4. First Order Linear Systems

Quite often in applications you must consider systems of differential equations. We shall consider a linear system of the form

$$\begin{aligned}
\frac{du_1}{dx} &= a_{11}(x)u_1 + a_{12}(x)u_2 + \cdots + a_{1n}(x)u_n + f_1(x) \\
\frac{du_2}{dx} &= a_{21}(x)u_1 + \cdots \qquad\qquad + a_{2n}(x)u_n + f_2(x) \\
&\vdots \\
\frac{du_n}{dx} &= a_{n1}(x)u_1 + \cdots \qquad\qquad + a_{nn}(x)u_n + f_n(x),
\end{aligned}$$

where the functions $a_{ij}(x)$ and $f_j(x)$ are continuous. If we anticipate the next chapter and write the derivative of a vector $U = (u_1, \ldots, u_n)$ as the derivative of its components,

$$\frac{d}{dx} U(x) = \left(\frac{du_1}{dx}, \frac{du_2}{dx}, \ldots, \frac{du_n}{dx}\right),$$

then the above system can be written in the clean form

$$\frac{dU}{dx} = A(x)U + F(x), \tag{22}$$

where,

$$A(x) = ((a_{ij})), \quad F = (f_1, f_2, \ldots, f_n)$$

and

$$U(x) = (u_1, u_2, \ldots, u_n).$$

The initial value problem for the system of differential equations (22) is to find a vector $U(x)$ which satisfies the equation as well as the initial condition

$$U(x_0) = U_0 , \qquad (23)$$

where U_0 is a vector of constants.

It is of considerable theoretical importance to realize that the initial value problem for a single linear equation of order n

$$u^{(n)} + a_{n-1}(x)u^{(n-1)} + \cdots + a_0(x)u = f(x)$$

$$u(x_0) = \alpha_1,\ u'(x_0) = \alpha_2, \ldots, u^{(n-1)}(x_0) = \alpha_n ,$$

can be transformed to the conceptually simpler problem (22)-(23). Let $u_1(x) \equiv u(x)$, $u_2(x) \equiv u'(x)$, ..., and $u_n(x) = u^{(n-1)}(x)$. Then the components of the vector $U(x) = (u_1, u_2, \ldots, u_n)$ must obviously satisfy the relations

$$\frac{du_1}{dx} = u_2$$

$$\frac{du_2}{dx} = u_3$$

$$\vdots$$

$$\frac{du_{n-1}}{dx} = u_n$$

$$\frac{du_n}{dx} = -a_0u_1 - a_1u_2 - \cdots - a_{n-1}u_n + f(x) ,$$

which may be written as

$$U' = AU + F ,$$

where

$$A(x) = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & & 0 \\ 0 & 0 & 0 & & 0 \\ 0 & 0 & . & & 1 \\ -a_0 & -a_1 & - & -a_{n-2} & -a_{n-1} \end{pmatrix} ,$$

and

$$F = (\underbrace{0, 0, \ldots, 0}_{n-1}, f) .$$

The initial conditions read

$$U(x_0) = (\alpha_1, \alpha_2, \ldots, \alpha_n) .$$

Conversely, if U is any solution of this system of equations with the proper initial conditions, then the first component $u_1(x)$ is a solution of the single n^{th} order equation. Thus, the general theory of a single n^{th} order linear O.D.E. is completely subsumed as a portion of the theory of a system of first order linear O.D.E.'s. You should be warned that this generalization is mainly of theoretical value and is of little use if you are seeking an explicit solution.

Both the existence and uniqueness theorems are true for systems, and supply an example where the theoretical advantages of systems becomes clear. To illustrate this, we shall prove the uniqueness theorem. Our proof is patterned directly after the uniqueness proof for a single equation (Theorem 1).

Theorem 9. (Uniqueness). Let $A(x)$ be a matrix whose coefficients $a_{ij}(x)$ are bounded $|a_{ij}(x)| \leq M$ for x in some interval, and let $F(x)$ be a continuous function. Then there is at most one solution $U(x)$ of the initial value problem

$$U' = AU + F, \quad U(x_0) = U_0.$$

Remark. The existence theorem states, if A is nonsingular and each element is integrable there is at least one solution. Thus, there is then exactly one solution.

Proof: Assume U_1 and U_2 are both solutions. Let

$$W = U_1 - U_2.$$

Then W satisfies the homogeneous equation and is zero at x_0,

$$W' = AW, \quad W(x_0) = 0.$$

Take the scalar product of both sides with W,

$$\langle W, W' \rangle = \langle W, AW \rangle.$$

But

$$\langle W, W' \rangle = w_1 w_1' + w w_2' + \cdots + w_n w_n'$$

$$= \frac{1}{2} \frac{d}{dx} (w_1^2 + w_2^2 + \cdots + w_n^2) = \frac{1}{2} \frac{d}{dx} \| W \|^2.$$

Thus,

$$\frac{1}{2} \frac{d}{dx} \| W \|^2 = \langle W, AW \rangle.$$

By Theorem 17, p. 173 and the hypothesis $|a_{ij}(x)| \leq M$, we know

$$\langle W, AW \rangle \leq \sqrt{\sum_{i,j=1}^{n} a_{ij}^2} \, \| W \|^2 \leq nM \| W \|^2,$$

so that

$$\frac{1}{2} \frac{d}{dx} \| W \|^2 \leq nM \| W \|^2.$$

Therefore, as on p. 462-3

$$\frac{d}{dx} (\| W \|^2) - 2nM \| W \|^2 \leq 0,$$

or

$$e^{2nMx} \frac{d}{dx} (e^{-2nMx} \| W \|^2) \leq 0.$$

Because e^{2nMx} is always positive, by the mean value theorem the quantity ( ) is a decreasing function. Its value for $x > x_0$ is then less than at x_0,

$$e^{-2nMx} \| W(x) \|^2 \leq e^{-2nMx_0} \| W(x_0) \|^2 , \quad x \geq x_0$$

Consequently

$$\| W(x) \| \leq e^{nM(x-x_0)} \| W(x_0) \| , \quad x \geq x_0 .$$

Since $W(x_0) = 0$ and the norm is non negative, we have

$$0 \leq \| W(x) \| \leq 0 , \quad x \geq x_0 ,$$

which implies

$$\| W(x) \| = 0 , \quad x \geq x_0 .$$

Therefore,

$$W(x) \equiv 0 \quad x \geq x_0 .$$

By replacing x with $-x$ in the original equation, the same statement is true for $x \leq x_0$. Thus, throughout the interval where $|a_{ij}(x)| \leq M$, we have proved $W(x) \equiv 0$, that is, $U_1(x) \equiv U_2(x)$, so the solution is indeed unique.

Because a single linear n^{th} order O. D. E. can be replaced by an equivalent system of equations, this theorem implies the uniqueness theorem for a single O. D. E. of order n if the coefficients $a_j(x)$ are bounded in some interval - which is certainly true in every interval if the a_j's are continuous.

With this theorem, a short section closes. Further developments in the theory of systems of linear O. D. E.'s makes elegant use of linear operators in general and matrices in particular. As you might well except, the exercises contain a few of the more accessible results.

Exercises.

1. Find functions $u_1(x)$, $u_2(x)$ which satisfy

$$u_1' = u_1$$

$$u_2' = u_1 - u_2 ,$$

with the initial conditions $U(0) \equiv (u_1(0), u_2(0) = (1, 0)$. Find the general solution too. [Hint: Solve the equation $u_1' = u_1$ first, then substitute. Answer: General solution is $U(x) = (\gamma_1 e^x, \frac{\gamma_1}{2} e^x + \gamma_2 e^{-x})$].

2 . Consider the system

$$u_1' = 2u_1 - u_2$$

$$u_2' = 3u_1 - 2u_2 ,$$

that is,

$$U' = AU , \text{ where } A = \begin{pmatrix} 2 & -1 \\ 3 & -2 \end{pmatrix} .$$

Let $\phi_1(x) = au_1 + bu_2$, $\phi_2(x) = cu_1 + du_2$, where a, b, c, and d are constants. Thus,

$$\Phi = SU,$$

where

$$S = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \Phi = (\phi_1, \phi_2).$$

a). By direct substitution, find the differential equations satisfied by the ϕ_j's and show they can be written as

$$\Phi' = SAS^{-1}\Phi.$$

b). Pick the coefficients of S so the matrix SAS^{-1} is a diagonal matrix,

$$SAS^{-1} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \equiv \Lambda.$$

c). Solve the resulting equation $\Phi' = \Lambda\Phi$. [Solution: $\phi_1 = \alpha e^x$, $\phi_2 = \beta e^{-x}$ - you might have ϕ_1 and ϕ_2 interchanged].

d). Use this solution to solve the original equations for U. [Hint: Recall $U = S^{-1}\Phi$].

3. By only a slight modification of Exercise 2, solve

$$v_1'' = 2v_1 - v_2$$

$$v_2'' = 3v_1 - 2v_2.$$

[Hint: Everything, even the algebra, is identical. The only difference is in part c) you have to solve $\Phi'' = \Lambda\Phi$. Then $V = S^{-1}\Phi$ as before].

4. A bathtub initially contains Q_1 gallons of gin and Q_2 gallons of vermouth, where $Q_1 + Q_2 = Q$, Q being the capacity of the tub. Pure gin enters from one faucet at a constant rate of R_1 gallons per minute, while pure vermouth enters from another faucet at a constant rate R_2 gallons per minute. The well stirred mixture of martinis leaves the drain at a rate $R_1 + R_2$ gallons per minute (so the total amount of fluid in the tub remains constant at Q gallons). Let $G(t)$ be the quantity of gin in the tub at time t and $V(t)$ be the quantity of vermouth.

a) Show

$$\frac{dG}{dt} = R_1 - \frac{G}{Q}(R_1 + R_2)$$

$$\frac{dV}{dt} = R_2 - \frac{V}{Q}(R_1 + R_2).$$

b). Integrate this simple system of equations to find $G(t)$ and $V(t)$. Also find their ratio $P(t) \equiv G(t)/V(t)$ which is the strength of the martinis at time t.

c). Prove

$$\lim_{t \to \infty} P(t) = \frac{R_1}{R_2}.$$

Compare this with your intuitive expectations.

d). If $Q_1 = 20$, $Q_2 = 0$, $R_1 = R_2 = 1$ gal/min, how long must I wait to get a perfect martini (for me, perfect is 5 parts gin to 1 part vermouth). [Needless to say, the mathematical model is applicable to many problems in the mixing of chemicals which do not react with each other. If the chemicals do interact, the model must be changed to account for the interaction].

5 . Consider the homogeneous equation $U' = A(x)U$, where A is non-singular (so $\det A \neq 0$). Assuming the validity of the existence theorem, prove there exists n linearly independent vectors $U_1(x), U_2(x), \ldots, U_n(x)$ which are solutions, $U_k' = AU_k$, $k = 1, \ldots, n$. [Hint: Construct n solutions which are linearly independent at $x = x_0$, and then prove a set of n solutions are linearly independent in an interval if and only if they are linearly independent at $x = x_0$, where x_0 is a point in the interval].

6 . Let $LU \equiv U' - A(x)U$ as in Exercise 5. Prove $\dim \mathcal{N}(L) = n$.

7 . Let $LU \equiv U' - A(x)U$. If a basis $U_1, \ldots, U_n$, for $\mathcal{N}(L)$ is known, prove the inhomogeneous equation $LU = F$ can be solved by variation of parameters. That is, seek a particular solution U_p of $LU = F$ in the form

$$U_p = \sum_{i=1}^{n} U_i v_i$$

where the $v_i(x)$ are scalar-valued functions (<u>not</u> vectors).

a). Compute U_p' and substitute into the O.D.E. to conclude U_p is a particular solution if

$$\sum_{i=1}^{n} U_i v_i' = F .$$

b). Let U be the $n \times n$ matrix whose columns are $U_1, U_2, \ldots, U_n$. Prove U is invertible and show

$$v_i'(x) = (U^{-1}F)_{i\text{th component}} .$$

c). Show

$$U_p(x) = \sum_{i=1}^{n} U_i(x) \int^x [U^{-1}(s)F(s)]_i \, ds .$$

This may also be written in the form

$$U_p(x) = U(x) \int^x U^{-1}(s) F(s) \, ds$$

d). Apply this procedure to find the general solution of

$$u_1' = u_1 + e^{2x} \qquad \text{(cf. Ex. 1)}$$
$$u_2' = u_1 - u_2 + 1 .$$

5. Translation Invariant Linear Operators

This section develops various extensions and applications of the procedure used to solve linear ordinary differential equations with constant coefficients. The results will be proved as a series of exercises interspersed by various remarks.

Definition. The translation operator T_t acting on functions $u(x)$ is defined by the property

$$(T_t u)(x) = u(x-t) . \qquad x, t \in \mathbb{R} .$$

Definition. A linear operator L is translation invariant if

$$LT_t = T_t L$$

for every t, that is, if

$$L(T_t u) = T_t(Lu)$$

for every t and for every function u for which the operators are defined.

Example 1. Let $(Lu)(x) \equiv 3u(x) - 2u(x-1)$. Then

$$[T_t(Lu)](x) = 3u(x-t) - 2u(x-t-1),$$

and

$$[L(T_t u)](x) = Lu(x-t) = 3u(x-t) - 2u(x-t-1).$$

Thus,

$$LT_t = T_t L ,$$

so the operator L is translation invariant.

2. Let $(Lu)(x) \equiv 3xu(x)$. Then

$$[T_t(Lu)](x) = 3(x-t)u(x-t),$$

and

$$[L(T_t u)](x) = Lu(x-t) = 3xu(x-t).$$

Thus

$$LT_t \neq T_t L ,$$

so this operator is not translation invariant.

Exercise 1. Which of the following linear operators (verify!) are also translation invariant?

a). $(Lu)(x) \equiv cu(x)$, $c \equiv$ constant

b). $(Lu)(x) \equiv \dfrac{u(x+h)-u(x)}{h}$, $h \equiv$ constant $\neq 0$.

c). $(Lu)(x) \equiv \displaystyle\int_{-\infty}^{x} k(x-s)u(s)ds$

d). $(Lu)(x) \equiv (x-1)u(x)$

e). $(Lu)(x) = \dfrac{du}{dx}(x)$.

f). Any linear ordinary differential operator with constant coefficients,

$$Lu \equiv a_n u^{(n)} + a_{n-1}u^{(n-1)} + \cdots + a_0 u , \qquad a_k \text{ constants.}$$

g). Any linear ordinary differential operator with <u>variable</u> coefficients.

h). $(Lu)(x) = \sum_{k=1}^{n} a_k u(x-\gamma_k)$, a_k and γ_k constants.

[Answers: All but d) and g) are translation invariant].

2. If L_1 and L_2 are translation invariant operators which map some linear space into itself, then so are

a). $AL_1 + BL_2$, A, B constants

b). L_1L_2 and L_2L_1

c). If in addition L is invertible, then L^{-1} is also translation invariant.

<u>Theorem 10.</u> If L is a translation invariant linear operator, then

$$L(e^{\lambda x}) = \phi(\lambda)e^{\lambda x}.$$

<u>Proof.</u> We know so little about L that all we can hope to do is compute $T_tL(e^{\lambda x})$ and $LT_t(e^{\lambda x})$ and see what happens. Let $Le^{\lambda x} = \psi(\lambda ; x)$, where ψ is some unknown function whose value depends on both λ and x. Then

$$T_tL(e^{\lambda x}) = \psi(\lambda ; x-t),$$

while

$$LT_te^{\lambda x} = Le^{\lambda(x-t)} = L(e^{-\lambda t}e^{\lambda x})$$

$$= e^{-\lambda t}Le^{\lambda x} = e^{-\lambda t}\psi(\lambda ; x).$$

Since $T_tL = LT_t$, we find

$$e^{-\lambda t}\psi(\lambda ; x) = \psi(\lambda ; x-t),$$

or

$$\psi(\lambda ; x) = \psi(\lambda ; x-t)e^{\lambda t}.$$

Because the left side does not contain t, the right side must not depend on which value of t is chosen. Using this freedom, we let $t = x$ and conclude

$$\psi(\lambda ; x) = \psi(\lambda ; 0)e^{\lambda x}.$$

By setting $\phi(\lambda) = \psi(\lambda, 0)$, we find

$$Le^{\lambda x} = \psi(\lambda ; x) = \phi(\lambda)e^{\lambda x}$$

as desired.

<u>Exercise 3.</u> By direct substitution, find $\phi(\lambda)$ for those operators in Exercise 1 which are translation invariant.

[Answers: a) $\phi(\lambda) = c$, b). $\phi(\lambda) = (e^{-ah}-1)/h$

c). $\phi(\lambda) = \int_{-\infty}^{0} k(-s)e^{\lambda s}ds$, d). $\phi(\lambda) = \lambda$,

f). $\phi(\lambda) = \sum_{k=0}^{n} a_k\lambda^k$ (the characteristic polynomial), h). $\phi(\lambda) = \sum_{k=1}^{n} a_k e^{-\lambda \gamma_k}]$.

4. With the same assumptions and notation as in the theorem, if $\phi(\lambda) = 0$ is a polynomial equation with N distinct roots $\lambda_1, \lambda_2, \ldots, \lambda_N$, so $\phi(\lambda_j) = 0$, $j = 1, \ldots, N$, prove any linear combination of the function $e^{\lambda_j x}$ is in $\mathcal{N}(L)$, that is,

$$Lu = 0 \quad \text{where} \quad u(x) = \sum_{1}^{N} c_j e^{\lambda_j x} .$$

5. Apply the theorem to find the solution of Exercise 4 for the equation $Lu = 0$, where

a). $Lu \equiv u'' - u' - u$.

b). $(Lu)(x) = u(x+2) - u(x+1) - u(x)$.

c). Find a special solution of b) which satisfies the "initial conditions" $u(0) = u(1) = 1$. Compute $u(2)$, $u(3)$ and $u(4)$ directly from b). The integers $u(n)$, $n \in \mathbb{Z}_+$ are called the Fibonacci sequence. [Answer: $u(2) = 2$, $u(3) = 3$, $u(4) = 5$, and surprisingly,

$$u(n) = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1} \right] .$$

6. Solve $u(x) - au(x-1) + b^2 u(x-2) = 0$ with the initial conditions $u(1) = a$, $u(2) = a^2 - b^2$. Compare with Exercise 17, p. 440.

7. Extend Exercises 5(b-c) and 6 to develop a theory of second order difference equations with constant coefficients. Thus

$$Lu \equiv a_2 u(x+2) + a_1 u(x+1) + a_0 u(x), \qquad a_2 \neq 0, \qquad x \in \mathbb{Z} .$$

In particular, you should,

a). Find two linearly independent solutions of $Lu = 0$. Remember the degenerate case $a_1^2 - 4a_0 a_2 = 0$.

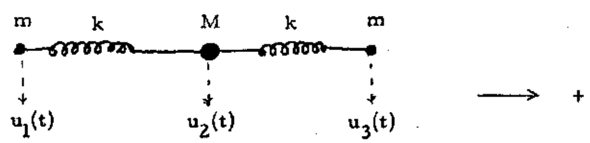
b). Prove there is at most one solution of the initial value problem $Lu = f$, $u(0) = \alpha_0$, $u(1) = \alpha_1$.

c). Prove $\dim \mathcal{N}(L) = 2$.

Remarks. The ideas presented above generalize immediately to the case where $X \in \mathbb{R}^n$ instead of just $\mathbb{R}^1$, as well as to the case where the u's are vectors and not scalars. These few concepts lie at the heart of any treatment of many linear operators with constant coefficients, especially ordinary and partial differential operators. This mildly abstract formulation manages to penetrate through the obscuring details of particular cases to observe a rather simple structure unifying many seemingly different problems.

6. A Linear Triatomic Molecule

A molecule composed of three atoms is called a triatomic. Consider a triatomic molecule whose equilibrium configuration is a straight line with two atoms of equal mass m situated on either side of a central atom of mass M.



To simplify the situation further, we shall only consider the motion along the straight line (axis) of these atoms, and shall assume the interatomic forces can be approximated by springs with equal spring constants k. $u_1(t)$, $u_2(t)$ and $u_3(t)$ will denote the displacements of the atoms (see fig.) from their equilibrium position.

Newton's second law, $m\ddot{u} = \sum F$, will give the equations of motion. The atom on the left only "feels" the force due to the spring attached to it, the force being equal to the spring constant k times the amount that spring is stretched, $u_2 - u_1$. Thus

$$m\ddot{u}_1 = k(u_2 - u_1).$$

The central atom "feels" two forces, one from each side, with the resulting equation of motion

$$M\ddot{u}_2 = -k(u_2-u_1) + k(u_3-u_2).$$

In the same way, the equation of motion for the remaining atom is

$$m\ddot{u}_3 = -k(u_3 - u_2).$$

Collecting our equations, we have

$$\ddot{u}_1 = -\frac{k}{m}u_1 + \frac{k}{m}u_2$$

$$\ddot{u}_2 = \frac{k}{M}u_1 - \frac{2k}{M}u_2 + \frac{k}{M}u_3$$

$$\ddot{u}_3 = \frac{k}{m}u_2 - \frac{k}{m}u_3.$$

These are a system of three linear ordinary differential equations with constant coefficients. They cannot be integrated as they stand since each equation involves functions from the other equations, that is, the equations are coupled (not surprising since we are considering coupled oscillators). Now we can integrate such a system immediately if they are in the simple form

$$\ddot{\phi}_1 = \lambda_1\phi_1$$

$$\ddot{\phi}_2 = \lambda_2\phi_2$$

$$\ddot{\phi}_3 = \lambda_3\phi_3$$

by integrating each equation separately. By using an important method, we will be able to place our system in this special form.

Before doing so, it is suggestive to rewrite the system in matrix form

$$\begin{pmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \ddot{u}_3 \end{pmatrix} = \begin{pmatrix} -\frac{k}{m} & \frac{k}{m} & 0 \\ \frac{k}{M} & -\frac{2k}{M} & \frac{k}{M} \\ 0 & \frac{k}{m} & -\frac{k}{m} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

Letting A denote the 3×3 matrix, our hope is to somehow change A into a <u>diagonal matrix</u> (one with zeroes everywhere except along the principal diagonal), for then the differential equations will be in a form mentioned above which can be immediately integrated.

The trick is to replace the basis u_1, u_2, u_3 by some other basis in which the matrix assumes a diagonal form. The differential equation can be written in the form

$$\ddot{U} = AU ,$$

where $U = (u_1, u_2, u_3)$, and the derivative of a vector being defined as the derivative of each of its components. Let $\phi_1(t), \phi_2(t)$, and $\phi_3(t)$ be three other functions - which we plan to use as a new basis. Then the ϕ_j's can be written as a linear combination of the u_j's,

$$\phi_1 = s_{11}u_1 + s_{12}u_2 + s_{13}u_3$$

$$\phi_2 = s_{21}u_1 + s_{22}u_2 + s_{23}u_3$$

$$\phi_3 = s_{31}u_1 + s_{33}u_2 + s_{33}u_3 ,$$

where s_{ij} are <u>constants.</u> Writing $S = ((s_{ij}))$ and $\Phi = (\phi_1, \phi_2, \phi_3)$, this last equation reads

$$\Phi = SU .$$

Taking the derivative of both sides (or going back to the equations defining ϕ_j in terms of the u_k's), we find

$$\ddot{\Phi} = S\ddot{U} .$$

Because both u_1, u_2, and u_3 as well as ϕ_1, ϕ_2, and ϕ_3 are bases for the solution, the matrix S must be non-singular (its inverse expresses the ϕ_j's in terms of the u_j's). Thus

$$\ddot{\Phi} = SAS^{-1}\Phi.$$

The problem has been reduced to <u>finding a matrix</u> S <u>such that the matrix</u> SAS^{-1} <u>is a diagonal matrix,</u>

$$SAS^{-1} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \equiv \Lambda.$$

Multiply by S^{-1} on the left:

$$AS^{-1} = S^{-1}\Lambda .$$

Since this equation is equality between matrices, their corresponding columns must be equal. Thus, if we denote by $\hat{S}_i$, the i^{th} column of

S^{-1}, the above equation then reads

$$A\hat{S}_i = \lambda_i \hat{S}_i ,$$

or

$$(A - \lambda_i I)\hat{S}_i = 0 .$$

For each i this is a system of three linear algebraic equations for the three components of $\hat{S}_i$. If there is to be a non-trivial solution, we know

$$\det(A - \lambda_i I) = 0.$$

Since

$$\det(A-\lambda_i I) = \begin{vmatrix} -\frac{k}{m}-\lambda_i & \frac{k}{m} & 0 \\ \frac{k}{M} & -\frac{2k}{M}-\lambda_i & \frac{k}{M} \\ 0 & \frac{k}{m} & -\frac{k}{m}-\lambda_i \end{vmatrix} ,$$

(algebra later)

$$= -\lambda_i(\frac{k}{m} + \lambda_i)[\lambda_i + (\frac{2}{M} + \frac{1}{m})k]$$

We see the three possible values of λ for $\det(A-\lambda_i I) = 0$ are

$$\lambda_1 = 0, \lambda_2 = -\frac{k}{m} , \quad \lambda_3 = -k(\frac{2}{M} + \frac{1}{m}).$$

These numbers λ_i are the <u>eigenvalues of A.</u> The non-trivial solution $\hat{S}_i$ of the homogeneous equations $(A - \lambda_i I)\hat{S}_i = 0$ corresponding to the i^{th} eigenvalue is called the <u>eigenvector</u> of A corresponding to the

eigenvalue λ_i. For example, $\hat{S}_2$ is the solution of $(A-\lambda_2 I)S_2 = 0$ corresponding to $\lambda_2 = -k/m$,

$$0\hat{s}_{12} + \frac{k}{m}\hat{s}_{22} + 0\hat{s}_{32} = 0$$

$$\frac{k}{M}\hat{s}_{12} - (\frac{2k}{M} - \frac{k}{m})\hat{s}_{22} + \frac{k}{M}\hat{s}_{32} = 0$$

$$0\hat{s}_{12} + \frac{k}{m}\hat{s}_{22} + 0\hat{s}_{32} = 0 .$$

We see $\hat{s}_{22} = 0$ while $\hat{s}_{12} = -\hat{s}_{32}$. Thus, one solution is

$$\hat{S}_2 = (1, 0, -1)$$

Similarly we find one solution for $\hat{S}_1$ is

$$\hat{S}_1 = (1, 1, 1) ,$$

while one solution for $\hat{S}_3$ is

$$\hat{S}_3 = (1, -\frac{2m}{M}, 1) .$$

The computation is over. All that remains is to put the parts together and interpret the solution. If you got lost, presumably this recapitulation will help. We have found a transformation S to new coordinates (ϕ_1, ϕ_2, ϕ_3) such that the differential equations for the ϕ_j's are in diagonal form, $\ddot{\phi}_j = \lambda_j \phi_j$.

$$\ddot{\phi}_1 = 0$$

$$\ddot{\phi}_2 = -\frac{k}{m}\phi_2$$

$$\ddot{\phi}_3 = -k\left(\frac{2}{M}+\frac{1}{m}\right)\phi_3 .$$

The solutions are

$$\phi_1(t) = A_1 + B_1 t ,$$

$$\phi_2(t) = A_2 \cos\sqrt{\frac{k}{m}}\,t + B_2 \sin\sqrt{\frac{k}{m}}\,t$$

$$\phi_3(t) = A_3 \cos\sqrt{k\left(\frac{2}{M}+\frac{1}{m}\right)}\,t + B_3 \sin\sqrt{k\left(\frac{2}{M}+\frac{1}{m}\right)}\,t .$$

Since $\Phi = SU$, and the $\hat{S}_j$ are the columns of S^{-1},

$$S^{-1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -\frac{2m}{M} \\ 1 & -1 & 1 \end{pmatrix} ,$$

we have $U = S^{-1}\Phi$,

$$u_1(t) = \phi_1(t) + \phi_2(t) + \phi_3(t)$$

$$u_2(t) = \phi_1(t) \qquad - \frac{2m}{M}\phi_3(t)$$

$$u_3(t) = \phi_1(t) - \phi_2(t) + \phi_3(t)$$

Although the solutions $\phi_1(t)$, $\phi_2(t)$, and $\phi_3(t)$ can now be substituted into the first set of equations for the u_i's, it is more

instructive to leave that step to your imagination and analyze the nature of the solution.

1. If $\phi_1(t) \neq 0$ but $\phi_2(t) = \phi_3(t) = 0$, then

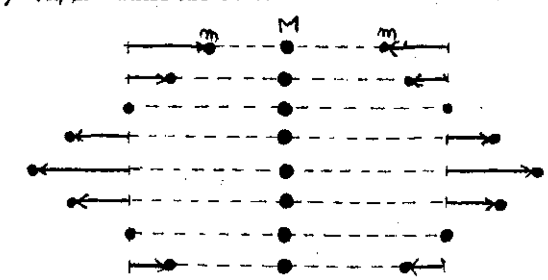
$$u_1(t) = u_2(t) = u_3(t) = A_1 + B_1 t .$$

Thus all three atoms - the whole molecule - moves with a constant velocity B_1. This is the trivial translation motion of the molecule, simply moving without internal oscillations at all.

2. If $\phi_2(t) \neq 0$ but $\phi_1(t) = \phi_3(t) = 0$, then

$$u_1(t) = \phi_2(t) = -u_3(t), \text{ and } u_2(t) = 0.$$

Thus, the two outside atoms vibrate in opposite directions with frequency $\sqrt{k/m}$ while the center atom remains still:

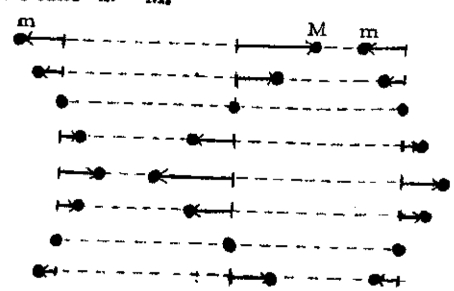


3. If $\phi_3(t) \neq 0$ but $\phi_1(t) = \phi_2(t) = 0$

$$u_1(t) = u_3(t) = \phi_3(t), \quad u_2(t) = -\frac{2m}{M}\phi_3(t) .$$

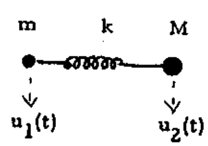
A bit more complicated. The two outside atoms move in the same direction with same frequency $\sqrt{k(\frac{2}{M} + \frac{1}{m})}$, while the center atom moves in a direction opposite to them and with the same frequency but a different amplitude (to conserve linear momentum $m\dot{u}_1 + M\dot{u}_2 + m\dot{u}_3 = 0$).

In the figure we take $m = M$.



These three simple motions are called the <u>normal modes of oscillation</u> of the molecule. They are the oscillations determined by the ϕ_1, ϕ_2, and ϕ_3. Every motion of the system is a linear combination of the normal modes of oscillation, the particular oscillation depending on what initial conditions are given. By an appropriate choice of the initial conditions, one or another of the normal modes will result. Otherwise some less recognizable motion will result.

<u>Exercise.</u> Consider the s... r model of a diatomic molecule



which we will represent as two masses joined by a spring with spring constant k.

a). Show the equations of motion are

$$m\ddot{u}_1 = k(u_2 - u_1)$$

$$M\ddot{u}_2 = -k(u_2 - u_1)$$

b). Introduce new variables, $\Phi = SU$,

$$\phi_1 = s_{11}u_1 + s_{12}u_2$$

$$\phi_2 = s_{21}u_1 + s_{22}u_2 ,$$

and find S so that the equation

$$\ddot{\Phi} = SAS^{-1}\Phi$$

is in diagonal form.

c). Solve the resulting equation and find the normal modes of oscillation. Interpret your results with a diagram.