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Energy Flow in Harmonic Linear Chain

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Recently Rieder et al.[1] analyzed the stationary state of a harmonic linear chain with fixed ends under the influence of heat reservoirs. Here we discuss the stationary state of the same system but with "free" ends. Consider a linear harmonic chain with nearest neighbour force and free ends, and let the particles be numbered from one end to the other as $1, 2, \cdots, N$. The displacement of the n-th particle from its equilibrium position and its velocity are denoted by x_n and v_n respectively. Equations of motion are

$$\begin{aligned} \dot{v}_1 &= k(-x_1+x_2)-\beta_1 v_1+f_1(t), \\ \dot{v}_i &= k(x_{i-1}-2x_i+x_{i+1}),\ i=2,\ \ldots,\ N-1, \quad (1) \\ \dot{v}_N &= k(x_{N-1}-x_N)-\beta_N v_N+f_N(t). \end{aligned}$$

Here k is the force constant, β_i the friction constant and $f_i(t)$ is the purely random Gaussian process with mean value zero:

$$\langle f_i(t) f_j(t')\rangle = 4\delta_{ij}\beta_i \kappa T_i \delta(t-t').$$

$\langle\cdots\rangle$ is the average and κ is Boltzmann's constant. The mass of particles is assumed to be unity but the modification is easy. The pair $(\beta_i, f_i(t))$ represents the heat reservoir of temperature T_i.[2] In the matrix form (1) is written as follows:

$$\dot{\boldsymbol{X}} = A\boldsymbol{X}+\boldsymbol{F}(t), \quad \boldsymbol{X}=\begin{pmatrix}\boldsymbol{x}\\ \boldsymbol{v}\end{pmatrix},$$

$$\boldsymbol{F}=\begin{pmatrix}0\\ \boldsymbol{f}(t)\end{pmatrix}, \quad A=\begin{pmatrix}0 & 1\\ K & B\end{pmatrix}.$$

$\boldsymbol{X}$ and $\boldsymbol{F}$ are $2N\times 1$ matrices and A is $2N\times 2N$. K is $N\times N$ and represents the coefficients of harmonic interaction. K is not regular. The formal solution is

$$\boldsymbol{X}(t)=e^{At}\boldsymbol{X}(0)+\int_0^t e^{A(t-s)}\boldsymbol{F}(s)\,ds. \qquad (2)$$

It can now be proved that when at least one of β_i's is positive [1] among eigenvalues $\{\lambda_i;\ i=1,\cdots,2N\}$ of A only λ_1 is zero and others have negative real parts, and [2] λ_i's are distinct in so far as β_i's are small. The eigenvector $\boldsymbol{e}_1$ corresponding to λ_1 represents the center-of-mass coordinate,

$$e_1{}^*=(1,1,\cdots,1;\ 0,0,\cdots,0)$$

where $*$ denotes the transpose. Now [2] assures that A can be diagonalized by a regular matrix P as $(PAP^{-1})_{ij}=\lambda_i\delta_{ij}$, and $(P^{-1})_{i1}$ is the i-th component of $\boldsymbol{e}_1$.

Let us discuss the correlation matrix

$$C(t)=\langle\boldsymbol{X}(t)\boldsymbol{X}(t)^*\rangle.$$

With (2) and [1] it can be established[3]

$$\begin{aligned}&(AC(t)+C(t)A^*)_{ij}=(Z(t)-G+S)_{ij},\\&(S)_{ij}=(P^{-1})_{i1}(PGP^*)_{11}(P^{-1})_{j1}\\&\quad=\begin{cases}s;\ 1\leqq i,\ j\leqq N,\\0;\ \text{otherwise},\end{cases}\qquad (3)\\&G=\langle\boldsymbol{F}(t)\boldsymbol{F}(t')^*\rangle/\delta(t-t'),\end{aligned}$$

where $Z(t)$ is the matrix that collects all terms that vanish as $t\to\infty$, and s is a constant. Equation (3) is the linear equation for $(C)_{ij}$. Let us decompose

$$C(t)=\begin{pmatrix}C_1 & C_2\\ C_2{}^* & C_3\end{pmatrix},\qquad \begin{aligned}C_1&=\langle\boldsymbol{x}(t)\boldsymbol{x}(t)^*\rangle,\\C_2&=\langle\boldsymbol{x}(t)\boldsymbol{v}(t)^*\rangle,\\C_3&=\langle\boldsymbol{v}(t)\boldsymbol{v}(t)^*\rangle.\end{aligned}$$

Because of zero the eigenvalue C_1 is $O(t)$ as $t\to\infty$, but C_2 and C_3 remain finite. Therefore we rewrite (3) in terms of C_i and put C_1 away. Then, with $t=\infty$ all initial conditions drop out and

$$\begin{aligned}&C_2+C_2{}^*=S_1,\\&KC_2B-BC_2{}^*K+KC_3-C_3K=0,\\&KC_2+C_2{}^*K+BC_3+C_3B=-D,\\&D=\langle f(t)f(t')^*\rangle/\delta(t-t'),\end{aligned}\qquad (4)$$

where S_1 is the $N\times N$ matrix whose elements are all s.

Since we have to operate the non-regular matrix K on (3) to obtain (4), (4) is only a necessary condition of (3). But it can be shown that for $N=2$, 3 and 4, (4) gives a "unique" solution; that is, its coefficient matrix (which is $N^2\times N^2$) is regular (for $N=4$ the determinant is $k^3(k+\beta_1\beta_4)^3(\beta_1+\beta_4)^4$). Therefore it would be safe to consider the solution of (4) to be always that of (3). The solution of (4) is as follows:

$$\langle x_iv_j\rangle=s+\begin{cases}b, & i<j,\\0, & i=j,\\-b, & i>j,\end{cases}$$

$$\langle v_iv_j\rangle=a\delta_{ij}+\begin{cases}\beta_1b, & i=j=1,\\\beta_Nb, & i=j=N,\\0, & \text{otherwise},\end{cases}$$

$$a=2\kappa\frac{(k+\beta_N{}^2)\beta_1T_1+(k+\beta_1{}^2)\beta_NT_N}{(\beta_1+\beta_N)(k+\beta_1\beta_N)},$$

$$b=\frac{2\kappa\beta_1\beta_N(T_1-T_N)}{(\beta_1+\beta_N)(k+\beta_1\beta_N)}.$$

Thus particles 2, $\cdots$, $N-1$ have all the same mean kinetic energy (temperature) in contrast with the result of 1). The rate of energy flow from i to $i+1$ is kb, and depends only on T_1-T_N. This is a kind of superconduction. Which of the end conditions be more realistic, the fixed or the free? The author believes it is the latter: this point will be discussed more fully in a forthcoming investigation.

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