R.Peierls's theory of thermal conductivity and the method of quasisolutions

Alexey Elokhin, NRU HSE

In 1929 R.Peierls published his work [1], where the theory of thermal conductivity in solids was described on a heuristic level of rigour. In this paper Peierls models the solid with a lattice of anharmonic oscillators where each of them interacts only with his nearest neighbors. Our goal is to continue his work, namely, we aim to provide a rigorous explanation of the thermal conductivity in a similar setting. Hence, we consider a periodic d-dimensional lattice

$$\mathbb{T}_L^d \stackrel{\text{def}}{=} L^{-1}[\mathbb{Z}^d/L\mathbb{Z}^d]$$

equipped with a Hamiltonian $H(z) = H_2 + \varepsilon H_4$, where

$$H_2(z) \stackrel{\text{def}}{=} \frac{1}{2}\sum_{\mathbf{j}\in\mathbb{T}_L^d}\left[p_{\mathbf{j}}^2 + \sum_{\mathbf{l}\in U_L}(q_{\mathbf{j}+\mathbf{l}} - q_{\mathbf{j}})^2\right]$$

$$H_4(z) \stackrel{\text{def}}{=} \sum_{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3,\mathbf{j}_4\in\mathbb{T}_L^d} c_{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3,\mathbf{j}_4} q_{\mathbf{j}_1}q_{\mathbf{j}_2}q_{\mathbf{j}_3}q_{\mathbf{j}_4}$$

Following Peierls, we perform a sequence of canonical transformations and proceed with adding small viscosity and noise. This gives the following equation of motion:

$$\dot{a}_{\mathbf{k}}^{\pm} = -i\rho L^{-d}\Psi_{\mathbf{k}}^{\pm}(\mathbf{a}, \tau\nu^{-1}) - \gamma_{\mathbf{k}}^{\pm}a_{\mathbf{k}}^{\pm} + b^{\pm}(\mathbf{k})\dot{\beta}_{\mathbf{k}}^{\pm}, \qquad \mathbf{k}\in\mathbb{T}_L^d,$$

where $\Psi_{\mathbf{k}}^{\pm}(\mathbf{a}, t)$ is the nonlinearity. We are interested in the energy spectrum of the solution since this is a physically measurable quantity. We also consider its expansion in the parameter ρ

$$\mathfrak{n}_{\mathbf{k}}^{\pm}(\tau) = \mathbb{E}|a_{\mathbf{k}}^{\pm}(\tau)|^2 = \sum_{i=1}^{\infty}\rho^i\mathfrak{n}_{\mathbf{k};\pm}^{(i)}$$

1

For now we limit our consideration only to the first three terms of the series. Our goal is to show that in the limit $L\to\infty$ and $\nu\to 0$ they obey a certain kinetic equation. It is easy to show that

$$\mathfrak{n}_{\mathbf{k};\pm}^{(0)} \sim 1, \quad \mathfrak{n}_{\mathbf{k};\pm}^{(1)} = 0$$

due to Wick theorem and certain relations on indexes. The next term

$$\mathfrak{n}_{\mathbf{k};\pm}^{(2)}(\tau) = \mathbb{E}|a_{\mathbf{k};\pm}^{(1)}|^2 + 2\Re\mathbb{E}a_{\mathbf{k};\pm}^{(2)}\overline{a_{\mathbf{k};\pm}^{(0)}}$$

is less trivial, and the first step of its analysis it to approximate it with the following integral expression as $L\to\infty$:

$$I_{\mathbf{k}}^{\sigma} = \nu^2\sum_{\sigma_1,\sigma_2,\sigma_3=\pm1}\int_{\mathcal{D}^3} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

$$\delta_{1,2,3}^{-k}\frac{F_{\mathbf{k}}^{\sigma_1,\sigma_2,\sigma_3,\sigma}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)}{\nu^2(\Gamma_{\mathbf{k}}^{\sigma_1,\sigma_2,\sigma_3,\sigma}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3))^2 + (\Omega_{\mathbf{k}}^{\sigma_1,\sigma_2,\sigma_3,\sigma}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3))^2}.$$

The next step is to obtain the asymptotics of the expression above in the limit $\nu\to 0$ and this is where the problem becomes difficult since we need to precisely examine the critical points of the function

$$\Omega_{\mathbf{k}}^{\sigma_1,\sigma_2,\sigma_3,\sigma}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3) = \sigma_1\omega_{\mathbf{k}_1} + \sigma_2\omega_{\mathbf{k}_2} + \sigma_3\omega_{\mathbf{k}_3} - \sigma\omega_{\mathbf{k}},$$

where

$$\omega_{\mathbf{k}}^2 = \sum_{i=1}^{d}\sin\pi k_i$$

is a dispersion relation. In order to ensure the convergence of the integral above, we need to show that there are no degenerate critical points in the domain $\{(\mathbf{k}_1,\mathbf{k}_2) : \Omega_{\mathbf{k}}^{\sigma_1,\sigma_2,\sigma_3,\sigma} = 0\}$.

2

3

In other words, we are studying the solutions of the following system of equations:

$$\begin{cases}\sigma_1\omega_{\mathbf{k}_1} + \sigma_2\omega_{\mathbf{k}_2} + \sigma_3\omega_{\mathbf{k}_3} - \sigma\omega_{\mathbf{k}} = 0,\\ \sigma_j\frac{\sin(2\pi(\mathbf{k}_j)_i)}{\omega_{\mathbf{k}_j}} + \sigma_3\frac{\sin(2\pi(\mathbf{k}_3)_i)}{\omega_{\mathbf{k}_3}} = 0,\\ \mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}\in\mathbb{Z}^d.\end{cases}$$

It appears that apart from certain arithmetic insights it is impossible to solve the system analytically, so we turned our attention to the numerical approach. We found out that:

1) The critical points almost always have a regular structure, i.e. the coordinates satisfy some simple relations (yet we were unable to prove this),
2) There is a submanifold $\mathcal{B}^1$, $\dim\mathcal{B}^1 = d-1$, such that if $\mathbf{k}\in\mathcal{B}^1$ then we have at least one degenerate critical point of the same regular structure,
3) There is a submanifold $\mathcal{B}^2$, $\dim\mathcal{B}^2 = d-2$, such that if $\mathbf{k}\in\mathcal{B}^2$ then we have degenerate critical points of different structure that becomes more complex with growth of d.

Thus, we can only obtain the asymptotics of the integral above for $\mathbf{k}\notin\mathcal{B}^1\cup\mathcal{B}^2$, i.e., for such $\mathbf{k}$ we have

$$|I_{\mathbf{k}}^{\sigma} - \nu\hat{I}_{\mathbf{k}}^{\sigma}| \le C(\mathbf{k})\nu^2\chi_{d,2}(\nu),$$

where

$$\hat{I}_{\mathbf{k}}^{\sigma} = \pi\sum_{\mathcal{K}_{3,\sigma}}\int_{\mathbb{M}_{\mathbf{k};\mathbf{k}_3}}\frac{\hat{F}_{\mathbf{k}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3(\mathbf{k}_1,\mathbf{k}_2))}{|\nabla\hat{\Omega}_{\mathbf{k}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3(\mathbf{k}_1,\mathbf{k}_2))|}d\mathbf{k}_1 d\mathbf{k}_2|_{\mathbb{M}_{\mathbf{k}}}$$

4

We aim to achieve the following result:

$$|\mathfrak{n}_{\mathbf{k};\sigma}^{\le 2}(\tau) - m(\tau;\mathbf{k})| \le C\varepsilon^2,$$

where $m(\tau;.)$ is a solution of the wave kinetic equation

$$\dot{m}(\tau;\mathbf{k}) = -2\gamma_{\mathbf{k}}^{\sigma}m(\tau;\mathbf{k}) + \varepsilon K(m(\tau;.))(\mathbf{k}) + 2b^{\sigma}(\mathbf{k}),$$

and $K(m(\tau;.))$ is a wave kinetic integral operator defined as

$$K(y)(\mathbf{k}) = 2\pi\sum_{\mathcal{K}_{3,\sigma}}\int_{\mathbb{M}_{\mathbf{k};\mathbf{k}_3}}\frac{d\mathbf{k}_1 d\mathbf{k}_2|_{\mathbb{M}_{\mathbf{k}}} y_1 y_2 y_3 y_{\mathbf{k}}}{|\nabla\Omega_{\mathbf{k}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3(\mathbf{k}_1,\mathbf{k}_2))|} \times\left(\frac{1}{y_{\mathbf{k}}} + \frac{1}{y_3} - \frac{1}{y_2} - \frac{1}{y_1}\right)$$

The key step in proof of the main result is to show that

$$\dot{\mathfrak{n}}_{\mathbf{k}}^{\le 2} = -2\gamma_{\mathbf{k}}^{\sigma}\mathfrak{n}_{\mathbf{k}}^{\le 2} + b^{\sigma}(\mathbf{k}) + \varepsilon K(\mathfrak{n}_{.}^{\le 2})(\mathbf{k}) + O(\varepsilon^4),$$

which is done via estimating the increments of $\mathfrak{n}_{\mathbf{k}}^{\le 2}$. Currently the work in this direction is ongoing.

References

[1] Peierls, R. (1929). Zur kinetischen Theorie der Wärmeleitung in Kristallen. In Annalen der Physik (Vol. 395, Issue 8, pp. 1055–1101). Wiley.
[2] Dymov, A., Kuksin, S. Formal Expansions in Stochastic Model for Wave Turbulence 1: Kinetic Limit. *Commun. Math. Phys.* **382**, 951–1014 (2021).
[3] Dymov, A.V. Asymptotic expansions for a class of singular integrals emerging in nonlinear wave systems. *Theor Math Phys* **214**, 153–169 (2023).