ON INTRINSIC LOCALIZED MODES, BREATHERS AND QUODONS

What are they?
Why do they exist?
Where do they exist?
Do they exist in crystals?
ILMs in germanium?
Quodons in mica muscovite?

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Discrete breather obtained with parcas MD code in Ge

Found by M. Klopop and V. Hizhnyakov using LAMMPS
Slice: discrete breather obtained with MD in Ge. $F=1.25$ THz
Fourier spectrum of the MD breather in Ge
Density of states for germanium

Breather frequency in Ge
So what is a discrete breather?

-Localized vibration in a periodic medium

-Two characteristics so far:
  -Localization
  -Nonlinear vibrations (some harmonics)
  -Well defined frequency outside the phonon spectrum

Many move

Typical energies: 0.5-5 eV
Are there other nonlinear intrinsic localized entities?

Yes:
-Solitons
-kinks
-Crowdions (replacement collisions cascade)
-Solelectrons and polarons
-Others: magnetic, spins

At least they exist in theory

ILMs for some is equal to breathers
Some basic maths

Suppose an 1D system:

\[ H = \sum_{n} \frac{1}{2} \dot{u}_n^2 + \sum_{n} V(u_n) + \sum_{n} W(u) \]

Linearized:

\[ H = \sum_{n} \frac{1}{2} \dot{u}_n^2 + \frac{1}{2} \sum_{n} \omega_0^2 u_n^2 + \frac{1}{2} \sum_{n} \epsilon(u_n - u_{n-1})^2 \]

Dynamical equations:

\[ \ddot{u}_n = -\omega_0^2 u_n + \epsilon(u_{n+1} + u_{n-1} - 2u_n) \]

Trial solution

\[ u_n = Ae^{i(qn - \omega t)} \]

Solutions for frequencies

\[ \omega^2 = \omega_0^2 + 4\epsilon \sin^2\left(\frac{q}{2}\right) \]
Phonons: \( u_n = A \cos(q n - \omega_q t) \)
Phonon spectrum

![Graph showing optical and acoustic phonon spectra. The optical spectrum has a non-zero frequency, while the acoustic spectrum has a zero frequency.]
Trial solution for frequencies outside the phonon spectrum

\[ u_n = Ae^{-\xi(n - Vt)} e^{i(qn - \omega t)} \quad ; \quad n > Vt \]

\[ \omega^2 = \xi^2 V^2 + \omega_0^2 + 2\varepsilon(1 - \cos(q)\cosh(\xi)) \]
\[ \omega\xi V = \varepsilon \sin(q)\sinh(\xi) \]
The further apart from the phonon band, the more localization
Hard potential (-- / Soft potential (...)

Hard: frequency increases with amplitude/energy
Soft: frequency decreases with amplitude/energy
Hard breathers / Soft breathers

Sometimes we may have both in the same system:
As in ClNa structure
Necessary conditions for breather existence

Nonresonance: \( n\omega_b \notin \text{phonon band} \)

Nonlinearity: \( \frac{\partial w_b}{\partial E} \neq 0 \)

Sufficient hardness if above the phonon band

In those conditions theorems establish that breathers are exact solutions.
So breathers exist in mathematical models, but do they exist in crystals?

In classical molecular dynamics
Ni, Nb, Fe, Cu, Ge, Si, NaCl, NaI, V, W, graphene, graphane, carbon nanotubes, C₆₀.

With DFT in graphane, ...

Some at finite temperature Fe 100K, Nb 300K,..

Not conclusive, but if they exist. Most likely:
They are not generic ➔ Few breathers, depending on the material and temperatures.
In the real world?

By Mike Russell. It helped two persons to get jobs

Also in electrical lattices, arrays of Josephson junctions, cantilever arrays, waveguide arrays, ...
In crystals:

**Manley et al., Uranium at 450-700K**


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**In germanium?** Archilla, Coelho, Auret, Dubinko, Hizhnyakov (2015)

**In mica muscovite?** Mike Russell, Eilbeck and coworkers since 1963
Plasma annealing of defects in germanium

Copra ICP Ar plasma source

Sb-doped Ge

Defect detection by DLTS

\[ N_{\text{Ge}} = 4.42 \times 10^{22} \text{ cm}^{-3} \]
\[ N_{\text{Sb}} = 1.03 \times 10^{15} \text{ cm}^{-3} \]
\[ N_{\text{T}} = 1.07 \times 10^{14} \text{ cm}^{-3} \]

Ge sample with an Au diode
Defects in germanium

- Can be produced by irradiation
- Some vital, some fatal
Concentration of E-center before and after plasma

Before plasma

- 4 eV, 30 minutes
- More T less effect
- 8 eV less effect
- 10^{-16} less energy than thermal annealing

After plasma

Quodons in mica muscovite

- Produced in the decay of $^{40}$K with 0.5 MeV.
- 3 per second per cm$^3$
- Tracks are Fe oxides, magnetite

FM Russell, From Nature 1967, Nature 216, 907 ; 217, 51 (1967) and many more
Mica muscovite. Cation layers

\[ K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4 \]

\( K^+ : \) 2D lattice of repulsive particles
Quodons: quasi one-dimensional excitations of the lattice in mica muscovite

Tracks: magnetite Fe$_3$O$_4$

Causes
- 0.1% Swift particles
- muons: after neutrino interaction
- Positrons: decay of 40K
- 99.9% unknown: most in lattice close packed directions

Anharmonic lattice vibrations?
The piece of mica in your hands

This is at 20° to chains.

Typical proton in the µ.

νucleon scattering giving cascades.
Experimental evidence of travelling excitations in mica muscovite

Trajectories were along lattice directions within the K$^+$ layer. Surface binding energy of ejected atoms unknown: typical values 3-8 eV

What about charge?

Almost all the decay modes of $^{40}$K leave a charge behind,


Table 2 Table of decays for $^{40}$K

<table>
<thead>
<tr>
<th>Decay</th>
<th>$\beta^-$</th>
<th>EC1</th>
<th>EC1+CE$^1$</th>
<th>EC2$^2$</th>
<th>$\beta^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intensity</td>
<td>89.25%</td>
<td>10.55%</td>
<td>0.001%</td>
<td>0.2%</td>
<td>0.001%</td>
</tr>
<tr>
<td>T (keV)</td>
<td>1311.07</td>
<td>1460</td>
<td>1460</td>
<td>1504.69</td>
<td>483.7</td>
</tr>
<tr>
<td>Emittted charged particle</td>
<td>e$^-$</td>
<td>e$^-$</td>
<td>e$^-$</td>
<td>e$^+$</td>
<td>e$^+$</td>
</tr>
<tr>
<td>Recoil from</td>
<td>$\nu$+e$^-$</td>
<td>$\gamma$</td>
<td>$\nu$</td>
<td>$\nu$+e$^+$</td>
<td></td>
</tr>
<tr>
<td>Max Recoil (eV)</td>
<td>42</td>
<td>29.2$^M$</td>
<td>49.7$^M$</td>
<td>31.1$^M$</td>
<td>10</td>
</tr>
<tr>
<td>Daughter ion (A=40)</td>
<td>Ca$^{++}$</td>
<td>Ar$^+$</td>
<td>Ar$^{++}$</td>
<td>Ar$^{++}$</td>
<td>Ar</td>
</tr>
<tr>
<td>Max V (Km/s)</td>
<td>14.4</td>
<td>12$^M$</td>
<td>15.7$^M$</td>
<td>12.2$^M$</td>
<td>7</td>
</tr>
<tr>
<td>Ionization of daughter (eV)</td>
<td>50.6</td>
<td>27.7</td>
<td>40.8</td>
<td>40.8</td>
<td>15.8</td>
</tr>
<tr>
<td>$\Delta q$ (e)</td>
<td>+1</td>
<td>0</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
</tr>
</tbody>
</table>

1 Subset of EC1 when the gamma is delivered to a shell electron; $^M$ Monocromatic
2 Direct decay to Ar ground state, recoil from neutrino emission; 3 KeV Auger e$^-$
EC: electron capture; CE: conversion electron; T: energy available excluding rest masses
Ionization energy of K$^+$ 31.6 eV
Quodons may have charge (2015)

- 90% of the decay modes leave a **positive** charge behind (beta – decay)
- Only positive swift particles leave tracks
- Positrons at near sonic speed leave the same tracks than quodons

Many thanks for your attention

Archilla, Russell and Coelho, Altea, Spain, 2013
To appear, Springer 2015
Many thanks for your attention

Archilla, Hizhnyakov and Dubinko, Tartu, Estonia, November 2012
Workshop: Lattice solitons and irradiation-induced nonlinear phenomena in solids,
Some bibliography

*Long range annealing of defects in germanium by low energy plasma ions*
JFR Archilla, SMM Coelho, FD Auret, VI Dubinko and V Hizhyakov

*Ultra-discrete kinks with supersonic speed in a layered crystal with realistic potentials,*

*Reaction rate theory with account of the crystal anharmonicity*
VI Dubinko, P.A. Selyshchev and JFR Archilla,
Phys Rev E 83 (2011) 041124

*Discrete breathers for understanding reconstructive mineral processes at low temperatures*
JFR Archilla, J Cuevas, MD Alba, M Naranjo and JM Trillo,