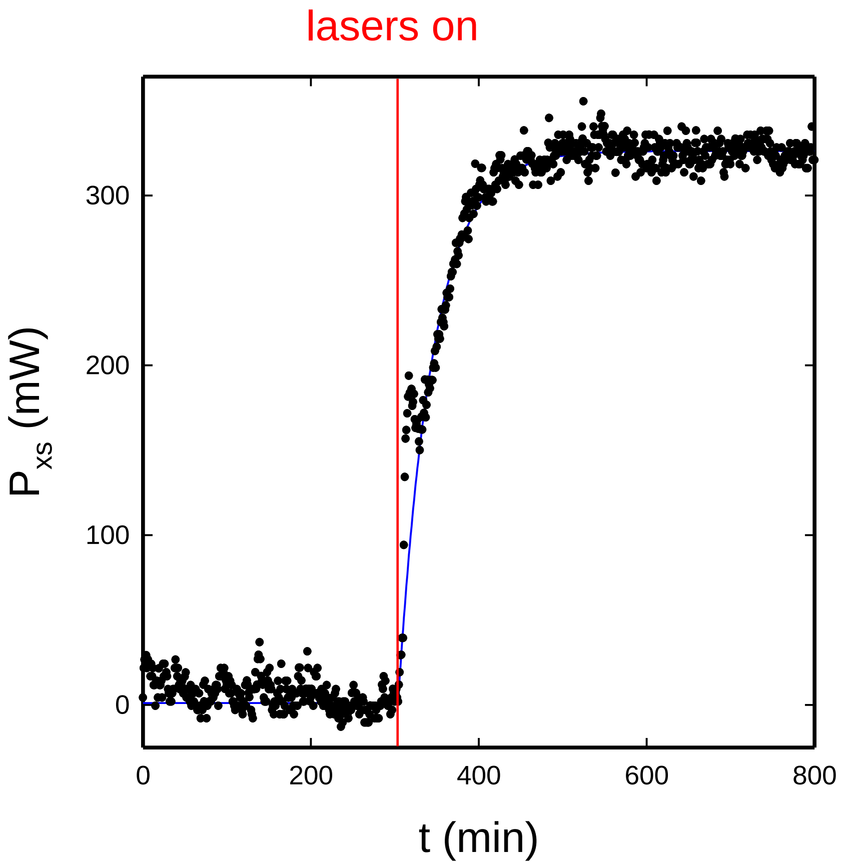


Figure 1. Schematic of the experimental set-up.

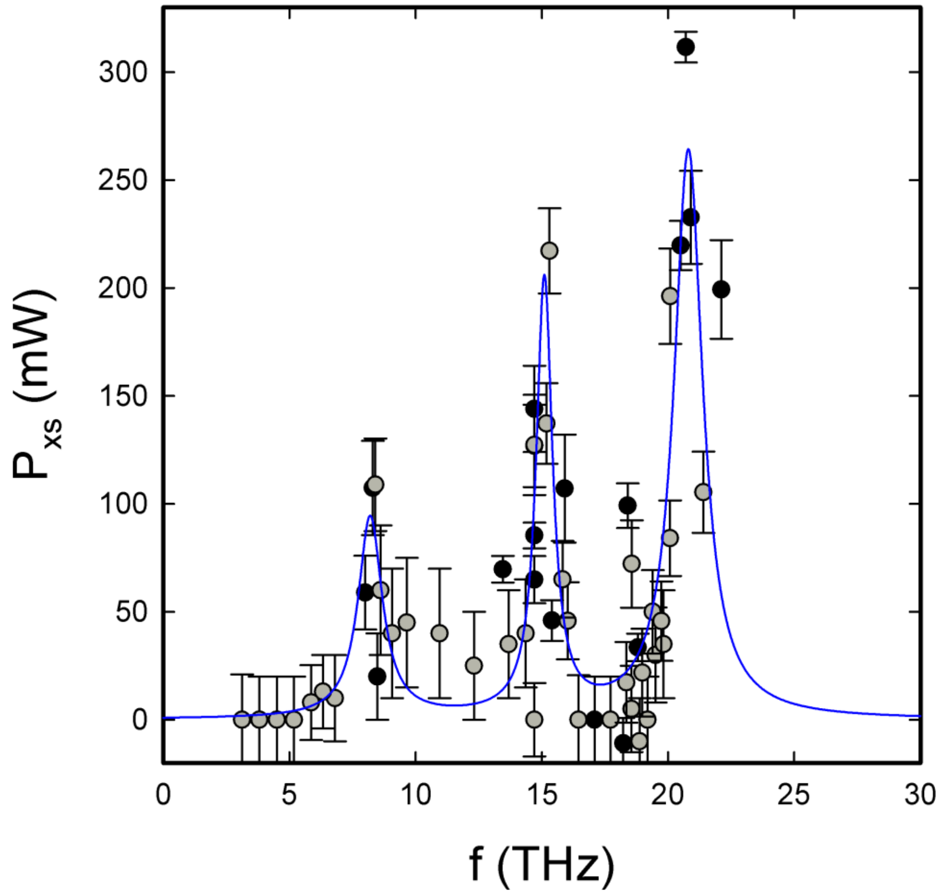
D. Letts, D. Cravens, and P.L. Hagelstein, *LENR Sourcebook* Volume 2, ACS: Washington DC. p. 81-93 (2009).

Excess power with 2 lasers

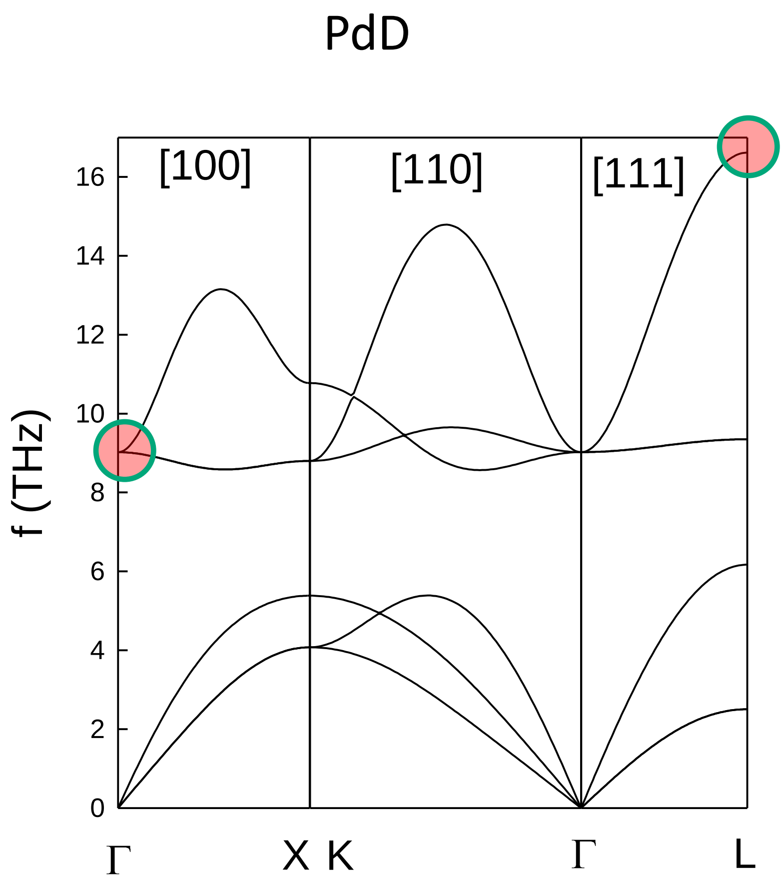


P. Hagelstein, D. Letts, and D. Cravens, *J Cond. Mat. Nucl. Sci.* **3** *59, 77 (2010)*

Sweet spots in the spectrum

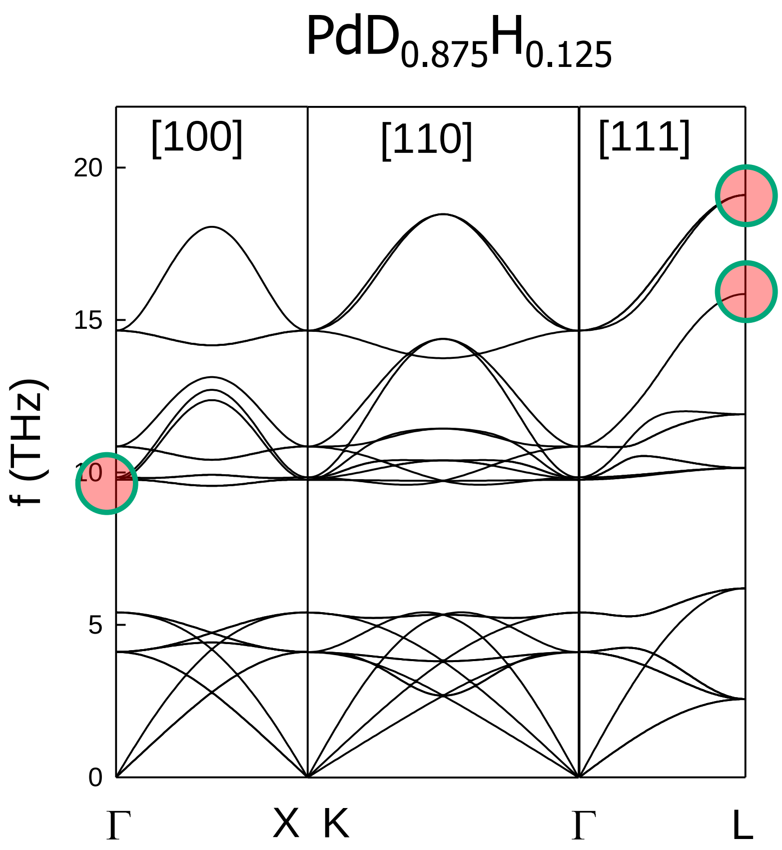


Dispersion curve for PdD



Operation was predicted on compressional modes with zero group velocity

Dispersion curve for PdD with some H



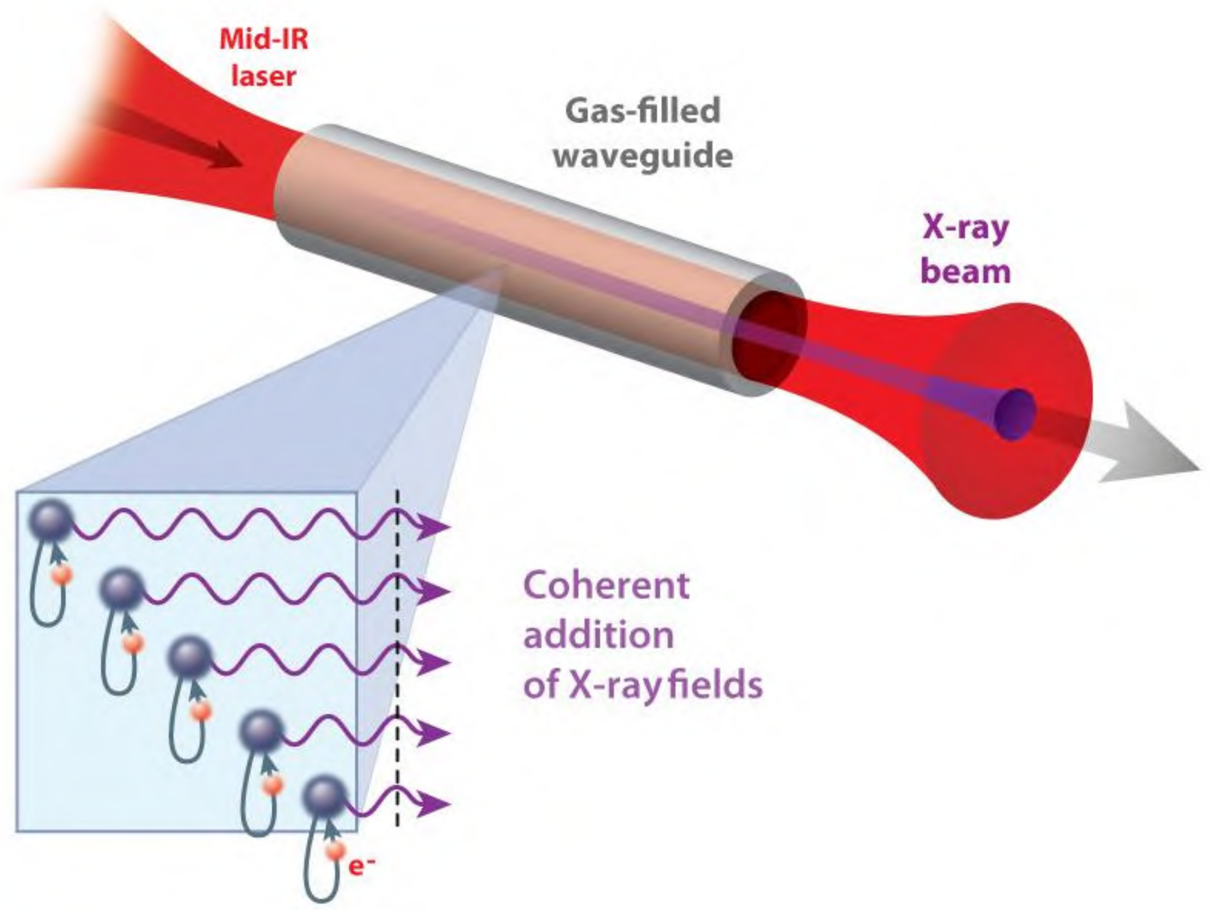
Take away message

•Excess power remains when lasers turned off in 2-laser experiment
•Propose that two-lasers initially stimulate optical phonon mode weakly at difference frequency
•Excitation of optical phonon mode allows new process to get going
•Energy from reaction proposed to go into optical phonon mode (in this experiment)
•Zero-group velocity modes favored (lower loss when phonon energy doesn't leave)
•Would explain why excess heat effect persists when lasers turned off

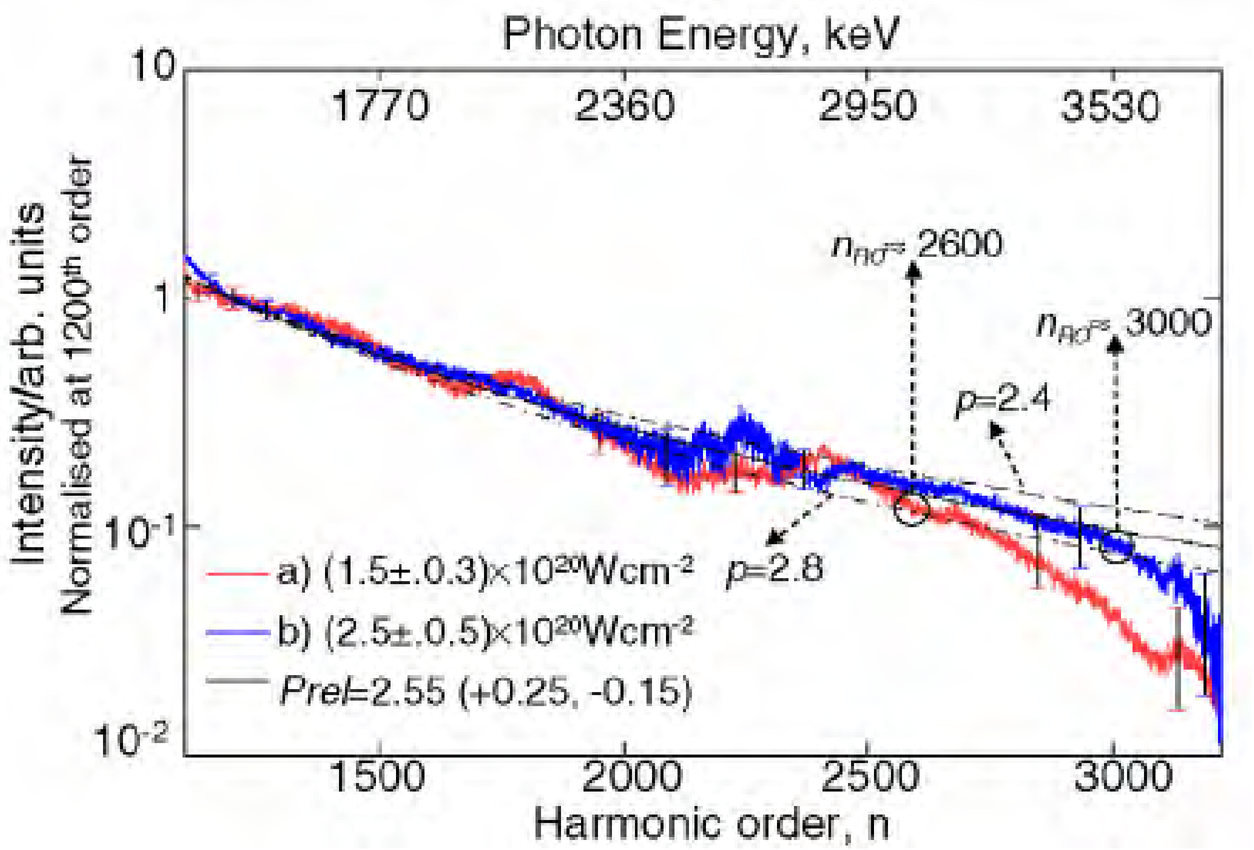
Biggest theory problem

- How to convert nuclear energy to vibrational energy?
- Problem is that nuclear energy quantum is big (MeV) and vibrational energy quantum is small (meV)
- Efficient energy exchange between systems with mismatched quantum is problematic

High harmonic generation



Collimated x-ray generation

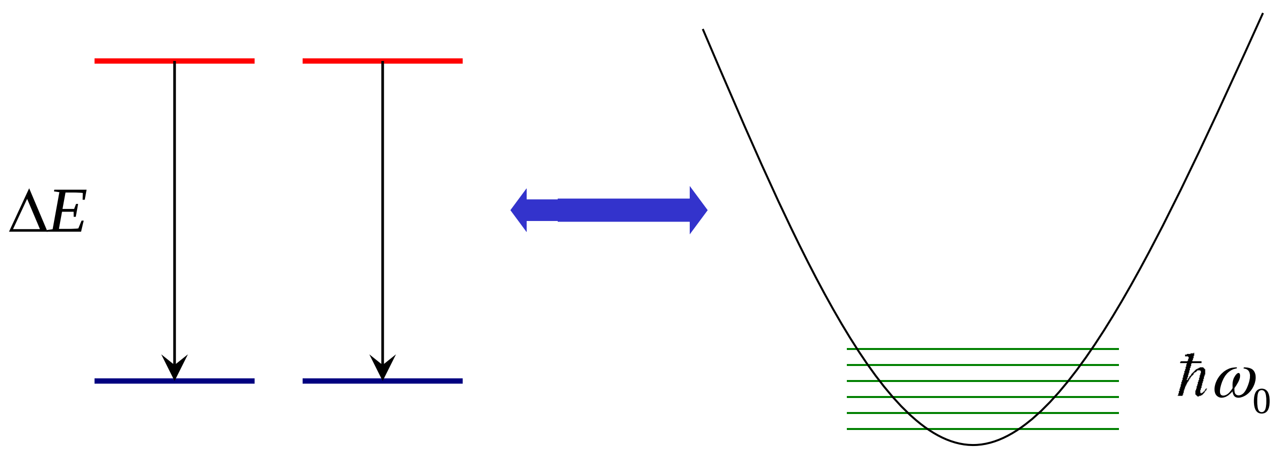


B. Dromey et al, *Phys. Rev. Lett.* **99** 085001 (2007).

Take away message

- Experiment suggests nuclear energy converted to optical phonons
- But nuclear quantum is O(MeV) and phonons are O(meV)
- Need to down-convert by nine orders of magnitude
- Coherent energy exchange with massive up and down conversion is known
- Few thousand quantum exchange in HHG by Corkum mechanism
- Not sure if possible
- But if it is going to happen, need a mechanism to do it!

Basic toy model



Two-level systems

Macroscopic excited mode

$$\boxed{\Delta E \;>>\; \hbar\omega_0}$$

Many-spin spin-boson model

Popularized by

C. Cohen-Tannoudji

$$\hat{H} = \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \hat{a}\hat{a}^\dagger + V \frac{2\hat{S}_x}{\hbar}\left(\hat{a} + \hat{a}^\dagger\right)$$

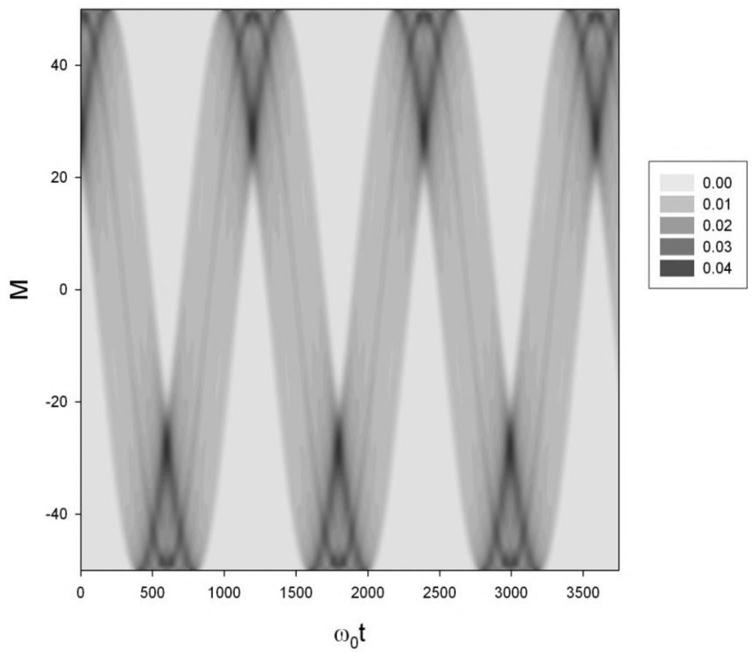
Two-level systems energy

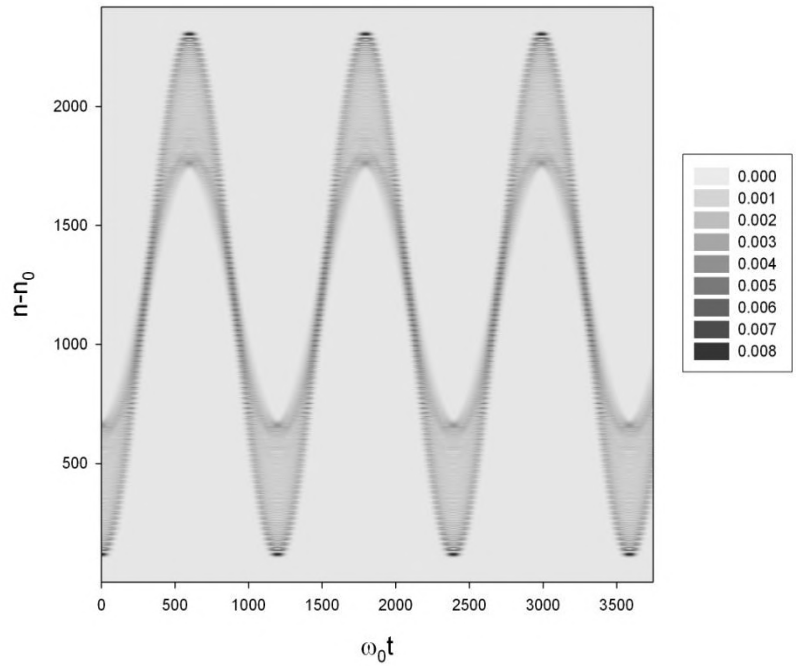
Harmonic oscillator energy

Linear coupling between two-level systems and oscillator

Earlier versions of the model due to Bloch and Siegert (1940)

Coherent energy exchange

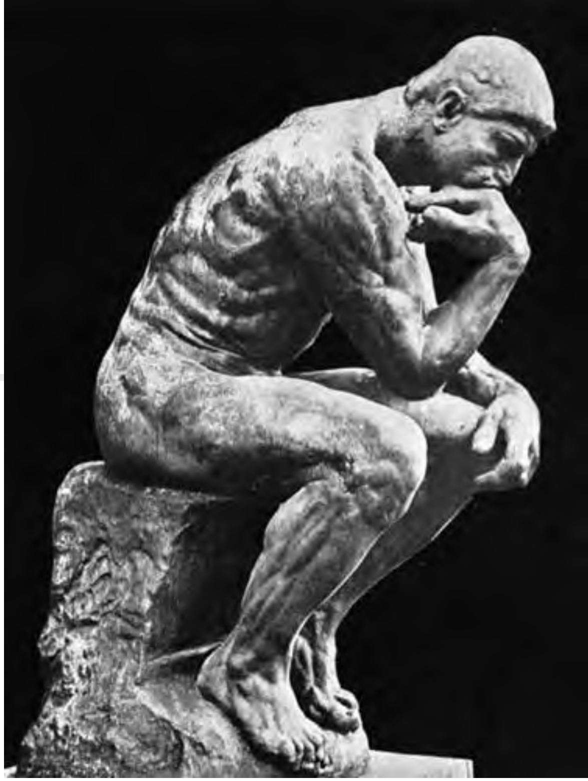




Numerical results for coherent energy exchange of 1700 oscillator quanta between 100 two-level systems and an oscillator

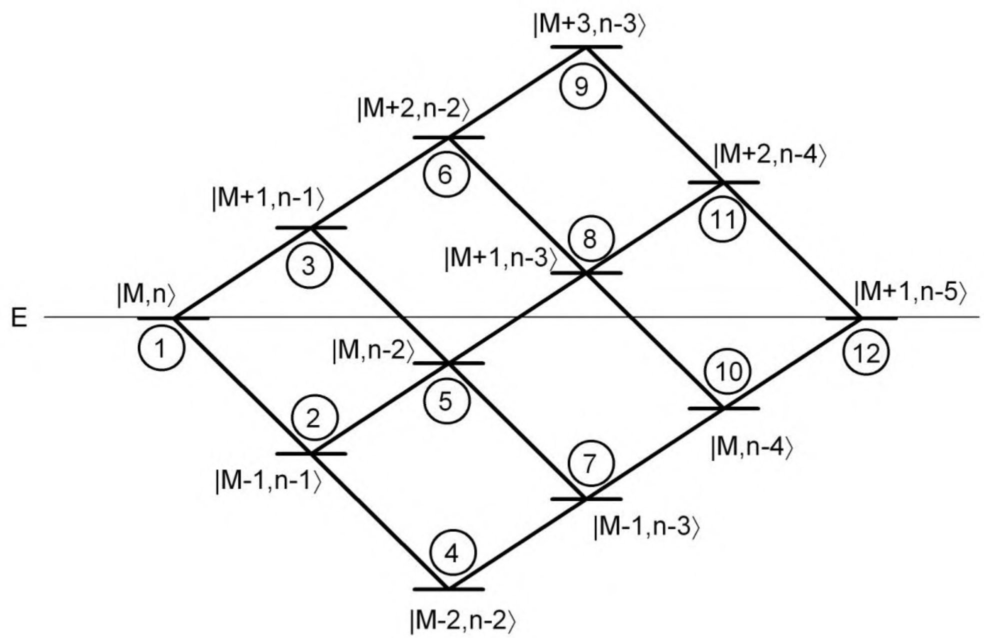
How does it work?

- Energy exchange from two-level system happens one quantum at a time
- You just keep exchanging quanta over and over again while maintaining coherence
- Agrees with analytic and numeric calculations



Wonder what limits number of quanta that can be exchanged…

Perturbation theory



Indirect coupling determined by contributions from all pathways, and large cancellation occurs

Finite basis approximation for $|n\rangle \otimes |M\rangle \rightarrow |n-5\rangle \otimes |M+1\rangle$

OK, the spin-boson model runs out of steam because of destructive interference effect. Contributions from different pathways cancel out nearly perfectly, so that overall rate is orders of magnitude smaller than individual pieces.

Lossy spin-boson model

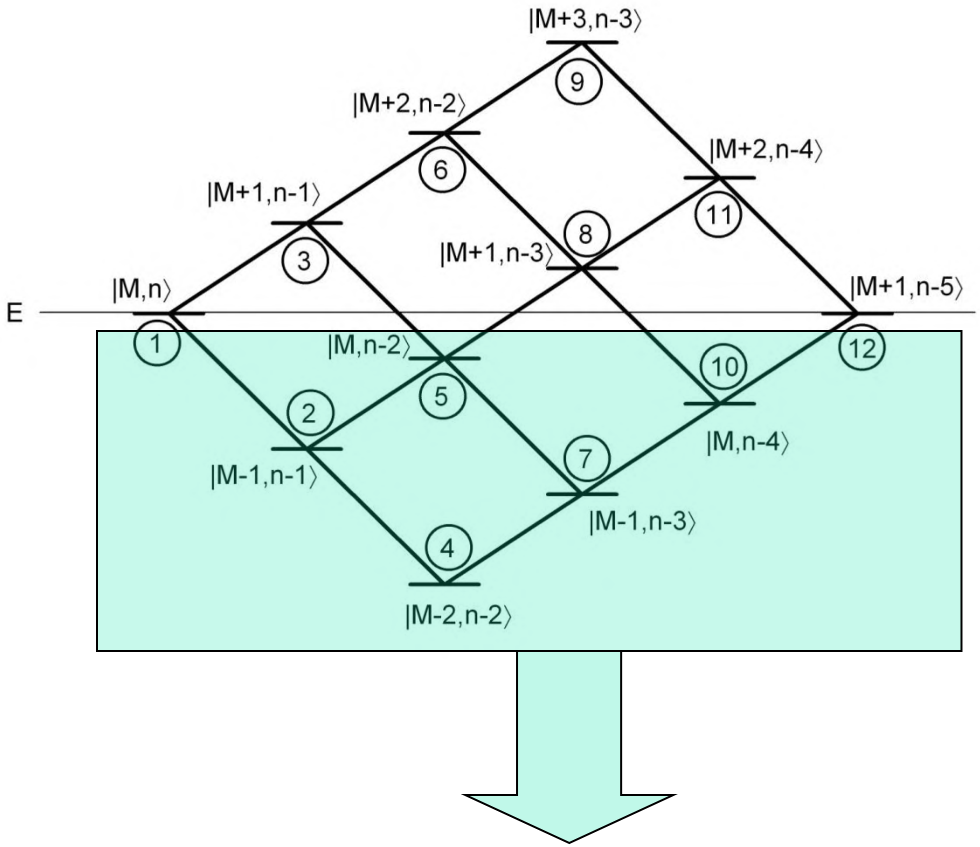
$$\hat{H} = \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \hat{a}\hat{a}^\dagger + V \frac{2\hat{S}_x}{\hbar}\left(\hat{a} + \hat{a}^\dagger\right) - i\frac{\hbar}{2}\hat{\Gamma}(E)$$

Loss term, which allows the system to decay when a large energy quantum is available

$$\frac{\Delta E}{\hbar\omega_0} = \Delta n$$

P. L. Hagelstein and I. U. Chaudhary, *J. Cond. Mat. Nucl. Sci.* **5** 52 (2011)

Perturbation theory



Loss channels available for off-resonant states with energy excess, which spoils the destructive interference

P. L. Hagelstein and I. U. Chaudhary, *J. Cond. Mat. Nucl. Sci.* **5** 52 (2011)

•Physical loss terms will be sensitive to the state energy
•Provides mechanism to eliminate destructive interference
•Resulting coherent energy transfer rate in perturbation theory larger by many orders of magnitude

Solution for simplest version

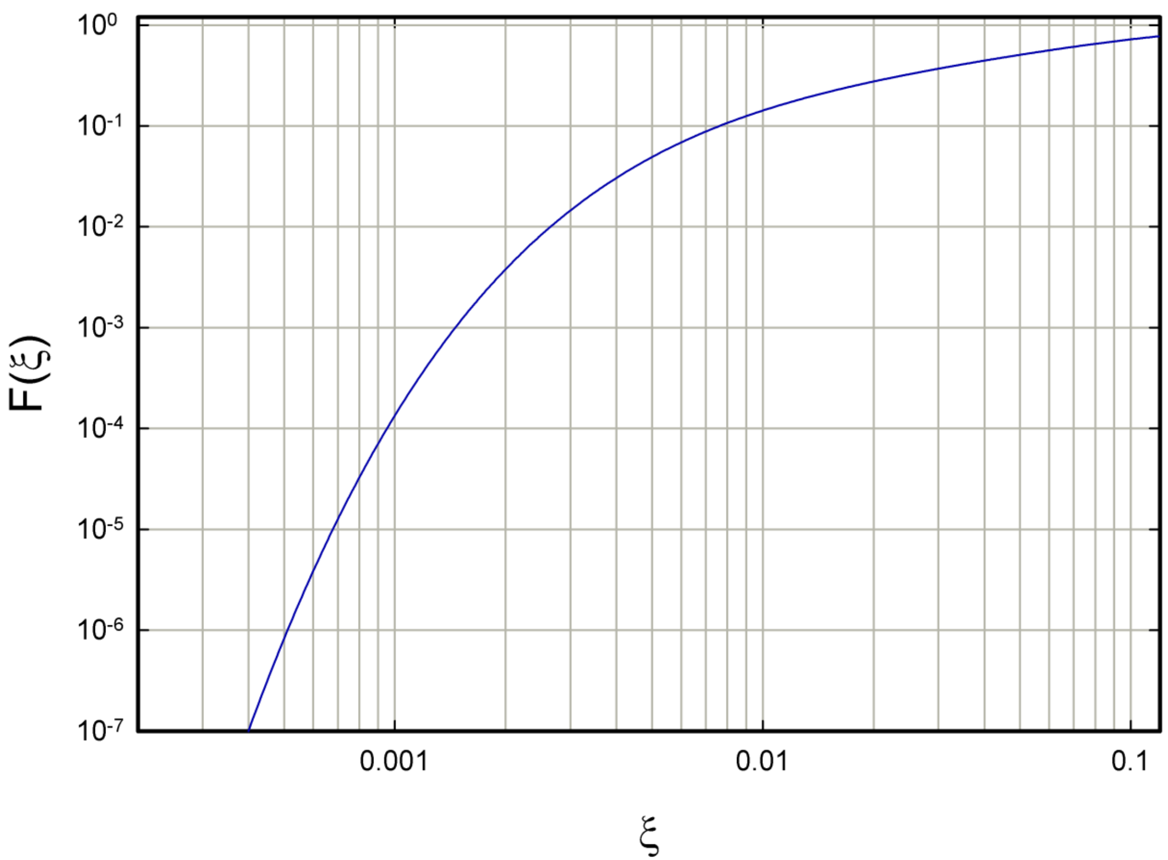
$$\frac{d^2}{dt^2}y(t) = -\Omega^2(y, g_{\max}, \Delta n)\, y(t)$$

$$y(t) = \frac{m(t)}{S} \qquad \Delta n = \frac{\Delta E}{\hbar\omega_0}$$

$$g_{\max} = \frac{V\sqrt{n}S}{\Delta E} \qquad \xi = \frac{g_{\max}}{\Delta n^2}\sqrt{1-y^2}$$

$$\Omega(y, g_{\max}, \Delta n) = \boxed{\frac{4}{\Delta n^2}\frac{V\sqrt{n}}{\hbar}\, F(\xi)}$$

Hindrance factor



If the coupling is sufficiently strong, then energy exchanges freely

Oscillation frequency

Maximum oscillation frequency is

$$\Omega_0 = \frac{4}{\Delta n^2}\frac{V\sqrt{n}}{\hbar}$$

Associated Rabi oscillation frequency

$$\Omega_0 = 4\frac{V\sqrt{n}}{\hbar}$$

Get $1/\Delta n^2$ penalty for transferring many oscillator quanta

P. L. Hagelstein and I. U. Chaudhary, *J. Cond. Mat. Nucl. Sci.* **5** 116 (2011)

We succeeded in analyzing the model, and we obtained the coherent energy exchange rate for a simplified version of the model in the strong coupling limit. The resulting rate can be fast as long as the coupling is sufficiently strong, and the scaling in the MeV to meV regime is gentle.

Fast forward…

- 10+ years experience with new models
- Focus on weakly-coupled donor / strongly-coupled receiver models
- Describe reactions just like what is needed
- $D_2/^4He$ transition ←→ weakly coupled donor
- Identification of receiver was problematic (hard to arrange for strong enough coupling)
- New (2012) model based on relativistic a*(cP) coupling appears to resolve outstanding issues

Start with relativistic model

Start with relativistic model for nucleons and electrons

$$\hat{H} = \left[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j m_j c^2 + \sum_{j<k} V_{jk}^{nn} \right]_{\text{nucleons}} + \left[\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\mathbf{p}}_j + \beta_j m_j c^2 + \sum_{j<k} V_{jk}^{ee} \right]_{\text{electrons}} + \sum_{jk} V_{jk}^{en}$$

P. L. Hagelstein and I. U. Chaudhary, *JCMNS* **7** 35 (2012)

Born-Oppenheimer approx

$$\hat{H} =$$

$$\sum_l \left\{ \boxed{\sum_j \frac{m_j}{M} \boldsymbol{\alpha}_j \cdot c\mathbf{P}} + \boxed{\sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \beta_j m_j c^2 + \sum_{j<k} (\text{same}) V_{jk}^{nn}} + \boxed{\sum_{j<k} (\text{different}) U_{jk}^{nn}} \right\}_l$$

center of mass | relative nuclear problem | nucleus-nucleus

Center of mass and nucleus-nucleus interaction given new condensed matter problem; get (new) interaction with relative states

Use nuclear basis states

$$\hat{H} = \boxed{\sum_j \frac{|\mathbf{P}_j|^2}{2M_j} + \sum_{j<k} U_{jk}} + \sum_j \left(\boxed{\mathbf{M}_j c^2} + \boxed{\mathbf{a}_j \cdot c\mathbf{P}_j - \frac{|\mathbf{P}_j|^2}{2M_j}} \right)$$

lattice vibrations basis state masses coupling counter-term

Now have model for phonon modes and nuclear states, with coupling and counter term

Harmonic lattice, and eliminate unphysical states

$$\hat{H} = \boxed{\sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k} + \sum_j \left(\boxed{\mathbf{M}_j c^2} + \boxed{\mathbf{a}_j \cdot c\mathbf{P}_j - \left(\mathbf{a}_j \cdot c\mathbf{P}_j\right)\left[E - \mathbf{M}_j c^2\right]^{-1}\left(\mathbf{a}_j \cdot c\mathbf{P}_j\right)} \right)_{\text{positive energy}}$$

phonon modes   basis state masses   coupling   counter-term

Most of the kinetic energy comes from coupling with negative energy states; counter term now from perturbation theory

$$\left(\mathbf{a}\cdot c\mathbf{P}\right)\left[E - \mathbf{M}c^2\right]^{-1}\left(\mathbf{a}\cdot c\mathbf{P}\right) \rightarrow \frac{|\mathbf{P}|^2}{2M} \quad \text{if all states included}$$

No new effects unless mode is highly excited

Focus on highly-excited mode, other modes assumed thermal

$$\hat{H} =$$

$$\hbar\omega_0 \hat{a}^\dagger \hat{a} + \sum_j \left(\mathbf{M}_j c^2 + \mathbf{a}_j \cdot c\mathbf{P}_j - \left(\mathbf{a}_j \cdot c\mathbf{P}_j\right) \left[E - \mathbf{M}_j c^2 \right]^{-1} \left(\mathbf{a}_j \cdot c\mathbf{P}_j\right) \right)_{\text{positive energy}}$$

This is our new basic model. It describes coherent energy exchange with fractionation, excess heat production, and other effects as well

Replacement for old donor and receiver model

$$\hat{H} = \hbar\omega_0 \hat{a}^\dagger \hat{a} + \sum_j \left(\mathbf{M}_j c^2 + \mathbf{a}_j \cdot c\mathbf{P}_j \right)_{\text{stable}} + \sum_j \left(\mathbf{M}_j c^2 + \mathbf{a}_j \cdot c\mathbf{P}_j \right)_{\text{unstable}}$$
$$- i \frac{\hbar \hat{\Gamma}(E)}{2}$$

Transitions with stable upper states can undergo coherent dynamics; transitions with unstable upper states mix with vibrational degree of freedom (and fractionate large quanta)

Counter terms very small compared to effects when loss present, so they are suppressed in this notation

Status

- Deuteron receiver for PdD excess heat with highly-excited optical phonon modes

- Transition matrix element now calculated (a = 0.003)

- Selection rules account for dependence of excess heat on magnetic field

- Transition matrix element now calculated for D_2/^4He transition

- Selection rules help understand requirement on local molecular D_2 environment

More status

- Earlier models simplified to make math simpler; new models under construction are much more complete and powerful
- New formulation for non-uniform highly-excited phonon mode
- Will shortly test model on Letts 2-laser experiments
- Connection with PdD hot spots (next talk)
- Connection with NiH (next talk)
- Same model gives Karabut collimated x-ray effect (next talk)