Modeling excess heat and related issues

Peter Hagelstein
Research Laboratory of Electronics
MIT

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Observation of a heat burst

$\Delta T = 27 \, ^\circ C$

Integrated energy

4 MJ/cm³ = 630 kJ

60 hours
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: \( \text{D}_2\text{O} + 0.1 \text{ M LiOD} \)

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

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

M4: Excess Power Correlation at SRI
[Closed, He-leak tight, Mass-Flow Calorimeter, Accuracy ±0.35%]

\[ P_{xs} = M (x - x^\circ)^2 (i - i^\circ) \frac{\dot{x}}{\dot{t}} \]

\[ x^\circ = 0.833, \quad i^\circ = 0.425, \quad r = 0.853 \quad 73\% \]

$^4\text{He}$ measurements

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

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

\[
(p_1 + p_2)_f = (p_1 + p_2)_i \\
\left( \frac{1}{2} m_1 |v_1|^2 + \frac{1}{2} m_1 |v_2|^2 \right)_f = \left( \frac{1}{2} m_1 |v_1|^2 + \frac{1}{2} m_1 |v_2|^2 \right)_i + Q
\]
Energy and momentum conservation

Initial state:

Final state:

\[
\frac{1}{2} M_1 |v_1|^2 = \left( \frac{M_2}{M_1 + M_2} \right) Q = \frac{3}{4} Q
\]

\[
\frac{1}{2} M_2 |v_2|^2 = \left( \frac{M_1}{M_1 + M_2} \right) Q = \frac{1}{4} Q
\]
Can learn about the reaction if we knew $^4$He energy

A proposed reaction scheme:

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

$$\frac{1}{2} M_{4\text{He}} \left| v_{4\text{He}} \right|^2 = \left( \frac{M_X}{M_{4\text{He}} + M_X} \right) 24 \text{ MeV}$$

$$\frac{1}{2} M_X \left| v_X \right|^2 = \left( \frac{M_{4\text{He}}}{M_{4\text{He}} + M_X} \right) 24 \text{ MeV}$$
Propose using PdD as detector
Stopping power from SRIM

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

$R(E)$

$E_{\alpha} (eV)$
Yield/energy for secondary neutrons

Examine d+d+X candidates

\[
d + d + \text{Pd} \rightarrow ^4\text{He}(23.0 \text{ MeV}) + \text{Pd}(0.85 \text{ MeV})
\]
\[
d + d + d \rightarrow ^4\text{He}(7.95 \text{ MeV}) + d(15.9 \text{ MeV})
\]
\[
d + d + e^- \rightarrow \text{He}(76 \text{ keV}) + e^-(23.77 \text{ MeV})
\]

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 $^4\text{He}$ observed correlated with $P_{xs}$
• Q-value consistent with $d+d\rightarrow^4\text{He}$
• But no commensurate nuclear radiation
• And $^4\text{He}$ born essentially at rest
• And no plausible Rutherford reaction consistent with experiment

• So, where does the energy go?
Letts 2-laser experiment

Excess power with 2 lasers

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

\[ PdD_{0.875}H_{0.125} \]
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

Mid-IR laser

Gas-filled waveguide

X-ray beam

Coherent addition of X-ray fields

e-
Collimated x-ray generation

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

$\Delta E \gg \hbar \omega_0$

Macroscopic excited mode
Many-spin spin-boson model

Popularized by C. Cohen-Tannoudji

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

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

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

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

\[
\frac{\Delta E}{\hbar \omega_0} = \Delta n
\]

Perturbation theory

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

• 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

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

\[
y(t) = \frac{m(t)}{S} \quad \Delta n = \frac{\Delta E}{\hbar \omega_0}
\]

\[
g_{\text{max}} = \frac{V \sqrt{nS}}{\Delta E} \quad \xi = \frac{g_{\text{max}}}{\Delta n^2} \sqrt{1 - y^2}
\]

\[
\Omega(y, g_{\text{max}}, \Delta n) = \frac{4}{\Delta n^2} \frac{V \sqrt{n}}{\hbar} F(\xi)
\]
Hindrance factor

If the coupling is sufficiently strong, then energy exchanges freely.
Oscillation frequency

Maximum oscillation frequency is

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

Associated Rabi oscillation frequency

\[ \Omega_0 = 4 \frac{V \sqrt{n}}{\hbar} \]

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

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
- $^2\text{D}/^4\text{He}$ transition $\leftrightarrow$ 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 for nucleons and electrons

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

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

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

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

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

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

\[ (\mathbf{a} \cdot \mathbf{cP}) \left[ E - \mathbf{Mc}^2 \right]^{-1} (\mathbf{a} \cdot \mathbf{cP}) \rightarrow \frac{|\mathbf{P}|^2}{2M} \quad \text{if all states included} \]
No new effects unless mode is highly excited

Focus on highly-excited mode, other modes assumed thermal

\[ \hat{H} = \hbar \omega_0 \hat{a}^\dagger \hat{a} + \sum_j \left( M_j c^2 + \mathbf{a}_j \cdot \mathbf{P}_j - \left( \mathbf{a}_j \cdot \mathbf{P}_j \right) \left[ E - M_j c^2 \right]^{-1} \left( \mathbf{a}_j \cdot \mathbf{P}_j \right) \right) \]

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

\[ \hat{H} = \hbar \omega_0 \hat{a} \hat{a}^\dagger + \sum_j \left( M_j c^2 + a_j \cdot c P_j \right) + \sum_j \left( M_j c^2 + a_j \cdot c P_j \right) \]

\[ -i \frac{\hbar \Gamma(E)}{2} \]

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.
• 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)