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# APPENDIX

# APPENDIX A

## THE EQUATIONS OF MOTION FOR INFINITE MONATOMIC AND DIATOMIC CHAINS

In the Classical Mechanics, the Hamiltonian,H, is equal to the summation of the kinetic energy,T, and the potential energy,V.

$$H = T + V \quad , \qquad (A.1)$$

where

$$T = \frac{P^2}{2m} \quad , \qquad (A.2)$$

and the potential energy of spring is

$$V = \frac{Cu^2}{2} \quad , \qquad (A.3)$$

Here P is the linear momentum, m is the mass, C is the spring constant and u is the displacement. Then, in the case of the infinite monatomic chain, the Hamiltonian is

$$H = (1/2m)\sum_{n=-\infty}^{\infty} P_n^2 + (C/2)\sum_{n=-\infty}^{\infty}(u_{n+1} - u_n)^2 \quad . \qquad (A.4)$$

From the definition of the linear momentum of mass m,

$$m\dot{u}_n = P_n \quad . \tag{A.5}$$

Taking the time derivative Eq. (A.5) yields

$$m\ddot{u}_n = \dot{P}_n \quad . \tag{A.5.1}$$

From Eq. (A.4) , H = H(P,u) and the Hamiltonian's equations of motion are

$$\dot{u} = \frac{\partial H}{\partial P}, and\ \dot{P} = \frac{\partial H}{\partial u}. \tag{A.6}$$

Consider $$\dot{P}_n = \frac{\partial H}{\partial u_n}. \tag{A.6.1}$$

Insert Eq.(A.4) and Eq.(A.5.1) into Eq.(A.6.1) and then obtain

$$m\ddot{u} = -\frac{C}{2}\frac{\partial(u_{n+1}-u_n)^2}{\partial u_n}$$
$$= -\frac{C}{2}[-2(u_{n+1}-u_n)] - \frac{C}{2}[2(u_n - u_{n-1})].$$

Therefore $$m\ddot{u} = C(u_{n+1}-u_n) + C(u_{n-1}-u_n) \quad . \tag{A.7}$$

Similarly, in the case of the infinite diatomic chain, the Hamiltonian is

$$\begin{aligned} H &= (1/2m_1)\sum_{n=-\infty}^{\infty} P_{s1,n}^2 + (C_1/2)\sum_{n=-\infty}^{\infty}(u_{s2,n}-u_{s1,n})^2 \\ &\quad + (1/2m_2)\sum_{n=-\infty}^{\infty} P_{s2,n}^2 + (C_2/2)\sum_{n=-\infty}^{\infty}(u_{s1,n+1}-u_{s2,n})^2 \end{aligned} \tag{A.8}$$

Since the definition of the linear momentum of mass m1 is

$$m\dot{u}_{s1,n} = P_{s1,n} \qquad . \tag{A.9}$$

Taking the time derivative of Eq.(A.9) yields

$$m\ddot{u}_{s1,n} = \dot{P}_{s1,n} \qquad . \tag{A.9.1}$$

Insert Eq.(A.8) and Eq.(A.9.1) into Eq.(A.6.1) and then obtain

$$\begin{aligned} m_1\ddot{u}_{s1,n} &= -\frac{C_1}{2}\frac{\partial(u_{s2,n}-u_{s1,n})^2}{\partial u_{s1,n}} - \frac{C_2}{2}\frac{\partial(u_{s1,n+1}-u_{s2,n})^2}{\partial u_{s1,n}}, \\ &= -\frac{C_1}{2}[-2(u_{s2,n}-u_{s1,n})] - \frac{C_2}{2}[2(u_{s1,n}-u_{s2,n-1})]. \end{aligned}$$

Therefore $$m_1\ddot{u}_{s1,n} = C_1(u_{s2,n} - u_{s1,n}) + C_2(u_{s2,n-1} - u_{s1,n}) \qquad . \tag{A.10}$$

Similarly, $$m_2\ddot{u}_{s2,n} = C_1(u_{s1,n} - u_{s2,n}) + C_2(u_{s1,n+1} - u_{s2,n}) \qquad . \tag{A.11}$$

## APPENDIX B

## THE EQUATIONS OF MOTION FOR SEMI-INFINITE MONATOMIC AND DIATOMIC CHAINS

In the Classical Mechanics, the Hamiltonian,H, is equal to the summation of the kinetic energy,T, and the potential energy,V.

$$H = T + V \quad , \qquad (B.1)$$

where

$$T = \frac{P^2}{2m} \quad , \qquad (B.2)$$

and the potential energy of spring is

$$V = \frac{Cu^2}{2} \quad , \qquad (B.3)$$

Here P is the linear momentum, m is the mass, C is a spring constant and u is the displacement. Then, in the case of the semi-infinite monatomic chain, the Hamiltonian is

$$H = (1/2m)\sum_{n=0}^{\infty} P_n^2 + (C/2)\sum_{n=0}^{\infty}(u_{n+1} - u_n)^2 \quad . \qquad (B.4)$$

From the definition of the linear momentum of mass m,

$$m\dot{u}_n = P_n \quad . \tag{B.5}$$

Taking the time derivative of Eq. (B.5) yields

$$m\ddot{u}_n = \dot{P}_n \quad . \tag{B.5.1}$$

From Eq. (B.4) , H = H(P,u) and the Hamiltonian's equations of motion are

$$\dot{u} = \frac{\partial H}{\partial P}, and\ \dot{P} = \frac{\partial H}{\partial u}. \tag{B.6}$$

Consider $$\dot{P}_n = \frac{\partial H}{\partial u_n}. \tag{B.6.1}$$

Insert Eq.(B.4) and Eq.(B.5.1) into Eq.(B.6.1) yields

$$\begin{aligned} m\ddot{u} &= -\frac{C}{2}\frac{\partial(u_{n+1}-u_n)^2}{\partial u_n} \\ &= -\frac{C}{2}[-2(u_{n+1}-u_n)] - \frac{C}{2}[2(u_n-u_{n-1})]. \end{aligned}$$

Therefore, the equation of motion for the first mass is

$$m\ddot{u}_1 = C(u_2 - u_1) \quad , \tag{B.7}$$

while the equation of motion for the other mass (n>1) is

$$m\ddot{u}_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) \quad , \tag{B.8}$$

Similarly, in the case of the semi-infinite diatomic chain, the Hamiltonian is

$$H = (1/2m_1)\sum_{n=0}^{\infty} P_{s1,n}^2 + (C_1/2)\sum_{n=0}^{\infty}(u_{s2,n} - u_{s1,n})^2$$
$$+ (1/2m_2)\sum_{n=0}^{\infty} P_{s2,n}^2 + (C_2/2)\sum_{n=0}^{\infty}(u_{s1,n+1} - u_{s2,n})^2$$

Since the definition of the linear momentum of mass m1 is

$$m\dot{u}_{s1,n} = P_{s1,n} \qquad \text{(B.10)}$$

Taking the time derivative of Eq.(B.9) yields

$$m\ddot{u}_{s1,n} = \dot{P}_{s1,n} \qquad \text{(B.10.1)}$$

Insert Eq.(B.8) and Eq.(B.9.1) into Eq.(B.6.1) yield

$$m_1\ddot{u}_{s1,n} = -\frac{C_1}{2}\frac{\partial(u_{s2,n}-u_{s1,n})^2}{\partial u_{s1,n}} - \frac{C_2}{2}\frac{\partial(u_{s1,n+1}-u_{s2,n})^2}{\partial u_{s1,n}},$$
$$= -\frac{C_1}{2}[-2(u_{s2,n}-u_{s1,n})] - \frac{C_2}{2}[2(u_{s1,n}-u_{s2,n-1})].$$

Therefore, the equation of motion for the first mass (s1) is

$$m_1\ddot{u}_{s1} = C_1(u_{s2} - u_{s1}) \quad , \qquad \text{(B.11)}$$

while the equation of motion for the other mass (n>0) is

$$m_1\ddot{u}_{s1,n} = C_1(u_{s2,n} - u_{s1,n}) + C_2(u_{s2,n-1} - u_{s1,n}) \; ; \; n \geq 1 \quad . \qquad \text{(B.12)}$$

Similarly, the equation of motion for the s2+n th mass (n>0) is

$$m_2 \ddot{u}_{s2,n} = C_1 (u_{s1,n} - u_{s2,n}) + C_2 (u_{s1,n+1} - u_{s2,n}) \; ; \; n \geq 0 \quad . \tag{B.13}$$

## APPENDIX C

## THE PROOF OF BLOCH'S THEOREM

Bloch's theorem follows from the fact that the potential function in the Schoedinger equation is periodic. The Schroedinger equation of two different cells of lattice is

$$\frac{-h^2}{2m}\nabla^2\Psi(r)+v(r)\Psi(r)=E\Psi(r), \tag{C.1}$$

$$\frac{-h^2}{2m}\nabla^2\Psi(r+R)+v(r+R)\Psi(r+R)=E\Psi(r+R), \tag{C.2}$$

Here **R** is a lattice vector connecting the two cells. Sence lattice is completely periodic v(**r**) = v(**r**+**R**) . The solution of Eq. (C.1) and (C.2) , Ψ(**r**)and Ψ(**r**+**R**) respectively,are translated from another by **R**. The solutions must be the same physical wave function, which they are equivalence. The function must he normalized, thus the multiple factor may be a complex number which has magnitude equal to one,exp i∝ , as (exp i∝ $)^2$ = 1.

$$\Psi(r)=e^{i\alpha}\Psi(r+R) \tag{C.3}$$

If two independent lattice translations, $\mathbf{R}_1$ and $\mathbf{R}_2$, are performed, the result must be a lattice translations which we call $\mathbf{R}_3$.

$$\Psi(r+R_1+R_2)=e^{i\alpha_2}\Psi(r+R_1)=e^{i(\alpha_1+\alpha_2)}\Psi(r) \qquad . \tag{C.4}$$

where $$\Psi(r+R_1+R_2)=\Psi(r+R_3)=e^{i(\alpha_3)}\Psi(r) \qquad . \tag{C.5}$$

then $$e^{i\alpha_3}=e^{i(\alpha_1+\alpha_2)} \qquad ,$$

and $$\alpha_3=\alpha_1+\alpha_2 \qquad . \tag{C.6}$$

This gives to be the linear in the distance of the translation, thus we can write the translation $\mathbf{R}_x$ in x direction as follows.

$$\alpha=k_xR_x \qquad .$$

or in the other direction (for three dimensions),

$$\alpha=k_xR_x+k_yR_y+k_zR_z=kR \qquad . \tag{C.7}$$

Then the solution of the Schroedinger equation must have the form

$$\Psi(r)=e^{i(kR)}\Psi(r+R) \qquad . \tag{C.8}$$

Multiply Eq.(C.8) by exp (**ikr**) on each side, then obtain

$$e^{i(kr)}\Psi(r)=e^{i(k(r+R))}\Psi(r+R) \qquad . \tag{C.9}$$

That it means the product exp (**ikr**) $\Psi$(**r**)is the periodic function which repeats itself within each cell of the lattice. If we call this function as u(**r**), then

$$e^{i(kr)}\Psi(r) = u(r) \quad , \qquad \text{(C.10)}$$

or

$$\Psi(r) = e^{-i(kr)}u(r) \quad , \qquad \text{(C.11)}$$

which is the Bloch's theorem.

**Reference**

C. A. Wert and R. M. Thomson, Physics of Solids, 2 nd. ed. (New York: McGraw-Hill, 1970) p.176-179.

## APPENDIX D

## THE RELATIONSHIP BETWEEN THE CAUSE AND THE EFFECT

In the special case of the simple harmonic motion,the force F applied on mass m is proportional to the displacement x from its equilibrium (in the opposite direction).

Thus,
$$F = -kx \quad , \tag{D.1}$$

and , according to the second law, F = ma . Hence

$$m\frac{d^2x}{dt^2} = -\omega^2 mx \quad ; \quad \omega = \sqrt{k/m} \ ,$$

therefore,
$$\frac{d^2x}{dt^2} + \omega^2 x = 0 \quad . \tag{D.2}$$

The one of the solution is

$$x = A\sin\omega t \quad . \tag{D.3}$$

If t = o, then x = 0, and it $t_n = (2n+1)\pi/2\omega$ ; n = 0,1,2,..., then x is maximum ($x = x_{max} = A$). Thus $\omega = (2n+1)\pi / 2t_n = \omega_n$ ,

and
$$x_n = A\sin\omega_n t = x_{max}\sin\omega_n t \quad . \tag{D.4}$$

To find $x_{max}$, differentiating the Eq. (D.4) two times with response to time t, hence

$$\frac{d^2x_n}{dt^2} = -x_{max}\omega_n^{\,2}\sin\omega_n t \quad .$$

Mutiplying the mass m on the both side yields

$$m\frac{d^2x_n}{dt^2} = -mx_{max}\omega_n^{\,2}\sin\omega_n t \quad .$$

Therefore, $$F = -mx_{max}\omega_n^{\,2}\sin\omega_n t \quad .$$

F will be maximum when $\sin\omega_n t = 1$, $F_{max} = F_0 = -mx_{max}\omega_n^2$ thus,

$$x_{max} = \frac{-F_0}{m\omega_n^{\,2}} \quad . \tag{D.5}$$

Insertiong Eq. (D.5) into Eq. (D.4) yields

$$x_n = \frac{-F_0}{m\omega_n^{\,2}}\sin\omega_n t \quad . \tag{D.6}$$

In the case of the solution which there is the phase factor

$$x_n = \frac{-F_0}{m\omega_n^{\,2}}\sin(\omega_n t - \delta) \quad , \tag{D.7}$$

where $\delta$ is the phase factor, or

$$x_n = \frac{-F_0}{m\omega_n^{\,2}}\sin\omega_n(t - \delta/\omega_n) \quad .$$

Let $\delta/\omega_n = t_n$ , hence

## APPENDIX E

## THE DEFINITION OF THE FOURIER TRANSFORM

## OF THE RESPONSE FUNCTION

The displacement of the first mass has the from $u_0(t) = u_0(\omega)\exp(i\omega t)$ and the force is $F(t) = F_0\exp(i\omega t)$. From the relationship between the cause and the effect in Eq. (4.2) in chapter IV, we can write the cause as

$$x(t) = F_0 \exp(i\omega t)\chi(\omega) \quad , \tag{E.1}$$

where x (t) means the effect such that x (t) is the acceleration of the first mass. Therefore

$$x(t) = \frac{d^2 u_0(t)}{dt^2} \quad . \tag{E.2}$$

Substitutiing $u_0(t) = u_0(\omega)\exp(i\omega t)$ into Eq.(E.2) yields

$$x(t) = -\exp(i\omega t)\omega^2 u_0 \quad , \tag{E.3}$$

Insert Eq. (E.3) into Eq. (E.1), we get

$$F_0 \exp(i\omega t)\chi(\omega) = -\exp(i\omega t)\omega^2 u_0 \quad , \tag{E.4}$$

therefore, $$F_0 \chi(\omega) = -\omega^2 u_0 \quad .$$

Insert the Harmonic motion, $\ddot{u}(\omega) = -\omega^2 u(\omega)$ into this last equation, can be written as

$$\ddot{u}(\omega) = F_0 \chi(\omega) \quad . \tag{E.5}$$

## APPENDIX F

## THE MATHCAD (MCAD) PROGRAM

The MCAD program for window is the high guality program. It can solve the complex equation of Mathematics (such as, integral, differential, numericalmethods, Matrix,etc.), plot the graphs (in 1-3 dimensions, polar, contour,etc.) , and so on.

In this thesis, we used the MCAD program for window to evaluate variables and to plot graphs.

**Program for Fig 4.1**

N := 15 , ω := 0.5 , m := 2 ,

T := 1..N , t := 1..N ,

$$\chi(T,t) := \frac{\cos(\omega t)\cos(\omega T)}{m\omega},$$

$$M_{(t,T)} := \chi(T,t)$$

**Program for Fig 4.2**

$N := 15$ , $\omega := 0.5$ , $m := 2$ ,

$T := 1..N$ , $t := 1..N$ ,

$$\chi(T,t) := \frac{\cos(\omega[T-t])}{m\omega},$$

$$M_{(t,T)} := \chi(T,t)$$

**Program for Fig 4.3**

$N := 15$ , $\omega := 0.5$ , $m := 2$ ,

$T := 1..N$ , $t := 1..N$ ,

$x(T,t) := T-t$ ,

$h(T,t) := \mathrm{if}(T<t, x(T,t), 0)$ ,

$$\chi(T,t) := \frac{\cos(\omega h[T,t])}{m\omega},$$

$$M_{(t,T)} := \chi(T,t)$$

**Program for Fig 5.2.3**

$m_1 := 5.8852\text{x}10^{-26}$ , $m_2 := 3.8163\text{x}10^{-26}$ ,

$M := 2.315\text{x}10^{-26}$ , $C := 78.4945$ ,

$\omega := -9.000\text{x}10^{13}, -8.995\text{x}10^{13} .. 9.000\text{x}10^{13}$

$$\chi_1(\omega) = \frac{\omega^2}{2C}\left[1 - \frac{(m_1 - m_2)C}{m_1 m_2 \omega^2 - (m_1 + m_2)C}\right]$$
$$\left[1 - \sqrt{1 + \frac{4C\ [(C\ +C\ ) - m_2\omega^2][m_1 m_2 \omega^2 - (m_1 + m_2)C\ ]}{\omega^2[m_1 m_2 \omega^2 - (m_1 + m_2)C\ - (m_1 - m_2)C\ ]^2}}\right]$$

**Program for Fig 5.2.4**

$m_1 := 5.8852\text{x}10^{-26}$ , $m_2 := 3.8163\text{x}10^{-26}$ ,

$M := 2.315\text{x}10^{-26}$ , $C := 78.4945$ ,

$\omega := -9.000\text{x}10^{13}, -8.995\text{x}10^{13} .. 9.000\text{x}10^{13}$

$$\chi_2(\omega) = \frac{\omega^2}{2C}\left[1 + \frac{(m_1 - m_2)C}{m_1 m_2 \omega^2 - (m_1 + m_2)C}\right]$$
$$\left[1 - \sqrt{1 + \frac{4C\ [(C\ +C\ ) - m_2\omega^2][m_1 m_2 \omega^2 - (m_1 + m_2)C\ ]}{\omega^2[m_1 m_2 \omega^2 - (m_1 + m_2)C\ - (m_1 - m_2)C\ ]^2}}\right]$$

**Program for Fig 5.3.1**

$m_1 := 5.8852\text{x}10^{-26}$ , $m_2 := 3.8163\text{x}10^{-26}$ ,

$M := 2.315\text{x}10^{-26}$ , $C := 78.4945$ ,

$\omega := -9.000\text{x}10^{13}, -8.995\text{x}10^{13} .. 9.000\text{x}10^{13}$

$$\chi_1(\omega) = \frac{\omega^2}{2C}\left[1 - \frac{(m_1 - m_2)C}{m_1 m_2 \omega^2 - (m_1 + m_2)C}\right]$$
$$\left[1 - \sqrt{1 + \frac{4C\,[(C \; + C \;) - m_2\omega^2][m_1 m_2 \omega^2 - (m_1 + m_2)C \;]}{\omega^2[m_1 m_2 \omega^2 - (m_1 + m_2)C \; - (m_1 - m_2)C \;]^2}}\right] ,$$

$$\chi_2(\omega) = \frac{\omega^2}{2C}\left[1 + \frac{(m_1 - m_2)C}{m_1 m_2 \omega^2 - (m_1 + m_2)C}\right]$$
$$\left[1 - \sqrt{1 + \frac{4C\,[(C \; + C \;) - m_2\omega^2][m_1 m_2 \omega^2 - (m_1 + m_2)C \;]}{\omega^2[m_1 m_2 \omega^2 - (m_1 + m_2)C \; - (m_1 - m_2)C \;]^2}}\right] ,$$

$$\frac{u_{s10,n}(\omega)}{u_{s20,n-1}(\omega)} = \frac{\chi_1(\omega)C}{\chi_1(\omega)C - \omega^2} ,$$

$$\frac{u_{s20,n}(\omega)}{u_{s10,n}(\omega)} = \frac{\chi_2(\omega)C}{\chi_2(\omega)C - \omega^2} .$$

# CIRRICURUM VITAE

Miss Orapin Niamploy was born on 22 August 1972; at Bangkok and received the Bachelor degree of Science in physics from the department of physics, faculty of science, Mahidol University in 1994. Miss Orapin Niamploy has been a student in the department of physics at the graduate school of Chulalongkorn University since 1994.