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SCATTERING OFF OF AN UNUSUAL BOUNDARY

Jerome Weston

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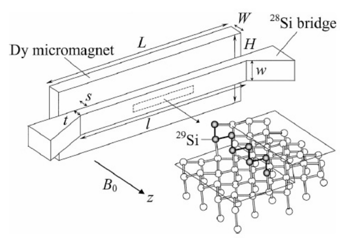
1. Introduction

The inspiration behind this project was based on an article written by a 6 man team (Abe, E., K. M. Itoh, T. D. Ladd, J. R. Goldman, F. Yamaguchi, and Y. Yamamoto. "Solid-State Silicon NMR Quantum Computer.") published in February 2003 and a follow up article written by one of the original members published in 2005.



Originally the purpose was to explore the quantum computing aspects of the paper from a purely mathematical standpoint. As time progressed focus shifted to the wave resonance properties of the silicon structure, specifically wave scattering off of the stair-like boundary of the structure. For this paper, we focus on the two-dimensional case of this structure by starting with base case of a 2-d lattice and build from there.

2. Focus

Consider an infinite net of beads, each of mass M with connection between each bead denoted as τ. For a particular bead, x_{n_1,n_2}, the force exerted on it relates to

$$F = M\,\ddot{x}_{n_1,n_2}$$
$$F = \tau(x_{n_1+1,n_2} + x_{n_1-1,n_2} + x_{n_1,n_2+1} + x_{n_1,n_2-1} - 4x_{n_1,n_2}),$$

where the first and second equations relate to Newton's 2nd law and a pseudo version of Hooke's law respectively.

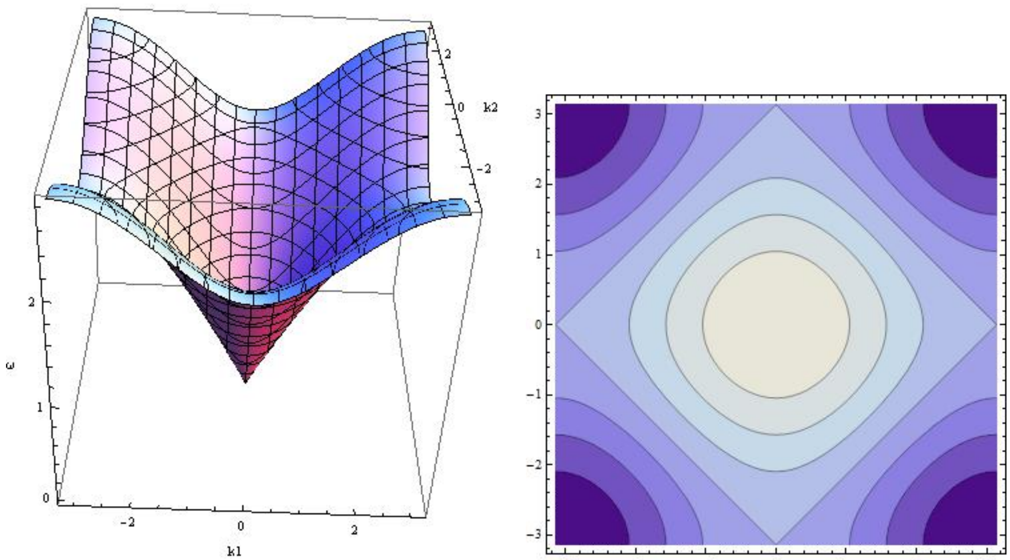


TABLE 1. dispersion relation with $\omega \in (0, 2\sqrt{2\alpha})$

We set the forces equal to each other to get

$$M\ddot{x}_{n_1,n_2} = \tau(x_{n_1+1,n_2} + x_{n_1-1,n_2} + x_{n_1,n_2+1} + x_{n_1,n_2-1} - 4x_{n_1,n_2}).$$

We look for harmonic solutions (i.e. separable in space and time) that represent the wave traveling through the lattice. So let

$$x_{n_1,n_2}(t) := e^{i(k_1 n_1 + k_2 n_2 - \omega t)},$$

where (k_1, k_2) represents the **wavevector** and ω its **frequency**. With the substitution of $x_{n_1,n_2}(t)$ into our previous equation, we get the following **dispersion relation**:

$$\cos(k_1) + \cos(k_2) = 2 - \frac{\omega^2}{2\alpha}$$

where $\alpha = \frac{\tau}{M}$.

The dispersion relation connects the components of the wavevector and frequency in a way such that the wave's **group velocity**, the velocity of which the shape of the wave's amplitudes move through space, and **phase velocity**, the velocity at which the phase of the wave moves through space, are easily expressed.

We now consider the effects of boundary conditions on our lattice structure.

Example 1: Suppose the lattice ends as an edge in free space (i.e. picture a sheet of paper). We represent this condition as

$$M\ \ddot{x}_{n_1,n_2} = \tau(x_{n_1+1,n_2} + x_{n_1-1,n_2} + x_{n_1,n_2-1} - 3x_{n_1,n_2}).$$

Let $U(n_1, n_2)$ represent the amplitude and phase shift of the wave and the line $n_2 = 0$ as the boundary. We have the following relation:

$$U(n_1, n_2) = Je^{i(k_1 n_1 + k_2 n_2)} + Re^{i(k_1 n_1 - k_2 n_2)}$$

where J and R are scalars representing the magnitude of an incoming and reflected wave respectively. Replace x_{n_1,n_2} with $U(n_1, n_2)e^{-i\omega t}$ and we have

$$J = -R\frac{\omega^2 - 3\alpha + \alpha\cos(k_1) + \alpha e^{ik_2}}{-\omega^2 + 3\alpha - \alpha\cos(k_1) - \alpha e^{-ik_2}}$$

Example 2: Suppose the lattice ends as an edge in free space with the beads, denoted y_{n_1,n_2}, at the boundary being of mass, M_2, different than the beads in bulk, y-y and y-x connections being denoted as τ_2, τ_3 respesctively. We represent this condition as

$$M_2\ \ddot{y}_{n_1,n_2} = \tau_2(y_{n_1+1,n_2} + y_{n_1-1,n_2} - 2y_{n_1,n_2}) + \tau_3(y_{n_1,0} - x_{n_1,-1}).$$

Using the same replacement of $U(n_1, n_2)e^{-i\omega t}$ for x and y leads to a different $J - R$ relation.

Now suppose that the bead in the original 2-d lattice problem is replaced with a cell of N beads, linearly connected of strength τ, each of mass M as before. With the previous example, it was assumed that the coordinate system was that of a standard Cartesian plane in (n_1, n_2). Under that assumption the current problem becomes a bit more difficult to understand clearly so we try a different approach. For examples in the current and following problems, it is assumed that $N = 4$.

Consider a transformation $T : (n_1, n_2) \longrightarrow (\tilde{n_1}, \tilde{n_2})$ such that

$$\tilde{n_1} = \tfrac{n_1}{N}$$
$$\tilde{n_2} = n_2.$$

For every cell shift in $\tilde{n_1}$, an arbitrary mode within a cell must shift N times in n_1 thus, under this transformation, the cell behaves similarly to bead in the original 2-d lattice problem. The wave numbers k_1, k_2 from before become $\tilde{k_1}$, $\tilde{k_2}$ such that

$$\tilde{k_1} = Nk_1$$
$$\tilde{k_2} = k_2.$$

We must look at for what fields $e^{ik_1 n_1}$ have $e^{i\tilde{k_1}}$ as a **Floquet multiplier** in $\tilde{n_1}$ variable. The Floquet multiplier gives a scaling and angular phase shift of a wave across a period. Since the cell contains N nodes, we need to find phase shifts for each mode in the cell in terms of $\tilde{k_1}$. Take $n_1 = 0, N$ (i.e. $\tilde{n_1} = 0, 1$). Then $e^{ik_1 0} = 1$ and $e^{ik_1 N} = e^{i\tilde{k_1}}$. We conclude that

$$e^{ik_1} = e^{i(\frac{\tilde{k_1}+2\pi j}{N})},$$

where $j \in \{0, 1, \cdots, N-1\}$. For example, under our assumed N,

$$k_1 \in \{\frac{\tilde{k_1}}{4}, \frac{\tilde{k_1}}{4} + \frac{\pi}{2}, \frac{\tilde{k_1}}{4} + \pi, \frac{\tilde{k_1}}{4} - \frac{\pi}{2}\}.$$

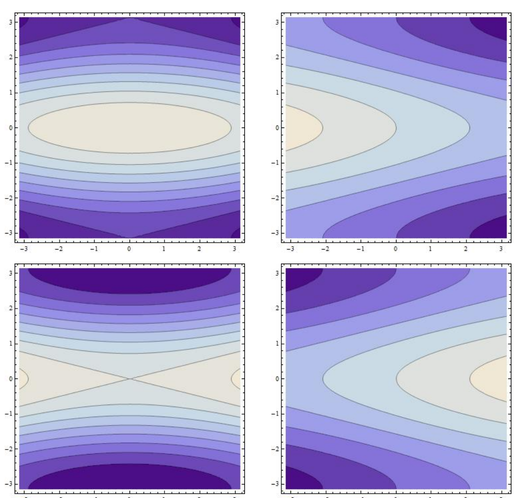
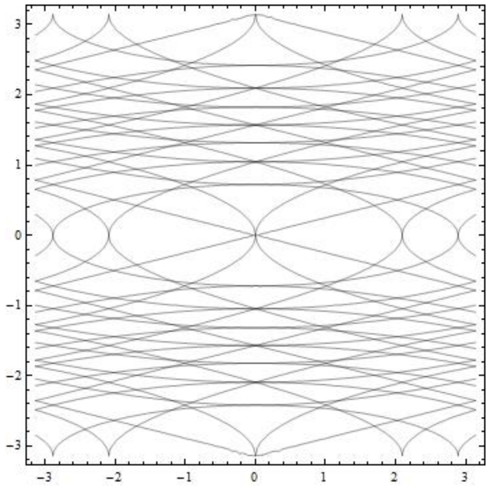


Table 2. Dispersion relations for $\tilde{k_1}$.

When plots are stacked,

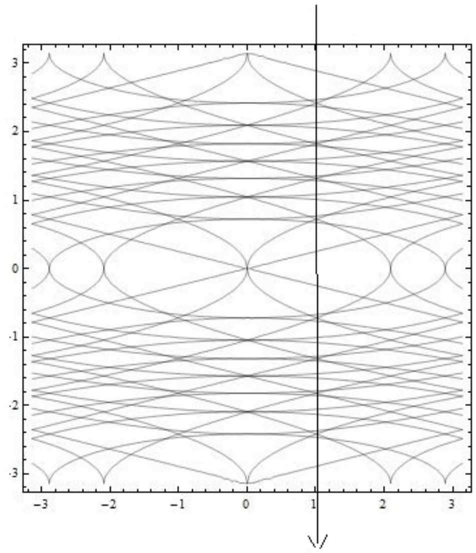


Now we look at scattering off of a periodic, free boundary. The boundary in this example has cells with N modes where the first mode in each cell is of different mass and has different connection τ_2 with surrounding modes.

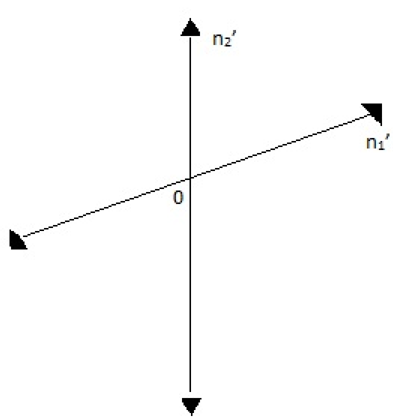
We can use the previous scattering problems as a basis for the geometry of the problem. Note that the scattering equation in this sense, turns into a vector equation with solution of the form:

$$S_1 \vec{J} = S_2 \vec{R},$$

where each component in the vectors $\vec{J}$, $\vec{R}$ correspond to an incoming and reflected wave for each mode in the cell respectively. S_1, S_2 are NXN matrices.



With respect to the above figure, choose an arbitrary $\tilde{k_1}$ (call it $\tilde{k_{1_0}}$). For a given frequency (i.e. the individual rings of the contour plot), the $\tilde{k_2}'s$ at which the line $\tilde{k_1} = \tilde{k_{1_0}}$ intersect the rings are the $\tilde{k_2}'s$ for which there are propagating and **evanescent waves** for that $\tilde{k_{1_0}}$. Evanescent waves are waves that decay exponentially over distance from their source.
We've taken for granted that our coordintate axes have been orthogonal so far. So let's consider the 2-d cluster problem with coordinate axes similar to this:



Consider a transformation $T' : (\tilde{n_1}, \tilde{n_2}) \longrightarrow (n'_1, n'_2)$ such that

$$n'_1 = \tilde{n_1}$$
$$n'_2 = \tilde{n_2} - \tilde{n_1}.$$

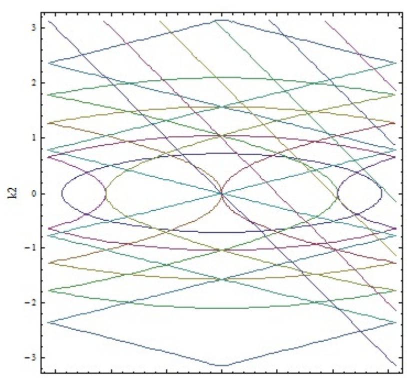
The justification goes as follows: A vertical shift of an arbitrary cell in n'_2 is equivalent to a horizontal shift in $\tilde{n_1}$ and a vertical shift in $\tilde{n_2}$. The resulting cell would have a higher value in $\tilde{n_2}$ than in n'_2 and the difference would be the amount of horizontal shifts in $\tilde{n_1}$. The wave numbers $\tilde{k_1}$, $\tilde{k_2}$ from before become k'_1, k'_2 such that

$$k'_1 = \tilde{k_2} + \tilde{k_1}$$
$$k'_2 = \tilde{k_2}.$$

By definitions of k'_1, k'_2, it is apparent that the fields $e^{i\tilde{k_1}\tilde{n_1}}$ that have $e^{ik'_1}$ as a Floquet multipler in n'_1 variable are the same with shifts equal to the value of k'_2.

Now we consider scattering under this new non-orthogonal coordinate system. The resulting $J - R$ relation is similar to that of the standard cluster problem from before of the form

$$S'_1 \vec{J} = S'_2 \vec{R},$$



Luckily, we can use a contour plot similar to the previous form with different orientation. Choose an arbitrary k'_1, denoted by choosing one of the colored slanted lines. As before the k'_2's at which a slanted line intersects a given frequency ring denotes which k'_2's have propagating and evanescent waves for an arbitrary k'_1.

3. Further Ideas

Ideas to be studied on in the future:

- Consider finite case of 3rd problem (2-d Lattice: Skewed).
- Extend ideas to 3 dimensions.
- Investigate connection between wave resonance, scattering, and quantum computing.

4. Acknowledgements

I would like to thank Dr. Stephen Shipman for his guidance through the development of this thesis, Professors Jonathan Dowling and Jimmie Lawson for their participation on the committee, and the Honors College.

References

[1] Abe, E., K. M. Itoh, T. D. Ladd, J. R. Goldman, F. Yamaguchi, and Y. Yamamoto. "Solid-State Silicon NMR Quantum Computer." Journal of Superconductivity: Incorporating Novel Magnetism 16.1 (2003): 175-78. Web.

[2] Itoh, Kohei M. "An All-silicon Linear Chain NMR Quantum Computer." Solid State Communications 133 (2005): 747-52. 25 Jan. 2005. Web. 26 Sept. 2012.