IP326. Lecture 8. Tuesday, Jan. 29, 2019

In the model of linked 1-d harmonic oscillators introduced in the last lecture, we found that the dynamics of the 2N light particles and the single heavy one that defined the model could be described by the following equation

$$[m+(M-m)\delta_{k,0}]\ddot{x}_k(t)=b[x_{k-1}(t)-2x_k(t)+x_{k+1}(t)] \tag{1}$$

where, as we'd stated earlier, M is the mass of the heavy particle, m the mass of the light particles, b the stiffness of the springs connecting adjacent particles, and $x_i(t)$ the position of the ith particle at time t.

As the first step in the solution of this equation (which is actually a set of *coupled* equations), we'll introduce a new variable q_j, called a *normal mode* or a collective coordinate, that will allow us to *decouple* these equations. This variable is defined through the relation:

$$x_k=\frac{1}{\sqrt{2N+1}}\sum_{j=-N}^{N}q_j\exp[-2\pi ijk/(2N+1)] \tag{2}$$

where i now refers to $\sqrt{-1}$ (and not to a particle label.) Equation (2) is the discrete representation of a Fourier integral.

The next step in the solution of Eq. (1) is to rewrite it in terms of this new variable. But to do so, we first need to *invert* Eq. (2), i.e., to express q_j as a function of the x_k's . This can be done exactly, but the necessary algebra – though fairly routine – is somewhat involved. It turns out, however, that one can get to essentially the same final result much more simply by making a few approximations, of which the key is to assume that because N is large (it could be on the order of Avogadro's number, for instance), the discrete variable j can be regarded as continuous, and that the sum over this variable in Eq. (2) can therefore be replaced by an integral. If we do this, we get

$$x_k=\frac{1}{\sqrt{2N}}\int_{-N}^{N}dj\,q_j\exp(-i\pi jk/N) \tag{3}$$

Now multiply both sides of this equation by $\exp(\pi ikl/N)$ (l being another variable that can take on values from $-N$ to $+N$), and integrate over k (which like j – and l – we'll treat *for the moment* as continuous.) This leads to

$$\int_{-N}^{N}dk\,x_k\exp(i\pi kl/N)=\frac{1}{\sqrt{2N}}\int_{-N}^{N}dj\int_{-N}^{N}dk\,q_j\exp[i\pi k(l-j)/N]$$

$$= \frac{1}{\sqrt{2N}} \int_{-N}^{N} dj \int_{-N}^{N} dk\, q_j \left[\cos(\pi k(l-j)/N) + i \sin(\pi k(l-j)/N) \right] \quad (4)$$

By symmetry, there is no contribution to the above integral from the sine term, so after noting that the cosine term is an even function of *k*, Eq. (4) becomes

$$\int_{-N}^{N} dk\, x_k \exp(i\pi kl/N) = \sqrt{\frac{2}{N}} \int_{-N}^{N} dj \int_{0}^{N} dk\, q_j \cos(\pi k(l-j)/N)$$

$$= \sqrt{\frac{2}{N}} \int_{-N}^{N} dj \int_{0}^{N} dk\, q_j \cos(\pi k(l-j)/N)$$

$$= \sqrt{\frac{2}{N}} \int_{-N}^{N} dj\, q_j \left. \frac{\sin(\pi k(l-j)/N)}{\pi(l-j)/N} \right|_{0}^{N} \quad (5)$$

When the sine function on the right hand side of Eq. (5) is evaluated at $k = 0$ (the lower limit), the result is 0; when it is evaluated at $k = N$ (the upper limit), the result is $\sin(\pi(l-j))$. Now we'd said that *l* and *j* were to be treated as continuous variables, but if we revert temporarily to their original meaning and consider them again as integers, then $\sin(\pi(l-j))$ will vanish whenever $l \neq j$. But what if $l = j$? Ordinarily, the function would be 0 in this limit too, but in Eq. (5) the function is also divided by $l - j$, which also vanishes. So the ratio of $\sin(\pi(l-j))$ to $l - j$ is indefinite, and its value must be determined by a limiting procedure, either by l'Hospital's rule, or by first expanding the sine in series, and only then setting *l* to *j*. Either way the result is unity. This means we can write

$$\frac{\sin(\pi k(l-j)/N)}{\pi(l-j)/N} \xrightarrow{k=N} N\delta_{j,l} \quad (6a)$$

Therefore,

$$\int_{-N}^{N} dk\, e^{i\pi k(l-j)/N} = 2N\delta_{l,j} \quad (6b)$$

After substituting Eq. (6a) into (5), and carrying out the trivial integral over q_j, we end up with

$$q_l = \frac{1}{\sqrt{2N}} \int_{-N}^{N} dk\, x_k \exp(i\pi kl/N) \quad (7a)$$

which, formally, is the inverse of the expression in Eq. (3). Had we carried out these operations exactly, by treating *j*, *k* and *l* as discrete variables from the outset, we would have found that

$$q_l = \frac{1}{\sqrt{2N+1}} \sum_{k=-N}^{N} x_k \exp[2\pi ikl/(2N+1)] \tag{7b}$$

We can now return to Eq. (1), and we proceed to find its solution by multiplying both sides by $\frac{1}{\sqrt{2N}}\exp(i\pi kl/N)$ and integrating over *k*. The left hand side of the equation then becomes

$$\frac{m}{\sqrt{2N}}\frac{d^2}{dt^2}\int_{-N}^{N} dk\, x_k e^{i\pi kl/N} + \frac{M-m}{\sqrt{2N}}\int_{-N}^{N} dk\, \ddot{x}_k e^{i\pi kl/N}\delta_{k,0} = m\ddot{q}_l(t) + \frac{M-m}{\sqrt{2N}}\ddot{x}_0(t) \tag{8}$$

As for the right hand side of Eq. (1), we'll treat the terms there one by one, starting with the term involving x_{k-1}, which after carrying out the indicated steps becomes

$$\begin{aligned}
\frac{1}{\sqrt{2N}}\int_{-N}^{N} dk\, x_{k-1} e^{i\pi kl/N} &= \frac{1}{2N}\int_{-N}^{N} dk \int_{-N}^{N} dj\, q_j e^{-i\pi(k-1)j/N} e^{i\pi kl/N} \\
&= \frac{1}{2N}\int_{-N}^{N} dj\, q_j \int_{-N}^{N} dk\, e^{i\pi k(l-j)/N} e^{i\pi j/N} \\
&= \int_{-N}^{N} dj\, q_j \delta_{l,j} e^{i\pi j/N} \\
&= q_l(t) e^{i\pi l/N}
\end{aligned} \tag{9}$$

In the same way, for the term in x_{k+1}, we have

$$\frac{1}{\sqrt{2N}}\int_{-N}^{N} dk\, x_{k+1} e^{i\pi kl/N} = q_l(t) e^{-i\pi l/N} \tag{10}$$

while for the term in x_k, we have already derived the relevant result: it is given in Eq. (7a). So putting Eqs. (7a), (8) – (10) together, we find the following equation for the variable q_l:

$$m\ddot{q}_l(t) + \frac{M-m}{\sqrt{2N}}\ddot{x}_0(t) = b\left[q_l(t)e^{i\pi l/N} - 2q_l(t) + q_l(t)e^{-i\pi l/N}\right]$$

$$= 2bq_l(t)[\cos(\pi l/N) - 1] \tag{11}$$

If we substitute the definitions $Q = (M - m)/m$ and $\omega_l^2 = \frac{2b}{m}[1 - \cos(\pi l/N)]$ into the above equation, we're finally left with

$$\ddot{q}_l(t) + \frac{Q}{\sqrt{2N}}\ddot{x}_0(t) = -q_l(t)\omega_l^2 \tag{12}$$

This is now truly a *single* equation in the variable $q_l(t)$ and $x_0(t)$, and the way we'll treat it is by a technique known as Laplace transformation. The Laplace transform of a function $f(t)$ is, by definition, a new function $\hat{f}(s)$ that is obtained from the old by multiplying it by e^{-st} and then integrating the product over *t* from 0 to ∞. That is

$$\hat{f}(s) = \int_0^\infty dt e^{-st} f(t) \tag{13}$$

The great utility of Laplace transforms lies in what they do when they're applied to the derivative of a function. So consider the Laplace transform of $d^2 f(t)/dt^2$, which by definition is the integral

$$\hat{I}(s) \equiv \int_0^\infty dt e^{-st} \frac{d^2 f(t)}{dt^2} \tag{14}$$

which is a function of the Laplace variable *s*. Suppose we integrate $\hat{I}(s)$ by parts twice; the result is

$$\hat{I}(s) = e^{-st}\frac{df(t)}{dt}\bigg|_0^\infty + s\left\{ e^{-st} f(t)\Big|_0^\infty + s\int_0^\infty dt e^{-st} f(t) \right\} \tag{15}$$

The variable *s* is actually complex, but so long as $\mathrm{Re}(s) > 0$ and $f(t)$ and its derivatives are finite at ∞, the surface terms in Eq. (15) vanish at the upper limit. So we're left with

$$\hat{I}(s) = -\dot{f}(0) - sf(0) + s^2\hat{f}(s),$$

which is an algebraic function of $\hat{f}(s)$ and of two initial conditions, $\dot{f}(0)$ and $f(0)$, both of which, typically, are known or can be specified; the derivative has been eliminated. Thus, when a Laplace transform is applied to a differential equation, it leads to an algebraic equation in the Laplace transformed function, which is usually easily solved. But then to recover the original function, the solution to this algebraic equation must be *Laplace inverted*; that step – about which more later – can sometimes be hard.

With this background, let's Laplace transform both sides of Eq. (12). This leads to

$$-\dot{q}_l(0) - sq_l(0) + s^2\hat{q}_l(s) + \frac{Q}{\sqrt{2N}}\left[-v_0(0) - sx_0(0) + s^2\hat{x}_0(s)\right] = -\omega_l^2\hat{q}_l(s) \qquad (16)$$

which as advertised is an algebraic equation in Laplace transformed functions. But it also includes terms involving the initial values of the original functions. We're free to specify what these values are, and we'll make the choice $x_l(0) = 0$ for all *l*, and $\dot{x}_l(0) \equiv v_l(0) = 0$ for all l except $l = 0$. We're assuming, therefore, that all the particles start out at the same point, and all of them, except the heavy particle, start out with 0 velocity. If for the moment we revert once again to the discrete representation of the normal modes (see Eq. (7b)), these conditions mean that

$$q_l(0) = 0 \quad \text{and} \quad \dot{q}_l(0) = \frac{v_0}{\sqrt{2N}}$$

When these initial conditions are substituted into Eq. (16), we find, after gathering like terms and rearranging, that

$$(s^2 + \omega_l^2)\hat{q}_l(s) = \frac{v_0(0)}{\sqrt{2N}}(Q+1) - \frac{Q}{\sqrt{2N}}s^2\hat{x}_0(s)$$

or

$$\hat{q}_l(s) = \frac{1}{\sqrt{2N}(s^2 + \omega_l^2)}\left[\frac{M}{m}v_0(0) - Qs^2\hat{x}_0(s)\right] \qquad (17)$$

Since we're interested in the dynamics of the heavy particle, we'd like to eliminate the collective coordinates $\hat{q}_l(s)$ in the above equation in favour of the coordinate $\hat{x}_0(s)$ of this particle. The relation between these two is contained in Eq. (3); if we set k to 0 in that equation, and then Laplace transform both sides, we get

$$\hat{x}_0(s) = \frac{1}{\sqrt{2N}}\int_{-N}^{N} dj\,\hat{q}_j(s) = \frac{1}{\sqrt{2N}}\int_{-N}^{N} dl\,\hat{q}_l(s)$$

So if we multiply Eq. (17) by $1/\sqrt{2N}$ and integrate both side over *l* from $-N$ to N, we transform the equation to

$$\hat{x}_0(s) = \hat{\phi}(s)\left[\frac{M}{m}v_0(0) - Qs^2\hat{x}_0(s)\right] \qquad (18a)$$

where $\hat{\phi}(s)$ is the function

$$\hat{\phi}(s) = \frac{1}{2N}\int_{-N}^{N} dl \, \frac{1}{s^2 + \omega_l^2} \tag{18b}$$

Equation (18a) is more usefully rewritten as

$$\hat{x}_0(s) = \frac{M}{m}\frac{v_0(0)\hat{\phi}(s)}{1 + Qs^2\hat{\phi}(s)} \tag{19}$$

In this form, we can make a connection to the velocity of the heavy particle at time *t*, which is what we need to finally obtain an expression for the particle's velocity autocorrelation function, the quantity we're interested in. This connection is made by taking the Laplace transform of $v_0(t)$, an operation we'll now represent by the symbol $\mathcal{L}$. So acting $\mathcal{L}$ on $v_0(t)$ we get

$$\begin{aligned}
\mathcal{L}v_0(t) &\equiv \int_0^\infty dt e^{-st} v_0(t) \\
&= \int_0^\infty dt e^{-st} \frac{d}{dt} x_0(t) \\
&= e^{-st} x_0(t)\Big|_0^\infty + s\int_0^\infty dt e^{-st} x_0(t) \\
&= -x_0(0) + s\hat{x}_0(s) \\
&= s\hat{x}_0(s)
\end{aligned} \tag{20}$$

where the last line follows from our choice of initial condition, viz., $x_l(0) = 0, \ \forall l$.

It's possible to *formally* invert Eq. (20) by acting an inverse Laplace operator, $\mathcal{L}^{-1}$, on both sides of the equation; for the moment, we won't worry about what it actually means to perform this operation, and simply note that in combination with Eq. (19) it leads to the following

$$v_0(t) = \mathcal{L}^{-1} s\hat{x}_0(s)$$

$$= \frac{M}{m} v_0(0) \mathcal{L}^{-1} \frac{s\hat{\phi}(s)}{1 + Qs^2 \hat{\phi}(s)} \tag{21}$$

From here it's a simple matter to derive an expression for the velocity autocorrelation function – just multiply both sides of Eq. (21) by $v_0(0)$ and take the ensemble average. After dividing the result by $\langle v_0^2(0) \rangle$, we obtain the following *normalized* velocity autocorrelation function

$$\frac{\langle v_0(0) v_0(t) \rangle}{\langle v_0^2(0) \rangle} = \frac{M}{m} \mathcal{L}^{-1} \frac{s\hat{\phi}(s)}{1 + Qs^2 \hat{\phi}(s)} \tag{22}$$

This is the result we were after, but we still have to carry out one final step to complete the calculation and obtain a definite functional form of the autocorrelation function; that step is to Laplace invert the *s*-dependent function on the right hand side. What we mean by Laplace inverting a function $\hat{F}(s)$ is finding a function $F(t)$ that when Laplace transformed produces $\hat{F}(s)$. For some functions of *s* that's easy to do. For instance, if $\hat{F}(s)$ were given by $\hat{F}(s) = 1/s^{n+1}$, where n is, an integer, some guesswork would allow you to deduce that

$$\mathcal{L}^{-1} \hat{F}(s) = F(t) = \frac{1}{n!} t^n$$

a result that you can confirm to be correct by taking the Laplace transform of $F(t)$, and showing that it recovers the given $\hat{F}(s)$. By similarly working backwards, you could also figure out that the Laplace inverse of $\hat{F}(s) = 1/(s+a)$ is the function $F(t) = e^{-at}$. But for complicated functions of *s*, this approach is clearly not practical. There is, however, a formula for calculating Laplace inverses, which is

$$F(t) = \frac{1}{2\pi i} \oint_C ds e^{st} \hat{F}(s)$$

This is a contour integral that must be evaluated along a particular path *C*. The subject of contour integration lies outside the scope of this course, we won't attempt to determine Laplace inverses using the above formula. Instead we'll note that many textbooks provide tables of Laplace transforms and their inverses, and we'll simply refer to one of them to get the answer we want.

In the present problem, the function we need to invert is $\hat{G}(s) = s\hat{\phi}(s)/[1 + Qs^2 \hat{\phi}(s)]$ (cf. Eq. (22)). To carry out this operation, we have first have to determine the explicit dependence of $\hat{G}(s)$ on *s*, which in turns requires that we know how $\hat{\phi}(s)$ depends on *s*. We'll turn to this calculation next.