Fourier’s law of heat conduction in a three dimensional harmonic crystal: A retrospection

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We present an exact solution of the Langevin’s equation in the steady state limit in a three dimensional, harmonic crystal of slab geometry whose boundary surfaces along its length are connected to two stochastic, white noise heat baths at different temperatures. We show that the heat transport obeys Fourier’s law in the continuum limit.

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When a steady temperature gradient is established between the two ends of a piece of solid bar, heat current will flow from high to low temperature end. According to Fourier’s law of heat conduction the current density is proportional to the temperature gradient and mathematically it reads as

\[ J(x) = -\kappa \nabla T(x), \quad (1) \]

where the constant of proportionality \( \kappa \) is known as the thermal conductivity of the solid. Conduction of heat in solid by its very nature is a non-equilibrium process. This is an area of Physics, where the idea of non-equilibrium statistical mechanics can be applied in order to find the underlying physical conditions for the validity of this law in case of solid. Various numerical and analytical studies confirm that the heat transport in one dimensional system exhibits anomalous \[ 1 \] behaviour. It means that thermal conductivity for such a system is not found to be an intrinsic property of the material. It shows a power law dependence \( \kappa \sim N^\alpha \), where \( N \) be the linear size of the system. There are studies on different models which predict divergent \( (0 < \alpha < 1) \) thermal conductivity \[ 1 \[2\]. \] There are also some oscillator models that give non-divergent \( (\alpha < 0) \) thermal conductivity \[ 3 \] in one dimension. The anomalous behaviour of thermal conductivity is also observed in two dimensional system. Numerical study indicates a logarithmic divergence \[ 1 \[2\] of thermal conductivity \( \kappa \sim \ln N \). A power law behaviour \[ 3 \] is also observed in such a system.

There are strong numerical evidences \[ 4 \] that indicate the validity of Fourier’s law of heat conduction in one and two dimensional systems with pining and anharmonicity. An extensive investigation on heat transport in a three dimensional disordered harmonic crystal has been carried out recently \[ 4 \]. The numerical simulation indicates the normal transport of heat when this system is subjected to an external pinning potential. Though it is not been verified numerically, but a finite conductivity is predicted for this disordered system from analytical arguments. A more recent simulation study \[ 5 \] establishes for the first time the validity of this law in three dimensional anharmonic crystal. It thus also establishes the fact that the process of heat conduction in three dimensional geometry is diffusive in nature. Apart from bringing in a temperature dependent contribution to the thermal conductivity, which is indeed the case for real systems, it is confirmed that anharmonicity provides a condition which is sufficient for normal heat transport in a solid. In this letter we give an exact analytical derivation of Fourier’s law of heat conduction in three dimensional harmonic crystal. We find that in the continuum limit the thermal conductivity is finite and does not depend on the system size.

We consider a cubic crystal in three dimension. The form of the Hamiltonian

\[ H = \sum_n \frac{x_n^2}{2} + \frac{1}{2} (x_n - x_{n+\hat{e}})^2. \quad (2) \]

The displacement field \( x_n \) is defined on each lattice site \( n = (n_1, n_2, n_3) \) where \( n_1 = 1, \cdots, N, \quad n_2 = 1, \cdots, W_2, \) and \( n_3 = 1, \cdots, W_3 \). Here \( \hat{e} \) denotes the unit vector in the three directions. We choose the value of mass attached to each lattice point and the harmonic spring constant as one. We have Langevin’s type heat baths that are coupled to the surfaces at \( n_1 = 1 \) and \( n_1 = N \) and are maintained at temperatures \( T_L \) and \( T_R \) \((T_L > T_R)\) respectively. Hence the equation of motion of a particle at the site \( n \) reads

\[ \ddot{x}_n = -\sum_{\hat{e}} (x_n - x_{n+\hat{e}}) - \gamma (\delta_{n_1,1} + \delta_{n_1,N}) \dot{x}_n + \gamma \delta_{n_1,1} \eta_{n_{n_1,N}}^{L,R} + \gamma \delta_{n_1,N} \eta_{n_{n_1,1}}^{L,R}. \quad (3) \]

We have chosen the noises to be white and they are uncorrelated at different sites. Noise strength is specified by

\[ \langle \eta_{n_{n_1,N}}^{L,R}(t) \eta_{n_{n_1,N}}^{L,R}(t') \rangle = 2\gamma T_L \delta(t - t') \delta_{n_1,n_{n_1,N}}. \quad (4) \]

where we have chosen the Boltzmann constant \( k_B = 1 \). We use the periodic boundary conditions for the displacement field and the noises in \( n_2 \) and \( n_3 \) directions:

\begin{align*}
\eta_{n+(0,W_2,0)}^{L,R}(t) &= \eta_{n+(0,0,W_3)}^{L,R}(t) \\
\eta_{n+(0,W_2,0)}^{L,R}(t) &= \eta_{n+(0,0,W_3)}^{L,R}(t)
\end{align*} \quad (5)
These periodic boundary conditions lead to the following expansion of $x_n(t)$ and $\eta_{n}^{L,R}(t)$:

$$x_n(t) = \frac{1}{\sqrt{W_tw_2}} \sum_{p_2} \sum_{p_3} y_{n_1}(p_2, p_3, t) e^{i(p_2n_2+p_3n_3)a},$$

$$\eta_{n}^{L,R}(t) = \frac{1}{\sqrt{W_tw_2}} \sum_{p_2} \sum_{p_3} f_{n_1}(p_2, p_3, t) e^{i(p_2n_2+p_3n_3)a},$$

where $a$ be the lattice constant of the crystal. Upon substitution of Eqn. (6) and (7) into Eqn. (3) we obtain

$$\ddot{y}_{j} = -V_{jk} y_{k} - \gamma W_{jk} \dot{y}_{k} + f_{j}$$

where

$$W_{jk} = \delta_{j,1}\delta_{k,1} + \delta_{j,N}\delta_{k,N},$$

$$f_{j}(p_2,p_3,t) = \delta_{j,1} f_{L}(p_2,p_3,t) + \delta_{j,N} f_{R}(p_2,p_3,t)$$

the $N \times N$ matrix

$$V = \begin{pmatrix} 2\omega_{0}^{2} & -1 & 0 & 0 & \cdots \\ -1 & 2\omega_{0}^{2} & -1 & 0 & \cdots \\ 0 & -1 & 2\omega_{0}^{2} & -1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & -1 & 2\omega_{0}^{2} \end{pmatrix}$$

and

$$\omega_{0}^{2}(p_2,p_3) = 1 + 2\sin^{2}\left(\frac{p_2a}{2}\right) + 2\sin^{2}\left(\frac{p_3a}{2}\right).$$

Here $j, k = 1, \ldots, N$. We have also assumed here that $y_{0}(p_2,p_3,t) = 0 = y_{N+1}(p_2,p_3,t)$. To solve Eqn. (5) we diagonalize the matrix $V$. The solution of the $N$ order equation $|V - \alpha^{2}I| = 0$ gives the eigenvalues of $V$ as

$$\alpha_{k}^{2}(p_1,p_2) = 2\omega_{0}^{2}(p_1,p_2) + 2\cos\left(\frac{k\pi}{N+1}\right).$$

The $j$-th component of the normalized eigenvector corresponding to the eigenvalue $\alpha_{k}^{2}$ is given by

$$a_{j}^{(k)} = \sqrt{\frac{2}{N+1}} (-1)^{j+1} \sin \left(\frac{jk\pi}{N+1}\right).$$

The diagonalizing matrix $A$ thus reads as $A_{jk} = a_{j}^{(k)}$ such that $A^{T}A = I$ and $A^{T}VA = \alpha^{2}$, where $(\alpha^{2})_{jk} = \alpha_{j}^{2}\delta_{jk}$. We introduce a new set of coordinates $\xi_{j}$ as

$$y_{j}(p_2,p_3,t) = A_{jk}\xi_{k}(p_2,p_3,t).$$

The equation of motion of $\xi_{j}$ in matrix form can be written as

$$\ddot{\xi} = -\alpha^{2}\xi - \gamma Z\dot{\xi} + \bar{f},$$

where the symmetric matrix $Z = A^{T}WA$, and $\bar{f} = A^{T}f$. In the steady state limit ($t \gg 1/\gamma$) we are interested in the particular solution of the set of equations of motion of $\xi$. We use the Fourier transform of

$$\xi_{j}(t) = \int_{-\infty}^{\infty} d\omega \xi_{j}(\omega)e^{i\omega t} \quad \text{and} \quad f_{j}(t) = \int_{-\infty}^{\infty} d\omega f_{j}(\omega)e^{i\omega t}$$

in Eqn. (10) and obtain

$$(-\omega^{2}\delta_{jk} + \alpha_{j}^{2}\delta_{jk} + i\gamma\omega Z_{jk})\xi_{k}(\omega) = \bar{f}_{j}(\omega).$$

Since the dynamics of the system in the steady state is governed by the noises, we decompose $\xi_{j}(\omega)$ as

$$\xi_{j}(\omega) = b(\omega)\bar{f}_{j}(\omega)$$

and then using this decomposition into Eqn. (15) we obtain

$$b(\omega) = -\frac{1}{\omega^{2} - \alpha_{j}^{2} - i\gamma\omega}.$$
where
\[
\Delta_d(\beta_1, \beta_2) = (\cos \beta_1 - \cos \beta_2)^2 + \gamma^2 (2\omega_1^2 + \cos \beta_1 + \cos \beta_2),
\] (26)
\[I_c(t-t') = 2(\cos \beta_1 - \cos \beta_2) \cos(\omega_1 |t-t'|) + \frac{\gamma}{\omega_1} \{ (4\omega_1^2 + 3 \cos \beta_1 + \cos \beta_2) \times \sin(\omega_1 |t-t'|) \},
\] (27)
\[I_c(t-t') = 2(\cos \beta_1 - \cos \beta_2) \cos(\omega_1 |t-t'|) - \frac{\gamma}{\omega_1} \{ (4\omega_1^2 + \cos \beta_1 + 3 \cos \beta_2) \times \sin(\omega_1 |t-t'|) \},
\] (28)
\[\beta_{1,2} = \frac{\pi k_{1,2}}{N + 1},
\] (29)
\[\omega_{1,2} = \sqrt{\alpha_1^2 - \gamma^2/4}.
\] (30)

It is clear that \(I_c(t-t') \to 0\), when \(|t-t'| \to \infty\) and when \(t = t'\).
\[I_c(0) = \frac{\cos \beta_1 - \cos \beta_2}{2 \Delta_d(\beta_1, \beta_2)}.
\] (31)

For \(1 \leq |k_1 - k_2| \leq N - 1\), \(I_c(0)\) remains finite when \(N\) tends to infinity. According to Eqn. (14) the factor appeared in Eqn. (23) \(\langle a^{(k_1)}_n \rangle \langle a^{(k_2)}_n \rangle T_L + \langle a^{(k_1)}_n \rangle \langle a^{(k_2)}_n \rangle T_R = 2(T_L + (-1)^{k_1+k_2}T_R) \sin \beta_1 \sin \beta_2/(N+1)\). It implies that even for zero momentum modes \((p_{2,3} = 0)\), which appear owing to the periodic boundary conditions imposed on the displacement field in \(n_2\) and \(n_3\) directions, the equal time correlation in Eqn. (23) goes as \(N^{-\alpha} (1 \leq \alpha \leq 3)\) when \(N \to \infty\). The fall of this correlation as a negative power of \(N\) in the thermodynamic limit indicates that the ballistic transport remains absent from the conduction process of heat \([8]\).

Heat current density \(j_n\) from the lattice site \(n\) to \(n + \hat{e}_1\), where \(\hat{e}_1 = (1, 0, 0)\), is given by [1]
\[j_n = \frac{1}{2} ((x_n + \hat{e}_1 - x_n)(\dot{x}_n + \dot{\hat{e}}_1 + \dot{x}_n))
\] (32)
The average heat current density per bond [11]
\[J = \frac{1}{2W_2W_3(N-1)} \sum_{n_1=1}^{N-1} \sum_{n_2=1}^{N} \sum_{n_3=1}^{W_3} j_n.
\] (33)

We substitute Eqn. (6) and (15) in \(J\) and after performing the summations over \(n_2\) and \(n_3\) obtain the average heat current density per bond in the steady state limit as
\[J = \frac{1}{2W_2W_3(N-1)} \sum_{p_{2,3}}^{N} \sum_{k_{1,2}=1}^{N-1} (a^{(k_1)}_{n_1+1} - a^{(k_1)}_{n_1}) \times (a^{(k_2)}_{n_1+1} + a^{(k_2)}_{n_1}) (\xi_{k_1}(p_2,p_3,t) \xi_{k_2}(-p_2,-p_3,t)).
\] (34)

We now use Eqn. (14) to evaluate the sum
\[\sum_{n_1=1}^{N-1} (a^{(k_1)}_{n_1+1} - a^{(k_1)}_{n_1}) (a^{(k_2)}_{n_1+1} + a^{(k_2)}_{n_1}) = 2(1 - (-1)^{k_1+k_2}) \sin \beta_1 \sin \beta_2 \times \frac{1}{\cos \beta_2 - \cos \beta_1 - 1}
\] (35)
and then using (23) and (31) obtain
\[J = -\frac{2\gamma (T_L - T_R)}{(N+1)^2(N-1)W_2W_3} \sum_{p_{2,3}}^{N} \sum_{k_1,k_2=1}^{N} \times (1 - (-1)^{k_1+k_2}) \sin \beta_1 \sin \beta_2
\Delta_d(\beta_1, \beta_2).
\] (36)

The factor \((1 - (-1)^{k_1+k_2})\) ensures that the summation over \(k_1\) and \(k_2\) will be non zero only when \(k_1 + k_2\) is an odd number and hence we take the factor \((T_L + (-1)^{k_1+k_2}T_R)\) out of the summation as \((T_L - T_R)\). In the continuum limit, when \(a \to 0\) and \(W_{2,3} \to \infty\) keeping a \(W_{2,3}\) at fixed values, we convert the discrete sums over \(p_2\) and \(p_3\) into integrals:
\[\sum_{p_{2,3}} \to \frac{a}{W_2W_3} \int_{\pi}^{\pi} dp_{2,3}.
\] (37)

Evaluation of the integrals [12] over \(p_2\) and \(p_3\) gives
\[J = -\frac{2\gamma (T_L - T_R)}{(N-1)I(N, \gamma)}
\] (38)
where
\[I(N, \gamma) = \frac{1}{(N+1)^2} \sum_{k_1,k_2=1}^{N} (1 - (-1)^{k_1+k_2}) \times \frac{\sin^2 \beta_1 \sin^2 \beta_2}{\Delta(\beta_1, \beta_2)} F \left( \frac{1}{2}, \frac{1}{2}; 1; \frac{4\gamma^2}{\Delta(\beta_1, \beta_2)^2} \right).
\] (39)

Here the function
\[\Delta(\beta_1, \beta_2) = (\cos \beta_1 - \cos \beta_2)^2 + \gamma^2 (6 + \cos \beta_1 + \cos \beta_2).
\] (40)

\(I(N, \gamma)\) is zero if \(k_1\) and \(k_2\) simultaneously take even integer values or odd integer values. Assuming that \(N\) be an even number and using the fact that the summant of Eqn. (39) is symmetric in respect of the interchange of \(\beta_1\) and \(\beta_2\), we rewrite the double sum of
\[I(N, \gamma) = \frac{4}{(N+1)^2} \sum_{j_1,j_2=1}^{N/2} \frac{\sin^2 \beta_1 \sin^2 \beta_2}{\Delta(\beta_1, \beta_2)} \times F \left( \frac{1}{2}, \frac{1}{2}; 1; \frac{4\gamma^2}{\Delta(\beta_1, \beta_2)^2} \right),
\] (41)
where $\beta_1 = 2\pi j_0/(N + 1)$ and $\beta_2 = \pi(2j_2 - 1)/(N + 1)$. Again in the continuum limit we convert this double sum into integrals. In this limit $\alpha \to 0$ and $N \to \infty$ keeping $N\alpha$ at a fixed value. Defining the integration variables in this limit as $\theta_{1,2} = 2\pi j_{1,2}/(N + 1)$, we convert the discrete sums into integrals:

$$\frac{2}{N+1} \sum_{j_{1,2}=1}^{N/2} \to \frac{1}{\pi} \int_0^\pi d\theta_{1,2}. \quad (42)$$

$I(N, \gamma)$ thus takes the form

$$g(\gamma) = \lim_{N \to \infty} I(N, \gamma)$$

$$= \frac{1}{\pi^2} \int_0^\pi d\theta_1 \int_0^\pi d\theta_2 \frac{\sin^2 \theta_1 \sin^2 \theta_2}{\Delta(\theta_1, \theta_2)}$$

$$\times F\left(\frac{1}{2}, \frac{1}{2}, 1; \frac{4\gamma^2}{\Delta(\theta_1, \theta_2)}\right). \quad (43)$$

Hence we obtain the steady state current density per bond in the continuum limit

$$J = -\kappa \frac{(T_L - T_R)}{N - 1}. \quad (44)$$

where the conductivity

$$\kappa = 2\gamma g(\gamma). \quad (45)$$

Here $\kappa$ is found to be independent of the size of the system. The variation of the thermal conductivity $\kappa$ as a function of $\gamma$, as given by Eqn. (45), is plotted in Fig. 1.

Here $\gamma$ appears as a constant in the dissipative force term of the Langevin’s equation. Physically this force term denotes a viscous force experienced by the particles of Brownian like at the boundary surfaces of the crystal owing to collisions with the particles of fluid which seems to constitute the heat baths\[13]. The increase of $\gamma$, reduces the mobilities of the Brownian particles and thereby reducing their velocities\[13, 14]. Consequently, the velocities of the particles at the surfaces next to the boundaries will reduce the rate of flow of heat from the boundaries to the crystal itself and thereby reducing the thermal conductivity of the system. Hence, it justifies reasonably the nature of variation of $\kappa$ with $\gamma$ as shown in Fig. 1.

The average of the square of velocity of a layer at $n_1$ reads

$$v_{avg}^2(n_1) = \frac{1}{W_2} \sum_{n_2=1}^{W_2} \sum_{n_3=1}^{W_3} \langle \dot{x}_{n_1}^2 \rangle$$

$$= \frac{1}{W_2} \sum_{n_2=1}^{W_2} \sum_{n_3=1}^{W_3} a_{n_1}^{(k_1)} a_{n_1}^{(k_2)}$$

$$\times \langle \xi_{k_1}(p_2, p_3, t) \xi_{k_2}(p_2, p_3, t) \rangle. \quad (46)$$

We use Eqn. (21) to compute the velocity-velocity correlation as

$$\langle \xi_{k_1}(p_2, p_3, t) \xi_{k_2}(p_2, p_3, t) \rangle$$

$$= \frac{2\gamma^2}{N+1} \left( T_L + (-1)^{k_1+k_2} \sin \beta_1 \sin \beta_2 \right)$$

$$\times \frac{2\alpha^2 + \cos \beta_1 + \cos \beta_2}{\Lambda(\beta_1, \beta_2)} \quad (47)$$

Upon substitution of Eqn. (47) into Eqn. (46) and evaluation of $p_2$ and $p_3$ sum in the continuum limit along $n_2$ and $n_3$ directions, give

$$v_{avg}^2(n_1) = h_L(n_1, N)T_L + h_R(n_1, N)T_R \quad (48)$$

where

$$h_L(n_1, N) = \frac{4}{(N+1)^2} \sum_{k_1, k_2=1}^{N} \Lambda(\beta_1, \beta_2) \Delta(\beta_1, \beta_2)$$

$$\times \sin(n_1 \beta_1) \sin(n_1 \beta_2) \sin \beta_1 \sin \beta_2, \quad (49)$$

$$h_R(n_1, N) = \frac{4}{(N+1)^2} \sum_{k_1, k_2=1}^{N} (-1)^{k_1+k_2} \Lambda(\beta_1, \beta_2) \Delta(\beta_1, \beta_2)$$

$$\times \sin(n_1 \beta_1) \sin(n_1 \beta_2) \sin \beta_1 \sin \beta_2, \quad (50)$$

$$\Lambda(\beta_1, \beta_2) = \{ (\cos \beta_1 - \cos \beta_2)^2 \}$$

$$\times [1 - F(1/2, 1/2, 1; 4\gamma^2 / \Delta(\beta_1, \beta_2)^2)] + \gamma^2 (6 + \cos \beta_1 + \cos \beta_2). \quad (51)$$

Our evaluation suggests that for $\gamma = 0.01$, $h_L$ tends to 0.0396 and $h_R$ tends to 0 and 0.0396 at $n_1 = 1$ and $n_1 = N$ respectively when $N \to \infty$. It indicates that as $h_L$ and $h_R$ are monotonically decreasing and increasing functions of $n_1$ respectively, $v_{avg}^2$ attains a minimum at
any layer in the region between $n_1 = 1$ and $n_1 = N$ and it is also evident from our plots given in Fig. 2 and 3. Since, $v_{avg}^2(n_1)$ is proportional to $T(n_1)$, the temperature of the layer at $n_1$, $T(n_1)$ also exhibits a minimum in the region $1 < n_1 < N$. This concave upward nature of $T(n_1)$ has also been predicted in Ref. [11].

In summary, we have given an exact analytical derivation of Fourier’s law of heat conduction in a three dimensional harmonic crystal. It shows that in three dimensions without introducing any pinning or disorder, harmonicity alone can give rise to a normal transport of heat in the crystal in the continuum limit.

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