REPRESENTATION THEORY OF
FINITE ABELIAN GROUPS APPLIED TO A
LINEAR DIATOMIC CRYSTAL

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ABSTRACT. After a brief review of matrix representations of finite abelian groups,

projection operators are defined and used to compute symmetry coordinates for

systems of coupled harmonic oscillators. The Lagrangian for such systems is

discussed in the event that the displacements along the symmetry coordinates are

complex. Lastly, the natural frequencies of a linear, diatomic crystal are deter-

mined through application of the Born cyclic condition and the determination of

the symmetry coordinates.

KEY WORDS AND PHRASES. Abelian groups, Born cyclic condition, Group representations,
Harmonic oscillators, Lagrangian mechanics, Natural Frequencies, Projection operators.

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1. <u>INTRODUCTION</u>.

    A classic application of abstract algebra is found in the use of the

representation theory of finite groups in the separation of the equations of

motion for symmetrically coupled harmonic oscillators. Although the literature

on the subject is extensive [3], [4], [5], [6], [9], we shall present a brief

review of certain pertinent facts. We shall define projection operators in the

event that the group under consideration is abelian and use the projection

operators to compute the symmetry coordinates for a physical system. Thereafter

we shall discuss the effect of the transformation to symmetry coordinates upon

a Lagrangian function. Finally, we shall find the natural frequencies of a one

dimensional, diatomic crystal.

2. <u>GROUP REPRESENTATIONS AND PROJECTION OPERATORS</u>.

    Let S denote a system of finitely many coupled, harmonic oscillators, and

let G be a finite symmetry group acting on S . Then, if M(n) denotes the

multiplicative group of n × n matrices over the complex numbers, $\mathbb{C}$, and if

$\Gamma: G \rightarrow M(n)$ is a homomorphism of groups, the image of Γ , given by

$\Gamma(G) = \{\Gamma(g) \mid g \varepsilon G\}$, is a matrix representation of dimension n for the symmetry

group, G .

    If $\Gamma(G)$ is unitary and if there exists no similarity transformation to

convert $\Gamma(G)$ into the block diagonal form $\bigoplus_{j=1}^{k} \Gamma_j(G)$ where $\Gamma_j(G)$ is a matrix

representation of G with dimension less than n for each j , then $\Gamma(G)$ is

said to be a unitary, irreducible matrix representation of G . The number of

nonequivalent, unitary, irreducible matrix representations is finite. In fact,

there are precisely as many of these as there are conjugacy classes in G . If

there are ℓ conjugacy classes in G and if the dimensions of the nonequivalent,

unitary, irreducible matrix representations are n(1) , n(2) , ... , n(ℓ) , we

know that

$$\sum_{j=1}^{\ell} (n(j))^2 = |G|$$

where $|G|$ is the order of the finite group [6].

If G is abelian, then $\ell = |G|$ and $n(j) = 1$, implying that all irreducible representations will be one dimensional. This fact is quite useful. Indeed, if the full symmetry group of the system, S, is nonabelian, it is often desirable to choose an abelian subgroup of the larger group to act as G, thereby obtaining significant advantages in the computational procedures.

EXAMPLE 2.1. Let $G = \{E, R, R^2, R^3\}$ be the cyclic four-group generated by R, a 90° rotation about a fixed axis. There are four irreducible, unitary representations:

$$\Gamma_1(G) : \Gamma_1(E) = \Gamma_1(R) = \Gamma_1(R^2) = \Gamma_1(R^3) = 1 ;$$

$$\Gamma_2(G) : \Gamma_2(E) = \Gamma_2(R^2) = 1, \ \Gamma_2(R) = \Gamma_2(R^3) = -1 ;$$

$$\Gamma_3(G) : \Gamma_3(E) = 1, \Gamma_3(R) = i, \ \Gamma_3(R^2) = -1,$$

$$\Gamma_3(R^3) = -i ;$$

$$\Gamma_4(G) : \Gamma_4(E) = 1, \ \Gamma_4(R) = -i, \ \Gamma_4(R^2) = -1,$$

$$\Gamma_4(R^3) = i .$$

Suppose that there is associated with each oscillator in S a point mass, m_i. If the displacement of the i-th mass is taken to be $\vec{v}_i$, the smallest vector space containing all linear combinations of these displacement vectors for all particles is the solution space, $\mathcal{V}$, of the physical system, S.

Now for each element, g, of the symmetry group, G, there is induced exactly one linear operator, $\phi(g)$, which acts on the basis vectors of $\mathcal{V}$.

Furthermore, it can then be shown that $A(\phi(G)) = \{ \sum\limits_{g \in G} a_g \phi(g) \mid a_g \in \mathbb{C}\}$ is an algebra

over $\mathbb{C}$.

In $A(\phi(G))$, there is a subset of operators upon which we fix attention.

DEFINITION 2.1. Let G be abelian and let $\Gamma_i(g)$ belong to $\Gamma_i(G)$,

the i-th unitary, irreducible, one dimensional representation of G . Then the

linear operator $P_i \in A(\phi(G))$ is defined by $P_i = \sum\limits_{g \in G} (\Gamma_i(g))\phi(g)$, and

$\{P_i \mid i = 1,2,\ldots, |G|\}$ is the set of projection operators in the algebra $A(\phi(G))$.

We emphasize that, in this definition, G is abelian. The reader may easily

find the general definition of the projection operators when G is not required

to be abelian [1], [9], [10].

EXAMPLE 2.2. $G = \{E, R, R^2, R^3\}$ as in Example 2.1. Then the projection

operators are

$$P_1 = \phi(E) + \phi(R) + \phi(R^2) + \phi(R^3) \ ,$$

$$P_2 = \phi(E) - \phi(R) + \phi(R^2) - \phi(R^3) \ ,$$

$$P_3 = \phi(E) + i\phi(R) - \phi(R^2) - i\phi(R^3) \ , \quad \text{and}$$

$$P_4 = \phi(E) - i\phi(R) - \phi(R^2) + i\phi(R^3) \ .$$

Now suppose that the solution space, $\mathcal{V}$, has the orthonormal basis

$B = \{\hat{u}_1, \hat{u}_2,\ldots,\hat{u}_n\}$. Then the symmetry coordinates for the physical system can

be obtained from B as indicated in the next definition.

DEFINITION 2.2. Suppose that $P_i(\hat{u}_\ell)$ is not the zero vector. Then the

distinct unit vectors of the form

$$\frac{P_i(\hat{u}_\ell)}{|P_i(\hat{u}_\ell)|}$$

are the symmetry coordinates of the physical system.

There are exactly $n = \dim \mathcal{V}$ distinct nonzero vectors which can be obtained

from this definition, and these are mutually orthogonal [1]. This set of vectors

establishes a new basis for $\mathcal{V}$ matching the symmetry of S and determines the

transformation of coordinates which will separate the equations of motion to the

greatest extent possible through the use of symmetry alone. We denote the new

basis of symmetry coordinates by $\{\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_n\}$ and to exhibit their use, we

give a simple example.

EXAMPLE 2.3. Four identical masses, m , are uniformly spaced and inter-

connected by identical springs on a frictionless, circular loop fixed in a plane.

The spring constant for each spring is k . All motion of the masses is confined

to the loop. We find the natural frequencies of motion [1], [2].

SOLUTION: The physical system is shown below. The symmetry group is taken to

be the rotation group $G = \{E, R, R^2, R^3\}$.
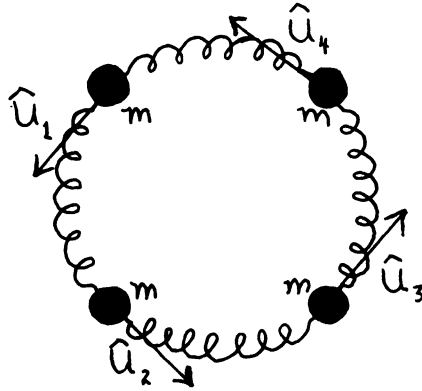
The basis for the solution space is the set of unit tangents $\{\hat{u}_1, \hat{u}_2, \hat{u}_3, \hat{u}_4\}$.

The projection operators are given in Example 2.2 and the symmetry coordinates

are

$$\hat{e}_1 = \frac{1}{2} P_1(\hat{u}_1) = \frac{1}{2} [\phi(E) + \phi(R) + \phi(R^2) + \phi(R^3)]\hat{u}_1$$

$$= \frac{1}{2} (\hat{u}_1 + \hat{u}_2 + \hat{u}_3 + \hat{u}_4) ,$$

$$\hat{e}_2 = \frac{1}{2} (\hat{u}_1 - \hat{u}_2 + \hat{u}_3 - \hat{u}_4) ,$$

$$\hat{e}_3 = \frac{1}{2} (\hat{u}_1 + i\hat{u}_2 - \hat{u}_3 - i\hat{u}_4) , \text{ and}$$

$$\hat{e}_4 = \frac{1}{2} (\hat{u}_1 - i\hat{u}_2 - \hat{u}_3 + i\hat{u}_4) .$$

These equations serve to define the unitary, transformation matrix U such that

$$\text{col}(\hat{e}_1 \ \hat{e}_2 \ \hat{e}_3 \ \hat{e}_4) = U \text{ col}(\hat{u}_1 \ \hat{u}_2 \ \hat{u}_3 \ \hat{u}_4) .$$

Thus

$$U = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{pmatrix} .$$

If the displacements of the masses along the unit tangents are x_1, x_2, x_3, x_4 and their velocities are $\dot{x}_1$, $\dot{x}_2$, $\dot{x}_3$, $\dot{x}_4$, we can write the displacements and velocities as the column vectors $X = \text{col}(x_1 \ x_2 \ x_3 \ x_4)$ and $\dot{X} = \text{col}(\dot{x}_1 \ \dot{x}_2 \ \dot{x}_3 \ \dot{x}_4)$.

Then the Lagrangian of the system is $L = \frac{1}{2} m\tilde{\dot{X}}T\dot{X} - \frac{1}{2} k\tilde{X}VX$ where $\tilde{\dot{X}}$ and $\tilde{X}$ are row vectors obtained by taking the transposes of $\dot{X}$ and X ,

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \text{ and } V = \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}.$$

We next transform the Lagrangian to obtain a function of the displacements, η_1, η_2, η_3, η_4, and velocities $\dot{\eta}_1$, $\dot{\eta}_2$, $\dot{\eta}_3$, $\dot{\eta}_4$, with respect to the symmetry coordinates, $\hat{e}_1$, $\hat{e}_2$, $\hat{e}_3$, $\hat{e}_4$. Thus

$$L = \frac{1}{2} m \tilde{\dot{X}} U^{-1} U T U^{-1} U \dot{X}$$

$$- \frac{1}{2} k \tilde{X} U^{-1} U V U^{-1} U X$$

$$= \frac{1}{2} m \tilde{\dot{N}}* (U T U^{-1}) \dot{N} - \frac{1}{2} k \tilde{N}* (U V U^{-1}) N$$

where $N = \text{col}(\eta_1 \ \eta_2 \ \eta_3 \ \eta_4)$, $\dot{N} = \text{col}(\dot{\eta}_1 \ \dot{\eta}_2 \ \dot{\eta}_3 \ \dot{\eta}_4)$ and $\tilde{N}*$, $\tilde{\dot{N}}*$ are the transposed, complex conjugates of N, $\dot{N}$ respectively. Since

$$U T U^{-1} = T \quad \text{and} \quad U V U^{-1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix},$$

we have

$$L = \frac{1}{2} m (\dot{\eta}_1^* \dot{\eta}_1 + \dot{\eta}_2^* \dot{\eta}_2 + \dot{\eta}_3^* \dot{\eta}_3 + \dot{\eta}_4^* \dot{\eta}_4)$$

$$- \frac{1}{2} k (4\eta_2^* \eta_2 + 2\eta_3^* \eta_3 + 2\eta_4^* \eta_4).$$

The completely separated equations of motion are given by

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\eta}_j} \right) - \frac{\partial L}{\partial \eta_j} = 0 \qquad \text{(Equation 2.1)}$$

or equivalently by

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\eta}_j^*}\right) - \frac{\partial L}{\partial \eta_j^*} = 0 \qquad \text{(Equation 2.2)}$$

for $j \varepsilon \{1, 2, 3, 4\}$.

It follows immediately that the four natural frequencies for this

system are

$$0 \ , \ \frac{1}{2\pi}\sqrt{\frac{2k}{m}} \ , \ \frac{1}{2\pi}\sqrt{\frac{2k}{m}} \ , \ \frac{1}{\pi}\sqrt{\frac{k}{m}} \quad .$$

3. THE LAGRANGIAN WITH COMPLEX COORDINATES.

In the preceding example, the transformation to symmetry coordinates yielded

a real-valued Lagrangian function in the complex variables η_j , η_j^* . The

similarity transformations of the T and V matrices leave their eigenvalues

undisturbed. As these eigenvalues, in fact, determine the natural frequencies,

such transformations are quite permissible. However, we also wish to show that

in the equations of motion as given by Equations 2.1 and 2.2, the variables η_j

and their complex conjugates, η_j^* , will never appear together. To that end,

let us consider the following exercise in partial differentiation.

Let F be a function of the independent complex variables $\eta_j = x_j + iy_j$.

Furthermore, suppose that F is differentiable with respect to x_j and y_j .

If $\frac{\partial x_j}{\partial y_j} = \frac{\partial y_j}{\partial x_j} = 0$ and if we apply the chain rule for partial derivatives while

noting that $\eta_j^* = x_j - iy_j$, we obtain $\frac{\partial F}{\partial x_j} = \frac{\partial F}{\partial \eta_j} + \frac{\partial F}{\partial \eta_j^*}$ and $\frac{\partial F}{\partial y_j} = i\frac{\partial F}{\partial \eta_j} - i\frac{\partial F}{\partial \eta_j^*}$.

Formally, we write

$$\frac{\partial}{\partial x_j} = \frac{\partial}{\partial \eta_j} + \frac{\partial}{\partial \eta_j^*} \quad \text{and} \quad \frac{\partial}{\partial y_j} = i\frac{\partial}{\partial \eta_j} - i\frac{\partial}{\partial \eta_j^*} \quad .$$

Inverting these operational equations, we have

$$\frac{\partial}{\partial \eta_j} = \frac{1}{2}(\frac{\partial}{\partial x_j} - i \frac{\partial}{\partial y_j}) \quad \text{and}$$

$$\frac{\partial}{\partial \eta_j^*} = \frac{1}{2}(\frac{\partial}{\partial x_j} + i \frac{\partial}{\partial y_j}) \quad .$$

It immediately follows that $\dfrac{\partial \eta_j}{\partial \eta_j} = \dfrac{\partial \eta_j^*}{\partial \eta_j^*} = 1$ and $\dfrac{\partial \eta_j^*}{\partial \eta_j} = \dfrac{\partial \eta_j}{\partial \eta_j^*} = 0$.

Thus, whenever the Lagrangian of a physical system of harmonic oscillators is written in the matrix notation $L = \frac{1}{2} m \, \dot{\tilde{N}}^* T_0 \dot{N} - \frac{1}{2} k \, \tilde{N}^* V_0 N$, each summand of the expanded Lagrangian will be of the form $C_1 \dot{\eta}_j^* \dot{\eta}_k$ or $C_2 \eta_j^* \eta_k$ where C_1 and C_2 are constant.

Thus the differential equation

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\eta}_j} \right) - \frac{\partial L}{\partial \eta_j} = 0 \quad \text{contains}$$

only the complex conjugates η_k^* together with their second derivatives with respect to time and

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\eta}_j^*} \right) - \frac{\partial L}{\partial \eta_j^*} = 0 \quad \text{contains}$$

only the coordinates η_k and $\ddot{\eta}_k$. That is, in neither equation will coordinates and their complex conjugates be mixed. The proper frequencies can be obtained from equations of either form.

4. THE ONE-DIMENSIONAL DIATOMIC CRYSTAL.

We now consider a circular loop of alternating masses of two sorts, m and M , connected by identical springs having force constant β [2]. Let there be 2N masses in all with N of each kind. If N is taken to be very large, we have essentially applied the Born cyclic condition to a linear, diatomic crystal

[1], [8] . We will now find the symmetry coordinates and natural frequencies of

the system.

The system is invariant with respect to rotations by $\frac{2\pi}{N}$, and, in the

neighborhood of the 2n-th and (2n+1)-th particles, the circular arrangement

appears as shown.

In the calculations to follow, two facts concerning the complex roots of

unity are required.
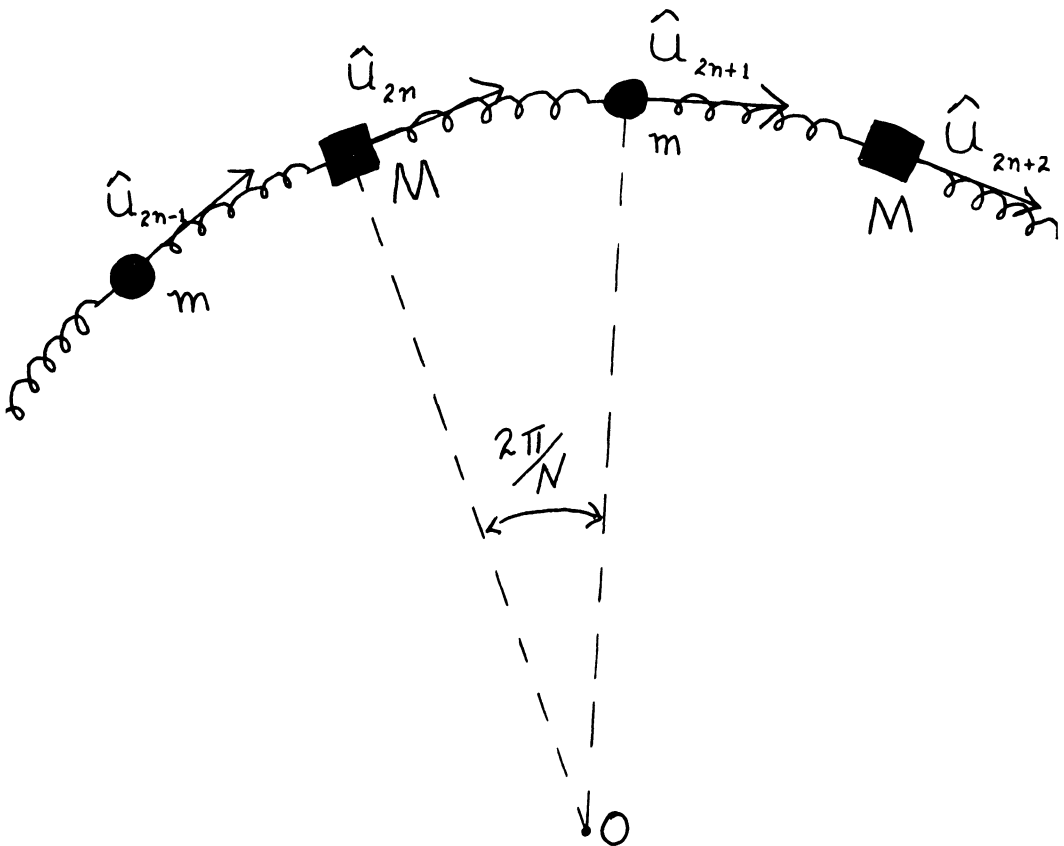
First, let exp $\frac{2\pi i}{K}$ be the primitive complex K-th root of unity. Then let

n_1 and $n_2 \in \{0,1,2,\ldots,K - 1\}$. By application of the Parallelogram Law of

Addition for Complex Numbers

$$\exp n_1 \left(\frac{2\pi i}{K}\right) + \exp n_2 \left(\frac{2\pi i}{K}\right) = 2 \left| \cos\left(\frac{n_1 - n_2}{2}\right) \frac{2\pi}{K} \right| \exp\left(\frac{n_1 + n_2}{2}\right) \frac{2\pi i}{K} . \quad \text{(Equation 4.1)}$$

In the event that we need to consider $\exp 2\pi i + \exp n \frac{2\pi}{K} i$ where $0 \le n \le K - 1$, we write

$$\exp 0i + \exp n \frac{2\pi i}{K} = 2 \left| \cos \frac{n}{2} \left(\frac{2\pi}{K}\right) \right| \exp \frac{n}{2} \left(\frac{2\pi i}{K}\right) .$$

Secondly we recall that the sum of the K complex K-th roots of unity is the complex number zero. That is

$$\sum_{n=0}^{K-1} \exp n \frac{2\pi i}{K} = 0 + 0i , \ K > 1 . \qquad \text{(Equation 4.2)}$$

The symmetry group of the circular arrangement is taken to be C_N, the group of rotations $\{R(\frac{2\pi \ell}{N}) \mid \ell = 1, 2, 3,\ldots, N\}$. The N one dimensional representations of the symmetry group are given by

$$\Gamma_k(G) : \Gamma_k(R(\frac{2\pi \ell}{N})) = \exp(\frac{2k\pi}{N}) \ell i$$

for $\ell = 1, 2, 3,\ldots, N$ [1].

Thus the projection operators are of the form

$$P_k = \sum_{\ell=1}^{N} (\exp(\frac{2k\pi}{N})\ell i)\phi(R(\frac{2\pi \ell}{N})) \quad \text{for} \quad k = 1, 2, 3,\ldots,N .$$

The symmetry coordinates are found by letting P_k act first upon the unit tangent $\hat{u}_{2N-1}$ and then upon $\hat{u}_{2N}$.

$$\hat{e}_{2k-1} = \frac{1}{\sqrt{N}} P_k \hat{u}_{2N-1} = \frac{1}{\sqrt{N}} \sum_{\ell=1}^{N} (\exp(\frac{2k\pi}{N})\ell i)\hat{u}_{2\ell - 1}$$

and

and

$$\hat{e}_{2k} = \frac{1}{\sqrt{N}} P_k \hat{u}_{2N} = \frac{1}{\sqrt{N}} \sum_{\ell=1}^{N} (\exp(\frac{2k\pi}{N})\ell i)\hat{u}_{2\ell} \quad \text{for } k = 1, 2, 3, \ldots, N \ .$$

The transformation matrix U is

$$\frac{1}{\sqrt{N}} \begin{pmatrix} \exp\frac{2\pi i}{N} & 0 & \exp\frac{4\pi i}{N} & 0 & \exp\frac{6\pi i}{N} & 0 & \cdots & 1 & 0 \\ 0 & \exp\frac{2\pi i}{N} & 0 & \exp\frac{4\pi i}{N} & 0 & \exp\frac{6\pi i}{N} & \cdots & 0 & 1 \\ \exp\frac{4\pi i}{N} & 0 & \exp\frac{8\pi i}{N} & 0 & \exp\frac{12\pi i}{N} & 0 & \cdots & 1 & 0 \\ 0 & \exp\frac{4\pi i}{N} & 0 & \exp\frac{8\pi i}{N} & 0 & \exp\frac{12\pi i}{N} & \cdots & 0 & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ 1 & 0 & 1 & 0 & 1 & 0 & \cdots & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & \cdots & 0 & 1 \end{pmatrix}$$

In terms of the displacements and velocities along the unit tangents, the Lagrangian of the system is

$$L = \frac{1}{2} m\tilde{\dot{X}}\dot{X} - \frac{1}{2}\beta \tilde{X}VX \quad \text{where} \quad X = \text{col}(x_1 \ x_2 \ \ldots \ x_{2N}) \ ,$$

$$\dot{X} = \text{col}(\dot{x}_1 \dot{x}_2 \ \ldots \ \dot{x}_{2N}) \ ,$$

$$T = \begin{pmatrix}
1 & 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\
0 & \frac{M}{m} & 0 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\
0 & 0 & 1 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\
0 & 0 & 0 & \frac{M}{m} & \cdot & \cdot & \cdot & 0 & 0 \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
0 & 0 & 0 & 0 & \cdot & \cdot & \cdot & 1 & 0 \\
0 & 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 & \frac{M}{m}
\end{pmatrix}, \text{ and}$$

$$V = \begin{pmatrix}
2 & -1 & 0 & 0 & \cdot & \cdot & \cdot & 0 & -1 \\
-1 & 2 & -1 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\
0 & -1 & 2 & -1 & \cdot & \cdot & \cdot & 0 & 0 \\
0 & 0 & -1 & 2 & \cdot & \cdot & \cdot & 0 & 0 \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & & & & \cdot & \cdot \\
0 & 0 & 0 & 0 & & & & 2 & -1 \\
-1 & 0 & 0 & 0 & & & & -1 & 2
\end{pmatrix}$$

The transformed Lagrangian is

$$L = \frac{1}{2} m \; \dot{\tilde{N}}{*}(UTU^{-1})\dot{N} - \frac{1}{2}\beta\tilde{N}{*}(UVU^{-1})N$$

where $N = \mathrm{col}(n_1 n_2 \ldots n_{2N})$ with respect to the symmetry coordinates. It is easily shown that $UTU^{-1} = T$.

The computation of UVU^{-1} is straightforward but tedious. However, by the use of the identities given in Equations 4.1 and 4.2, the matrix product becomes

$$\begin{pmatrix} 2 & -2\cos\frac{\pi}{N}\exp\frac{\pi i}{N} & 0 & 0 & \cdots & 0 & 0 \\ -2\cos\frac{\pi}{N}\exp(-\frac{\pi i}{N}) & 2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 2 & -2\cos\frac{2\pi}{N}\exp(\frac{2\pi i}{N}) & \cdots & 0 & 0 \\ 0 & 0 & -2\cos\frac{2\pi}{N}\exp(-\frac{2\pi i}{N}) & 2 & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & 2 & -2 \\ 0 & 0 & 0 & 0 & \cdots & -2 & 2 \end{pmatrix}$$

The k-th 2×2 block along the principal diagonal of the matrix UVU^{-1} is

$$\begin{pmatrix} 2 & -2\cos\frac{k\pi}{N}\exp(\frac{k\pi i}{N}) \\ -2\cos\frac{k\pi}{N}\exp(-\frac{k\pi i}{N}) & 2 \end{pmatrix} .$$

Thus, for n_{2k-1} and n_{2k} we have

$$L(n_{2k-1}, n_{2k}) = \frac{1}{2} m \ (\dot{n}_{2k-1}^* \dot{n}_{2k}^*) \begin{pmatrix} 1 & 0 \\ 0 & \frac{M}{m} \end{pmatrix} \begin{pmatrix} \dot{n}_{2k-1} \\ \dot{n}_{2k} \end{pmatrix}$$

$$- \frac{1}{2} \beta (n_{2k-1}^* n_{2k}^*) \begin{pmatrix} 2 & -2 \cos \frac{k\pi}{N} \exp(\frac{k\pi i}{N}) \\ -2 \cos \frac{k\pi}{N} \exp(-\frac{k\pi i}{N}) & 2 \end{pmatrix} \begin{pmatrix} n_{2k-1} \\ n_{2k} \end{pmatrix}$$

$$= \frac{1}{2} \left(m \ \dot{n}_{2k-1}^* \dot{n}_{2k-1} + M \dot{n}_{2k}^* \dot{n}_{2k} \right)$$

$$- \beta \left(n_{2k-1}^* n_{2k-1} - \cos \frac{k\pi}{N} \exp(- \frac{k\pi i}{N}) n_{2k}^* n_{2k-1} \right.$$

$$\left. - \cos \frac{k\pi}{N} \exp(\frac{k\pi i}{N}) n_{2k-1}^* n_{2k} + n_{2k}^* n_{2k} \right) .$$

The equations of motion are

$$\frac{1}{2} m \ \ddot{n}_{2k-1} + \beta n_{2k-1} - \beta \cos \frac{k\pi}{N} \exp(\frac{k\pi i}{N}) n_{2k} = 0 \quad ,$$

$$\frac{1}{2} M \ \ddot{n}_{2k}^* + \beta n_{2k} - \beta \cos \frac{k\pi}{M} \exp(- \frac{k\pi i}{N}) n_{2k-1} = 0 \quad .$$

The frequencies satisfy the secular determinant

$$\det \begin{pmatrix} -\frac{2\beta}{m} + 4\pi^2 f^2 & \frac{2\beta}{m} \cos \frac{k\pi}{N} \exp \frac{k\pi i}{N} \\ \frac{2\beta}{M} \cos \frac{k\pi}{N} \exp(- \frac{k\pi i}{N}) & -\frac{2\beta}{M} + 4\pi^2 f^2 \end{pmatrix} = 0 \quad .$$

Thus $\quad f = \frac{\sqrt{\beta}}{2\pi} \sqrt{(\frac{1}{m} + \frac{1}{M}) \pm \sqrt{(\frac{1}{m} + \frac{1}{M})^2 - \frac{4}{Mm} \sin^2 \frac{k\pi}{N}}} \quad .$

Recognizing that, in solid state physics, the wave number for the vibration

is $\quad K = \frac{k\pi}{Na} \quad$, where $\quad a$ is the separation of neighboring particles, the result

may be rewritten as

$$f = \frac{\sqrt{\beta}}{2\pi}\sqrt{(\frac{1}{m} + \frac{1}{M}) \pm \sqrt{(\frac{1}{m} + \frac{1}{M})^2 - \frac{4\sin^2 Ka}{Mm}}} \qquad .$$

The value $K = \frac{\pi}{2a}$ defines the boundary of the first Brillouin zone in reciprocal

lattice space. The familiar forbidden frequency gap appears since, for

$K = \frac{\pi}{2a}$,   f   will have the separated values

$$\frac{\sqrt{\beta}}{2\pi}\sqrt{\frac{2}{m}} \quad \text{or} \quad \frac{\sqrt{\beta}}{2\pi}\sqrt{\frac{2}{M}} \qquad [7] .$$

REFERENCES

1. Boyd, J.N. and Raychowdhury, P.N., "An Application of Projection Operators to a One Dimensional Crystal", Bulletin of the Institute of Mathematics, Academia Sinica 7(1979), 133-144.

2. Boyd, J.N. and Raychowdhury, P.N., "Projection Operator Techniques in Lagrangian Mechanics: Symmetrically Coupled Oscillators", to appear in International Journal of Mathematics and Mathematical Sciences.

3. Duffey, G.H., Theoretical Physics, Houghton Mifflin Company, Boston, 1973.

4. Gamba, A., "Representations and Classes in Groups of Finite Order", Journal of Mathematical Physics 9 (1968), 186-192.

5. Hamermesh, M., Group Theory and Its Application to Physical Problems, Addison Wesley Publishing Company, Reading, Mass., 1962.

6. Joshi, A.W., Elements of Group Theory for Physicists, Halsted Press, New York, 1973.

7. Kittel, C., Introduction to Solid State Physics (Second Edition), John Wiley and Sons, New York, 1959.

8. Mariot, L., (translated by A. Nussbaum), Group Theory and Solid State Physics, Prentice-Hall, Englewood Cliffs, N.J., 1964.

9. Nussbaum, A., "Group Theory and Normal Modes", American Journal of Physics 36, 529-539.

10. Wilde, R.E., "A General Theory of Symmetry Coordinates", American Journal of Physics 32(1964), 45-52.