# Update on Phonon-Coupled SU[n] Models

Peter L. Hagelstein Research Laboratory of Electronics Massachusetts Institute of Technology

# Outline

- Introduction
- Maximization of Overlap
- Inclusion of Lattice in Nuclear Problem
- Site-other-site processes
- Null reaction
- Phonon-coupled SU(N) models
- Conclusions



Studies of metal deuterides indicate the existence of new physical effects:

- Low-level dd-fusion
- •Fast alpha emission
- Kasagi d+d+d reaction
- Excess heat
- •Helium
- •Tritium

## Fundamental issues

- Why should there be any new effects?
- How can deuterons come together?
- Is it possible for reaction energy to be expressed as lattice energy?
- Do there exist new reaction mechanisms in a lattice that can compete with vacuum d+d reactions?

Theory effort

Theory pursued since 1989:

- •Was not obvious where to start
- •Was not clear which effects real
- •Theory in field viewed as impossible
- Assessment of roughly 150 different approaches, models, and variants
- •Edisonian approach initially sought to learn lessons from failed schemes

*No consensus in field on theory – this presentation focuses on one approach to the problem* 

## Maximization of Overlap

Models based on d+d reactions need for deuterons to get together, so we need to understand what maximizes overlap

We studied this problem using a simple two deuteron model based on:

$$\hat{H} = -\frac{\hbar^2 \nabla_1^2}{2M} - \frac{\hbar^2 \nabla_2^2}{2M} + V_{lat}(\mathbf{r}_1) + V_{lat}(\mathbf{r}_2) + V_{mol}(\mathbf{r}_2 - \mathbf{r}_1)$$

Conclusion

Deuterons at adjacent sites



Tunneling from one site to another is hindered

Double occupancy



Tunneling is like D<sub>2</sub> but probability of double occupancy is low

## Pd lattice structure (fcc)



## PdD lattice structure (fcc)



## **Double occupation**



# Connection with experiment

Double occupancy appears to be maximized under conditions favorable for anomalies:

- •High loading: D/Pd ratio near or over unity
- •Defects [single host metal atom vacancies]
- •Elevated temperature:

$$P_{xs} \square e^{-\Delta E/kT}$$

where  $\Delta E$  observed to be 670 meV by Storms, which is near the energy associated with double occupancy

#### Thermodynamics - bulk $p = \frac{g_{DD} e^{-(\varepsilon - 2\mu)/kT}}{1 + g_D e^{-(\varepsilon - \mu)/kT} + g_{DD} e^{-(\varepsilon - 2\mu)/kT}}$ Two deuterons 600 meV 500 10-8 10-6 10-7 450 10<sup>-9</sup> 10-10 Unoccupied 400 -0 meV 10<sup>-8</sup> ¥ 350 ⊢ 10<sup>-9</sup> 10<sup>-10</sup> -80 meV 300 Single deuteron 250 -200

0.2

0.4

D/Pd

0.6

0.8

## Vacancies in host lattice



Vacancies in host metal lattice are thermodynamically favored at high loading

## PdD Host lattice vacancy



Deuterium atoms relax toward host vacancy

#### Thermodynamics - vacancies



## **Increase in Occupation**



Vacancies improve double occupancy most at lower temperatures

# Inclusion of Lattice in the Nuclear Problem

Since the 1930s, physicists have considered reactions between nuclei to occur the same in solids as would be expected in vacuum



What happens if we include the lattice in the problem at the outset?

# **Resonating Group Method**

Early efforts at modeling fusion reactions were based on the resonating group method

The premise of the method is that the internal nuclear states are fixed, and the separation is described using channel factors  $F_i$ 

$$\psi_T = \sum_j \Phi_j F_j$$

The optimization of the channel separation factors leads to coupled-channel equations:

$$EF_{j} = \left\langle \Phi_{j} \left| \hat{H} \right| \Phi_{j} \right\rangle F_{j} + \sum_{k \neq j} \left\langle \Phi_{j} \left| \hat{H} - E \right| \Phi_{k} F_{k} \right\rangle$$

See J. A. Wheeler, Phys. Rev. 52, 1107 (1937).

## Now Include the Lattice

Generalize the resonating group method to include lattice effects

$$\Psi_T = \sum_j \Phi_j \Psi_j$$

The optimization of the lattice channel separation factors leads to new coupled-channel equations:

$$E\Psi_{j} = \langle \Phi_{j} | \hat{H} | \Phi_{j} \rangle \Psi_{j} + \sum_{k \neq j} \langle \Phi_{j} | \hat{H} - E | \Phi_{k} \Psi_{k} \rangle$$

New formulation now includes lattice effects on equal footing with nuclear problem

P. L. Hagelstein, ``A unified model for anomalies in metal deuterides," *Proceedings of the ICCF8*, Lerici (La Spezia), Italy, May 2000; p. 363.



Lattice resonating group method includes phonon exchange in reaction description

- Vacuum reaction physics included as subset
- •Angular momentum exchange with phonon exchange predicted
- Modification of vacuum selection rules
- •New site-other-site processes

### Site-other-site processes



Early proposal for mechanism for fast alpha emission

## In space...



Phononinduced disintegration at another site

Fusion at one site, with phonon exchange

## Second-order disintegration



Second-order disintegration in this case probably works more like photodisintegration

## Alpha spectrum from Pd



# Discussion

- New mechanism for alphas from PdD
- Predict fast alphas and protons from TiD
- Expect neutrons with exponential distribution
- Second-order reaction model gives rate orders of magnitude too small, so we know that mechanism is more complicated

# Ti p, $\alpha$ ejection energies



Alpha ejection energies from second-order mechanism in right range. Protons expected but not seen.

## **Absence of Protons**

Conjecture that angular momentum exchange with phonons leads to suppression of the proton channel

## Fastest site-other-site process

If site-other-site reactions can occur, then what is fastest possible reaction of this class?



Coupling to continuum

Coupling to discrete state





Early proposal for null reaction mechanism

## Null Reaction -- Observable?

For years after proposing the null reaction, we wondered whether there was any possibility of observing it – this was considered unlikely, since the initial state and final state products seemed to be the same, only exchanged in position

After analyzing the scheme, we understood that two deuterons created from helium dissociation as part of a site-other-site reaction would have trouble tunneling apart, and hence might be observable in a collision experiment

## Schematic of measurement



## The Kasagi Experiment



**Proton signals** 

Kasagi saw dd-fusion products; also fast protons and alphas from direct d+<sup>3</sup>He and from secondary <sup>3</sup>He+d reactions

A proton signal between 8 and 12 MeV was not accounted for; and a similar alpha signal below about 7 MeV

J. Kasagi et al, J. Phys. Soc. Japan 64, 777 (1995).



## Schematic of proton spectrum



Reactions that make fast protons and alphas:

 $d + {}^{3}He \rightarrow p + {}^{4}He$  (<sup>3</sup>He accumulates in the target)  $d + d \rightarrow n + {}^{3}He$  followed by  ${}^{3}He + d \rightarrow p + {}^{4}He$ 

# Discussion

Kasagi experiment interpreted as:

$$d + (d+d)_{compact} \rightarrow n + p + {}^{4}He$$

- •Where are d+<sup>4</sup>He and t+<sup>3</sup>He channel products?
- •Data consistent with 10<sup>-6</sup> of deuterons in compact states
- •How can compact states be so stable?

## Angular momentum



Suppression of the tunneling rate for the n+<sup>3</sup>He channel as a function of angular momentum
## Stabilization of compact states

- 20 units or more of angular momentum stabilizes compact states
- Two-body exit channels suppressed if large angular momentum present
- Phonon exchange capable of large angular momentum exchange

### Phonon interactions

General model is complicated, so we need to Simplify – propose reduced models to study

- •Only get effects when phonon exchange nonlinear
- Assume one phonon mode highly excited
- •All other modes thermal
- •Focus on two-site problem to see how it works
- Use simplified nuclear description initially

### **Position operators**

Can express the position operator in terms of phonon mode amplitudes

$$\hat{\mathbf{R}}_{j} = \sum_{m} \mathbf{u}_{m} [j] \, \hat{\boldsymbol{q}}_{m}$$

Position operator is local:  $\hat{\mathbf{R}}_{i}$ 

Phonon mode is nonlocal:  $\hat{q}_m$ 

How to model with strong (delocal phonon mode) and strong nuclear short range interaction?

### Hybrid description

Separation of lattice and nuclear degrees of freedom

$$\hat{\mathbf{R}}_{j} = \mathbf{u}_{j}[m] \, \hat{q}_{m} + \sum_{m' \neq m} \mathbf{u}_{j}[m'] \, \hat{q}_{m}$$

Define residual position operator:

$$\hat{\mathbf{R}}_{j} = \sum_{m' \neq m} \mathbf{u}_{j} [m'] \hat{q}_{m}$$

Leads to hybrid description:

$$\hat{\mathbf{R}}_{j} = \mathbf{u}_{j}[m] \, \hat{q}_{m} + \hat{\bar{\mathbf{R}}}_{j}$$

## Discussion

- Separation of local and nonlocal degrees of freedom
- Hybrid description allows direct computation of phonon exchange
- Results for scalar Gaussian nuclear models
- Work in progress on better nuclear models
- Duschinsky mechanism for phonon and angular momentum exchange

### Simplified Nuclear Interaction

Assume variational Gaussian wavefunctions and potential

$$\Phi_{d} = N_{2} e^{-\beta_{2} \left| \mathbf{r}_{1} - \mathbf{r}_{2} \right|^{2}}$$

$$\Phi_{He} = N_4 e^{-\beta_4 \left| \mathbf{r}_1 - \mathbf{r}_2 \right|^2} e^{-\beta_4 \left| \mathbf{r}_1 - \mathbf{r}_3 \right|^2} e^{-\beta_4 \left| \mathbf{r}_1 - \mathbf{r}_4 \right|^2} e^{-\beta_4 \left| \mathbf{r}_2 - \mathbf{r}_3 \right|^2} e^{-\beta_4 \left| \mathbf{r}_2 - \mathbf{r}_4 \right|^2} e^{-\beta_4 \left| \mathbf{r}_3 - \mathbf{r}_4 \right|^2}$$
$$V = -V_0 \sum_{i < j} e^{-\alpha \left| \mathbf{r}_i - \mathbf{r}_j \right|}$$

### Nuclear interaction

$$\left\langle \Phi_{dd} \middle| \hat{H} - E \middle| \Phi_{He} \right\rangle = -V_0 N_2^2 N_4 \int d^3 \mathbf{x}_{21} \int d^3 \mathbf{x}_{43} e^{-\beta_2 \left| \mathbf{x}_{21} \right|^2} e^{-\beta_2 \left| \mathbf{x}_{43} \right|^2} \\ \left[ e^{-\alpha \left| \mathbf{r}_1 - \mathbf{r}_3 \right|^2} + e^{-\alpha \left| \mathbf{r}_1 - \mathbf{r}_4 \right|^2} + e^{-\alpha \left| \mathbf{r}_2 - \mathbf{r}_3 \right|^2} + e^{-\alpha \left| \mathbf{r}_2 - \mathbf{r}_4 \right|^2} \right] \\ e^{-\beta_4 \left| \mathbf{x}_{21} \right|^2} e^{-\beta_4 \left| \mathbf{r}_1 - \mathbf{r}_3 \right|^2} e^{-\beta_4 \left| \mathbf{r}_1 - \mathbf{r}_4 \right|^2} e^{-\beta_4 \left| \mathbf{r}_2 - \mathbf{r}_3 \right|^2} e^{-\beta_4 \left| \mathbf{r}_2 - \mathbf{r}_4 \right|^2} e^{-\beta_4 \left| \mathbf{r}_4 \right|^2} e^{-$$

Separation between deuterons is a function of phonon mode coordinate:

$$\frac{1}{2}(\boldsymbol{r}_3 + \boldsymbol{r}_4) - \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2) = \bar{\boldsymbol{r}} + \Delta \boldsymbol{u}\hat{\boldsymbol{q}}$$

# Nuclear interaction in terms of phonon operators

Separation between deuterons is a function of phonon mode coordinate

$$\frac{1}{2}(\boldsymbol{r}_3 + \boldsymbol{r}_4) - \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2) = \bar{\boldsymbol{r}} + \Delta \boldsymbol{u}\hat{q}$$

WKB approximation:

$$\begin{split} \left\langle \Phi_{dd} \phi_{n} Y_{lm} \middle| \hat{H} - E \middle| \phi_{He} \phi_{n'} \right\rangle &= -4V_{0} \left[ \frac{8^{\frac{1}{4}} (2\beta_{2})^{\frac{3}{2}} (4\beta_{4})^{\frac{9}{4}}}{\pi^{\frac{1}{4}} (\beta_{2} + 2\beta_{4})^{\frac{3}{2}} (\beta_{2} + 2\beta_{4} + \frac{\alpha}{2})^{\frac{3}{2}}} \right] e^{-K \left| \vec{r} \right|^{2}} \sqrt{2l + 1} \delta_{m,0} \\ & \times \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-K \left| \Delta u \right|^{2} q_{\max}^{2} \sin^{2} \xi} i_{l} \left( 2K \bar{r} \middle| \Delta u \middle| q_{max} \sin \xi \right) \cos(\Delta n \xi) d\xi \end{split}$$

P. L. Hagelstein, ``Anomalies in metal deuterides," Proc. ICCF9 (2002)



### Thinking about results

- Approach allows for systematic calculation of phonon exchange
- If two deuterons are close together, they look like <sup>4</sup>He to lattice
- Hard to exchange phonons if initial and final states look so similar
- Need initial and final states to behave differently if we want to exchange 20 or more phonons

### Duschinsky in simple terms



Duschinsky mechanism can produce phonon and angular momentum exchange

Two site problem

$$\Psi = \sum_{n} A_{n} \left| \Phi_{He}^{a} \Phi_{He}^{b} \phi_{n} \right\rangle + \sum_{nlm} \left| \Phi_{dd}^{a} \Phi_{He}^{b} \phi_{n} Y_{lm} \right\rangle \frac{p_{nlm}^{a}(r)}{r}$$

$$+\sum_{nlm}\left|\Phi^{a}_{He}\Phi^{b}_{dd}\phi_{n}Y_{lm}\right\rangle\frac{p^{b}_{nlm}(s)}{s}$$

$$+\sum_{n}\sum_{lm}\sum_{l'm'}\left|\Phi^{a}_{dd}\Phi^{b}_{dd}\phi_{n}Y^{a}_{lm}Y^{b}_{l'm'}\right\rangle\frac{p^{ab}_{nlml'm'}(r,s)}{rs}$$

P. L. Hagelstein, Proc. ICCF9 (2001)

### **Coupled-channel equations**

-

$$\begin{split} EA_{n} &= \left[2E_{He} + \hbar\omega_{0}\left(n + \frac{1}{2}\right)\right]A_{n} + \sum_{n'lm}\int_{0}^{\infty}vl_{lm}^{nn'}(r)\left[P_{n'lm}^{a}(r)\right]dr\\ EP_{nlm}^{a}(r) &= \left[E_{He} + E_{dd} + \hbar\omega_{0}\left(n + \frac{1}{2}\right) - \frac{\hbar^{2}}{2\mu}\frac{d^{2}}{dr^{2}} + \frac{\hbar^{2}l(l+1)}{2\mu r^{2}} + V^{a}(r)\right]P_{nlm}^{a}(r)\\ &+ \sum_{n'}\left[v_{lm}^{nn'}(r)\right]^{*}A_{n'} + \sum_{n'}\sum_{l'm'}\int_{0}^{\infty}v_{l'm'}^{nn'}(s)P_{n'lml'm'}^{ab}(r,s)ds\\ EP_{nlm}^{b}(s) &= \left[E_{He} + E_{dd} + \hbar\omega_{0}\left(n + \frac{1}{2}\right) - \frac{\hbar^{2}}{2\mu}\frac{d^{2}}{ds^{2}} + \frac{\hbar^{2}l(l+1)}{2\mu s^{2}} + V^{b}(s)\right]P_{nlm}^{b}(s)\\ &+ \sum_{n'}\left[v_{lm}^{nn'}(s)\right]^{*}A_{n'} + \sum_{n'}\sum_{l'm'}\int_{0}^{\infty}v_{l'm'}^{nn'}(r)P_{n'lm'lm}^{ab}(r,s)dr \end{split}$$

$$E P_{nlml'm'}^{ab}(r,s) = \left[ 2E_{dd} + \hbar\omega_0 \left( n + \frac{1}{2} \right) - \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 l \left( l + 1 \right)}{2\mu r^2} + V^a \left( r \right) - \frac{\hbar^2}{2\mu} \frac{d^2}{ds^2} + \frac{\hbar^2 l' \left( l' + 1 \right)}{2\mu s^2} + V^b \left( s \right) \right] P_{nlml'm'}^{ab}(r,s) + \sum_{n'} \left[ v_{l'm'}^{nn'}(s) \right]^* P_{n'lm}^{ab}(r) + \sum_{n'} \left[ v_{lm'}^{nn'}(r) \right]^* P_{n'l'm'}^{b}(s)$$

### Analyze with unstable states

$$\psi(\mathbf{r},t) = \sum_{j} c_{j}(t)u_{j}(\mathbf{r})$$

$$i\hbar \frac{d}{dt}\mathbf{c}(t) = \mathbf{H} \cdot \mathbf{c}(t) - \frac{i\hbar}{2}\Gamma \cdot \mathbf{c}(t)$$

### Unstable basis model





## Coupled phonon SU(3) model

$$\begin{split} \hat{H} &= E_{He} \sum_{j} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{j} + E_{com} \sum_{j} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{j} + E_{mol} \sum_{j} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{j} + \hbar \omega_{0} \left( n + \frac{1}{2} \right) \\ &+ e^{-G} \sum_{jnn'} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{j} U_{nn'} \hat{\delta}_{nn'} + \sum_{jnn'} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}_{j} V_{nn'} \hat{\delta}_{nn'} \end{split}$$

### Augment model with loss effects

Start with model Hamiltonian

 $E\Psi = H_0\Psi + V\Psi$ 

Divide into 3 Hilbert space sectors:

 $\Psi = \Psi_1 + \Psi_2 + \Psi_3$ 

Get equivalent Brillouin-Wigner type flow calculation

$$\Psi_{2} = \left[ E - H_{2} - V_{23} \left[ E - H_{3} \right]^{-1} V_{32} \right]^{-1} V_{21} \Psi_{1}$$

P. L. Hagelstein, ``Anomalies in metal deuterides,'' Proc ICCF9 (2002)



$$\Psi_{2} = \left[ E - \hat{H}_{2} - i\hbar\hat{\Gamma}/2 \right]^{-1} \hat{V}_{21} \Psi_{1}$$

Weak coupling – Jones low-level dd-fusion



Moderate coupling and substantial angular momentum transfer – °1 accumulation of compact <sub>-2</sub> states, fast alpha emission



Strong coupling with large angular momentum transfer – massive coupling between nuclear and phonon degrees of freedom



# Coupling between nuclear and phononic degrees of freedom



Computations indicate that nuclear and phonon energy exchanged efficiently

# Nuclear and phonon energy exchange

Treat ratio of

 $\Delta E/\hbar\omega_0$ 

as a free parameter, and study transfer of nuclear energy to phonon energy



### Acceleration of Dynamics



### Massive excitation transfer I



DD/<sup>4</sup>He system transferring to <sup>4</sup>He/compact state system

### Massive excitation transfer II



DD/<sup>4</sup>He system transferring to Pd/compact state system

### Duschinsky for other cases



Duschinsky mechanism can produce phonon and angular momentum exchange for general nuclei in lattice

### Coherent excitation transfer



Results of model with 40 molecular state D<sub>2</sub> transferring excitation to 40 <sup>4</sup>He nuclei

$$\hat{V}' = e^{-G} \sum_{n'} V_{nn'} \hat{\mathcal{S}}_{nn'} \left( \hat{\Sigma}_{+}^{(1)} \hat{\Sigma}_{-}^{(2)} + \hat{\Sigma}_{-}^{(1)} \hat{\Sigma}_{+}^{(2)} \right)$$

t in units of 
$$\left[\frac{Ve^{-G}}{\hbar}\right]^{-1}$$

### Reaction rate in a burst





## **Connection with Experiment**

Model predicts relation between tunneling parameters, pulse length and maximum reaction rate

$$\frac{Ve^{-G}}{\hbar} = \frac{1}{2\pi\Gamma_{\max}\tau^2}$$

For a 5 hour pulse with  $\Gamma_{max} = 10^{12} \text{ sec}^{-1}$ , we get

$$e^{-G} = 3 \times 10^{-44}$$

This is close to the tunneling factor for  $D_2$ 

## Coupled phonon SU(4) model



### Coupled phonon SU(4) model

### Conclusions: I

- Double occupancy maximizes dd overlap
- Estimate of double occupancy in PdD
- Lattice resonating group method includes lattice in nuclear problem
- Proposal for new site-other-site reactions
- Proposed new explanation for fast alphas
- Proposal for new compact states
- Proposed explanation for Kasagi experiment

### Conclusions: II

- Proposal for new phonon/nuclear models
- Models appear to be relevant to heat effect, low-level dd-fusion effect, fast alpha emission, the Kasagi effect, and tritium
- New mechanism proposed for energy exchange between nuclei and lattice
- Accelerated tunneling mechanism proposed
- Mechanism proposed for interaction with host metal nuclei and other nuclei in lattice

# Simplified picture

Assume that active region is outer shell, and that phonons are produced by deuterium flux across drop in chemical potential
## Seek consistent parameters

$$\frac{E}{V} = \left(4 \times 10^{22} \text{ cm}^{-3}\right) \left[\frac{100 \text{ fm}}{0.2 \text{ A}}\right]^2 12 \text{ meV} = 190 \frac{\mu \text{J}}{\text{cm}^3}$$

$$\frac{P}{V} = \frac{1}{\tau} \frac{E}{V} = 5 \frac{\text{kW}}{\text{cm}^3}$$
Consistent with:
$$\frac{P}{A} = \frac{\ell}{\tau} \frac{E}{V} = 100 \frac{\text{mW}}{\text{cm}^2} \qquad \omega = 2\pi \left(1 \text{ GHz}\right)$$

$$\frac{P_{xs}}{V_{rod}} = \frac{E}{V} \frac{2\ell}{R} = 5 \frac{\text{W}}{\text{cm}^3} \qquad \tau = 40 \text{ nsec}$$