Thermal Conductivity Notes

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Please do not circulate this version around yet. Need lots of revision.

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CONTENTS

I. GEOMETRY EFFECT AND ANALOGY OF OHMS LAW

A. Review of Ohm's law

In introductory physics, we learn that voltage and current are proportional in many materials ($V \propto I$). The coefficient of this linear relation is resistance, R:

$$V = IR \tag{1}$$

The units of resistance, R, is in Ω (Ohms). This R depends both the geometry and the intrinsic property of the material. For a long bar shaped sample, if one wants to measure the resistance between a distance, L,

$$R = \rho \frac{L}{Wt}, \tag{2}$$

where W is the width and t is the thickness of the material. ρ is the intrinsic property of the material called **resistivity**. Often times, we express this intrinsic material property as an inverse called conductivity, $\sigma = 1/\rho$.

There is a differential version of Ohm's law, a slightly more advanced version.

$$\vec{j} = \sigma \vec{E}, \tag{3}$$

where j is the current density and E is the electric field. When the electric field does not change with time, we learn from electromagnetics that $\vec{E} = -\vec{\nabla}V$. Then, Eq. (3) can be expressed as:

$$\vec{j} = -\sigma\vec{\nabla}V, \tag{4}$$

Let me demonstrate that Eq. (1) can be derived from Eq. (3).

If the current density is uniform in a specific direction, we can integrate the current density with its cross section, A, to obtain the total current, I:

$$I = \int \vec{j} \cdot da = j \times A \tag{5}$$

Next, if we assume the electric field is also **constant** in a specific direction, say $\vec{x}$, and we are measuring the voltage difference of distance, L,

$$V = -\int \vec{E} \cdot d\vec{x} = EL, \tag{6}$$

or $V = E/L$. In addition, charge must be conserved. The differential version of charge conservation is the continuity equation:

$$\vec{\nabla} \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0. \tag{7}$$

Let us think of the region where no charge is built up. The second term of Eq. (7) is zero. Then, with $\vec{\nabla} \cdot \vec{j} = 0$, and Eq. (4),

$$\sigma\nabla^2 V = 0. \tag{8}$$

This is basically the Laplace equation. Therefore, in many cases, solving Ohm's law numerically for a given geometry is almost identical to solving a Laplace equation in electrostatics.

We shouldn't end here. Uniqueness theorem states that an electric potential (V) is only uniquely found with the boundary conditions. We review what those boundary conditions for determining voltage and resistance.

- Sample Boundary

Current cannot escape the boundary of the sample, unless a (current or voltage) source or drain (ground) is connected. This means that Neumann boundary condition must be satisfied at the sample boundary:

$$\hat{n} \cdot \vec{j} = 0, \tag{9}$$

except for the electrodes.

- Ground electrode boundary

$$V = 0 \tag{10}$$

by definition.

- Source Electrode boundary

Two kind of sources can be used: a constant voltage source or a constant current source. Mathematically, the constant voltage source is a Dirichlet boundary condition:

$$V = V_0 \tag{11}$$

The constant current source is similar to Eq. (9), but we impose another constraint. Integrating the area of the boundary should give the total current that is being applied to the sample:

$$\int_{\partial\Omega} -\hat{n} \cdot \vec{j}\, dS = I_0. \tag{12}$$

- Voltage Electrodes (Floating voltage)

The voltage measurements are measured by highly conductive metals that do not have a pre- well-defined electric potential. We rely on the fact that the electrode has $\sigma \to \infty$. Then, this would have no voltage change within the electrode geometry. This implies that a Voltage is constant within the electrode. Also, Neumann boundary conditions still apply.

$$V = \text{Constant} \tag{13}$$

and

$$\int_{\partial\Omega} -\hat{n}\cdot\vec{j}\, dS = 0. \tag{14}$$

B. Example: Simulation of a Bar-Shaped Sample

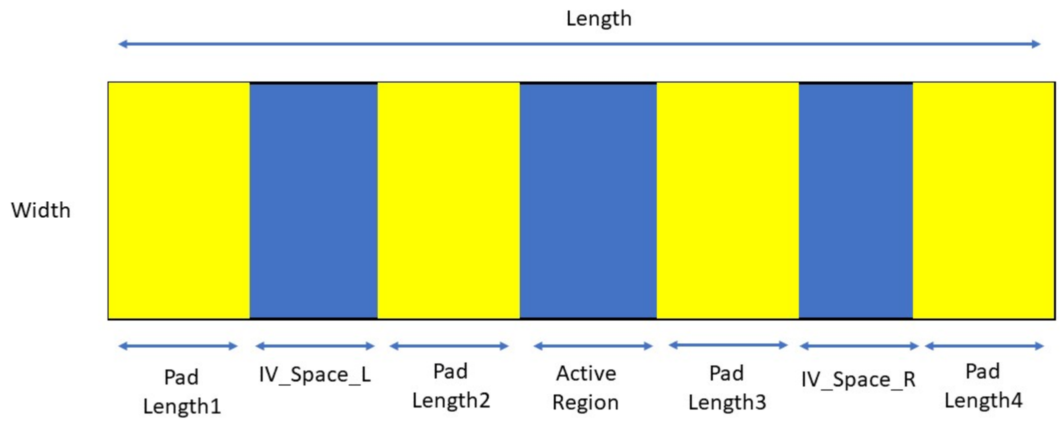

FIG. 1. Geometry of a Bar-Shaped Geometry. The blue color is the sample surface and the Yellow color is the electrode.

Let us try to mimic a transport geometry that many researchers use for their measurement. The schematic is shown in Fig. (1).

We try try the following dimensions:

- Length = 2 mm
- Width = 0.5 mm
- Thickness = 0.2 mm
- Pad Lengths are all 0.3 mm
- IV Space = IV Space = 0.266 mm
- Active Region = 0.266 mm

Now according to Eq. (2), the actual length that I need to use is not the total length of the sample, it is the active region. if I use σ = 1 Ω-cm, then I get 26.6 Ω. If I numerically estimate the resistance, I get 40 Ω. We know the reason. It is because the

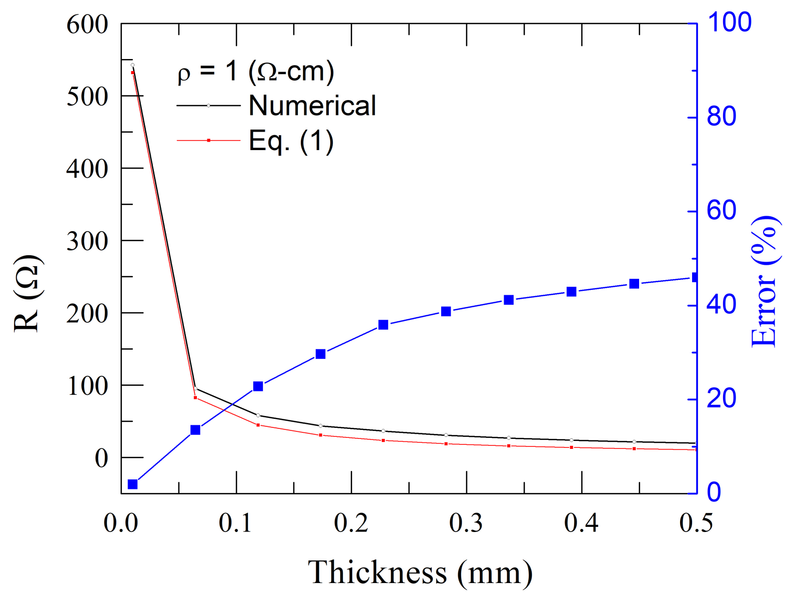

FIG. 2. Resistance simulation result by varying the thickness.

active region (channel length) is too short compared to the thickness, and therefore the current is not uniform along the thickness direction.

In Fig. (2), I show you how the estimated resistance from Eq. (2) compares with the numerical simulation. You can see that the error becomes significantly smaller when the thickness is smaller. This is a fun practice that demonstrates that your error can be off by roughly 50 percent. What does this mean?

A general form of resistivity and resistance relation is:

$$R = g\rho, \tag{15}$$

where all of the geometry information is in g. If I use Eq. (3), I am always using a smaller g value than what I am suppose to. Then, since I would estimate the resistivity by my resistance measurement as: $\rho = R/g$, I would be **overestimating** the resistivity value.

Let us imagine another case, you are in the lab and forgot to measure the dimensions of your sample. Can I roughly convert it to a reasonable resistivity? Yes. You **divide by roughly 30** and put units of **Ohm-cm**. I think you won't get terribly unphysical

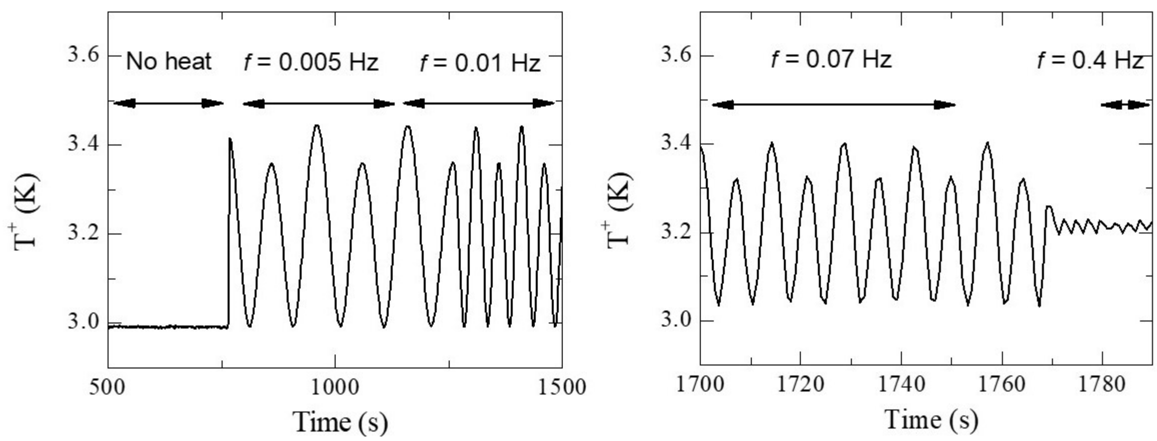

FIG. 3. Temperature change when an ac heat signal is applied through the UTe_2 sample. $T = 3$ K and an ac current of 0.3mA is sent through a 10kΩ heater.

resistivity values.

Let us think of the opposite case, if I measure UTe_2, the sample is in the mOhm-cm range at high temperatures. If I multiply by 30 and put units of Ohms, I get about 30 miliOhms. Good metals (such as gold or silver) have resistivity at room temperature in the 1 μ Ohm-cm range. Then, I should be able to measure in the 10s of μOhm range.

C. Geometry Calculation of Thermal Conductivity

I will do this part later when I feel like it.

II. ALTERNATING HEAT CURRENT

1. Experimental Observation

When applying an ac heat current, you see the following temperature change as shown in Fig. (3). Here I summarize the features:

- Roughly the thermometer signal repeats at twice the applied frequency (2ω).
- The amplitude becomes smaller at higher heat frequencies.

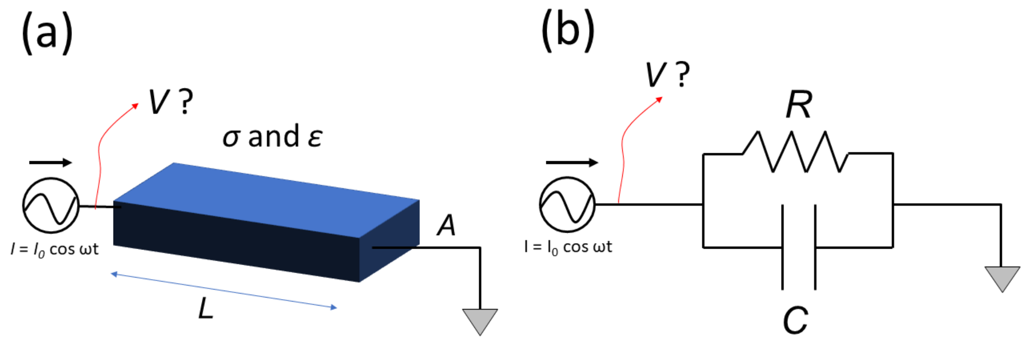

FIG. 4. (a) ac (constant) current flowing through a sample that has conductivity, σ, and permittivity, ϵ. (b) Equivalent circuit model.

- At a sufficiently high frequency, the temperature saturates at half the amplitude of the very low frequency heat case.
- Strictly speaking, the signal repeats at ω not 2ω. The amplitude of the peak is slightly different from the following peak.

From the previous section, I have shown you that a lot of our intuition from electrical conduction can be used in thermal conduction since the heat equation and continuity equation of charge have the same mathematical structure. So far, however, I have only considered the case in the dc limit ($\omega \to 0$).

A. Alternating electrical current

In this section, again using the analogy between heat conduction and electrical conduction, I will discuss what happens when heat current is alternating sinusoidally. Let us first consider the case when an ac electrical current flows through a uniform sample, as shown in Fig. (4) (a). I want to know what the electric potential is where the red arrow is located. Recall, in the dc case, we used Ohm's law:

$$\vec{j} = \sigma \vec{E} \tag{16}$$

If we take the divergence of this equation, we have:

$$\vec{\nabla} \cdot \vec{j} = \sigma \vec{\nabla} \cdot \vec{E} = 0 \tag{17}$$

This is the case of the continuity equation when there is no charge build up. ($\partial\rho/\partial t \to 0$). Let us restore the charge term again and look at the full version of the continuity equation.

$$\vec{\nabla} \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0. \tag{18}$$

To find a macroscopic equation for a uniform sample, we integrate over the entire volume:

$$\int dv\ \vec{\nabla} \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0. \tag{19}$$

In a linearly dielectric material,

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon}, \tag{20}$$

Using Gauss' law, the volume integral becomes an surface integral, where the surface is the boundary that encloses the volume:

$$\int dv\ \vec{\nabla} \cdot (\vec{j} + \epsilon \frac{\partial}{\partial t} \vec{E}) = \oint da\ (\vec{j} + \epsilon \frac{\partial}{\partial t} \vec{E}) = 0. \tag{21}$$

Calculating the first term is:

$$\int \vec{j} \to j \times A = I = (\sigma \times A/L) \times (E \times L) = V/R. \tag{22}$$

Integrating the second term is also a familiar one:

$$\int \epsilon \frac{\partial}{\partial t} E \to (\epsilon \times A/L) \times \frac{d}{dt}(E \times L) = C\frac{dV}{dt}, \tag{23}$$

where C is the capacitance. Therefore, if I send a total current of I_{total} through the material using a constant current source, I have the following conservation of current equation:

$$I_{total} = \frac{V}{R} + C\frac{dV}{dt} \tag{24}$$

This is identical to Kirchoff's equation for a resistor and capacitance connected in parallel, as shown in Fig. (4) (b). In circuit class, we solve this kind of circuit equation by letting voltage and current imaginary instead of sines and cosines. If $I_{total} = I_0 \sin(\omega t) = I_0 \mathrm{Im}[e^{i\omega t}]$, we can try $V = V_0 e^{i(\omega t+\phi)}$.

$$I_0 e^{i\omega t} = V_0(\frac{1}{R} + i\omega C)e^{i(\omega t+\phi)}. \tag{25}$$

We can use the beautiful Euler formula: $\exp(i\theta) = \cos(\theta) + i\sin(\theta)$.

$$\frac{1}{R} + i\omega C = \sqrt{\frac{1}{R^2} + (\omega C)^2}\exp(i\psi), \tag{26}$$

where

$$\psi \equiv \tan^{-1}(\omega RC) \equiv \tan^{-1}(\omega\tau). \tag{27}$$

I defined $\tau \equiv RC$ as the time constant.

Returning back to Eq. (25),

$$I_0 e^{i\omega t} = V_0\sqrt{\frac{1}{R^2} + (\omega C)^2}e^{i(\omega t+\phi+\psi)}. \tag{28}$$

Comparing the left hand side and right hand side, the amplitude part requires

$$V_0 = \frac{I_0}{\sqrt{\frac{1}{R^2} + (\omega C)^2}} = \frac{I_0 R}{\sqrt{1 + (\omega\tau)^2}}, \tag{29}$$

and the phase part requires

$$\phi = -\psi = -\tan^{-1}(\omega\tau) \tag{30}$$

We can plug these findings of amplitude and phase to $V = V_0 e^{i(\omega t+\phi)}$,

$$V = \frac{I_0 R}{\sqrt{1 + (\omega\tau)^2}}e^{i(\omega t - \tan^{-1}(\omega\tau))} \tag{31}$$

Taking the imaginary part,

$$\mathrm{Im}[V] = \frac{I_0 R}{\sqrt{1 + (\omega\tau)^2}}\sin(\omega t - \tan^{-1}(\omega\tau)). \tag{32}$$

Note, that if the current source was a cosine instead of a sine, you will need to take the real part

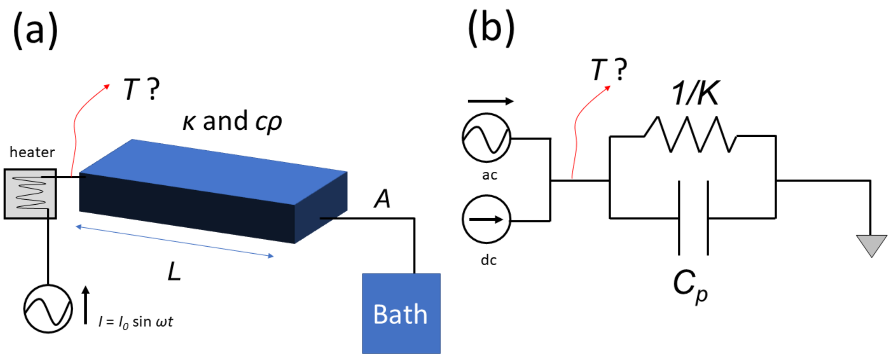

FIG. 5. (a) ac (constant) heat current flowing through a sample that has thermal conductivity, κ, density, ρ, and specific heat, c_p. (b) Equivalent circuit model.

$$\mathrm{Re}[V] = \frac{I_0 R}{\sqrt{1+(\omega\tau)^2}} \cos\left(\omega t - \tan^{-1}(\omega\tau)\right). \tag{33}$$

B. Alternating Heat Current

In ac electrical transport, I used the (charge) continuity equation and showed that this can be viewed as a circuit of a resistor and capacitor connected in parallel. For heat conduction, we consider the heat equation, which has a similar form as the continuity equation:

$$-\kappa\vec{\nabla}^2 T + \rho c_p \frac{\partial T}{\partial t} = 0, \tag{34}$$

where ρ is the density of the material and c_p is the specific heat. Again, let us consider the case where an ac heat current is flowing uniformly through the sample, as shown in Fig. (5) (a). This time, want to know the temperature where the red arrow is located. We can integrate the entire volume,

$$\int -\kappa\vec{\nabla}^2 T dv = \oint jda \rightarrow -\kappa\vec{\nabla}T \times A = (\kappa \times A/L) \times T = KT, \tag{35}$$

and

$$\int c_p\rho\frac{\partial T}{\partial t}dv \rightarrow \int c_p\rho\ dv \times \frac{\partial T}{\partial t} = C_p\frac{\partial T}{\partial t}, \tag{36}$$

where the total heat capacity is:

$$C_p \equiv \int c_p \rho dv \tag{37}$$

Then, we have

$$KT + C_p \frac{\partial T}{\partial t} = \dot{Q}_{source} \tag{38}$$

$\dot{Q}_{source}$ is the power from the heat source. Typically, an ac current, $I = I_0 \sin(\omega t)$, flows through a high resistance heater, R_{heater} and heats the sample by Joule heating:

$$\dot{Q}_{source} = I^2 R_{heater} = I_0^2 R_{heater} \sin^2(\omega t) = (\frac{I_0^2 R_{heater}}{2})(1 - \cos(2\omega t)). \tag{39}$$

The heat source can be viewed as a sum of a dc heat source and an ac heat source, oscillating with 2ω.

$$\dot{Q}_{source} = (\frac{I_0^2 R_{heater}}{2}) - (\frac{I_0^2 R_{heater}}{2}) \cos(2\omega t) = \dot{Q}^{dc}_{source} + \dot{Q}^{2\omega}_{source}. \tag{40}$$

Remember that Eq. (38) is a linear differential equation, meaning that the superposition principle holds. We can, therefore, separate this equation into two and solve them independently and later superimpose the two solutions:

$$KT^{dc} + C_p \frac{\partial T^{dc}}{\partial t} = \dot{Q}^{dc}_{source}, \tag{41}$$

and

$$KT^{ac} + C_p \frac{\partial T^{ac}}{\partial t} = \dot{Q}^{2\omega}_{source}, \tag{42}$$

Next, we need to set the initial condition. In equilibrium, $\dot{Q}_{source} = 0$, the entire sample is the same temperature as the bath temperature, i.e., $T = T_{bath}$. The solution for the dc heat equation, Eq. (41), is:

$$T^{dc}(t) = T_{bath} + \frac{T_0}{2}(1 - \exp(-C_p/\tau_q), \tag{43}$$

where I have defined

$$\frac{T_0}{2} \equiv \frac{I_0 R^2}{2K}, \tag{44}$$

and

$$\tau_q \equiv \frac{C_p}{K} \tag{45}$$

The solution for the ac problem is similar to the electrical circuit example from the previous subsection.

We replace the following quantities:

$$V \rightarrow T, \tag{46}$$

$$\omega \rightarrow 2\omega, \tag{47}$$

$$I_0 \rightarrow -\frac{I^2 R_{heater}}{2}, \tag{48}$$

$$\frac{1}{R} \rightarrow K, \tag{49}$$

$$C \rightarrow C_p \tag{50}$$

Then,

$$\text{Re}[T^{ac}] = \frac{-T_0/2}{\sqrt{1+4\omega^2\tau_q^2}} \cos(2\omega t + \tan^{-1}(2\omega\tau_q)) \tag{51}$$

The total solution is:

$$T = T^{dc} + T^{ac} = T_{bath} + \frac{T_0}{2}(1 - \exp(-t/\tau_q) + \frac{T_0/2}{\sqrt{1+4\omega^2\tau_q^2}} \cos(2\omega t + \tan^{-1}(2\omega\tau_q)) \tag{52}$$

Technically, the superposition principle have coefficients in front of T^{dc} and T^{ac}, and boundary or initial conditions determine those coefficients. Instead of going through that boring process, I try to convince you in the following that this solution is correct by considering extreme limits.

- Waiting for a long time ($t \gg \tau$)

  After waiting for a long time, the temperature will only oscillate with 2ω

$$T(t) \approx T_{bath} + \frac{T_0}{2} + \frac{T_0/2}{\sqrt{1+4\omega^2\tau_q^2}} \cos(2\omega t + \tan^{-1}(2\omega\tau_q)) \tag{53}$$

- dc limit ($\omega \to 0$):

  In the dc limit, $T(t) \to T_{bath} + T_0$, or $T_0 - T_{bath} = I_0^2 R/K$. This is exactly the same formula for finding the temperature change for dc thermal conductivity measurements. Remember, for finding the thermal conductivity experimentally, the most important information we want to measure is T_0.

- Low frequency limit:

  In the low frequency limit, $\omega\tau \ll 1$, therefore:

$$T(t) \approx T_{bath} + \frac{T_0}{2}(1 + \cos(2\omega t)) = T_{bath} + T_0 \cos^2(\omega t) \tag{54}$$

- High frequency limit :

  In the high frequency limit, $\omega\tau \gg 1$, we have

$$T(t) \approx T_{bath} + \frac{T_0}{2} + \frac{T_0}{2}\frac{\sin(2\omega t)}{2\omega\tau_q} \tag{55}$$

  In the very high frequency limit, $\omega \to \infty$, the sample temperature will only change half of the dc case $T \to T_{bath} + \frac{T_0}{2}$.

So far, this explains almost all the features of our experimental observation of Fig. (3). There is one more feature we did not capture: the signal has another periodicity of ω in addition to 2ω. This can be explained if the resistance of the heater changes with the magnitude of the current,

$$R \approx R_0 + \alpha I = R_0 + \alpha I_0 \sin\omega t, \tag{56}$$

where I have defined $\alpha \equiv (dR/dI)|_{I_0}$. The heat current becomes;

$$\dot{Q}_{heater} = I^2 R \approx I_0^2 \sin^2(\omega t)(R_0 + \alpha I_0 \sin\omega t) = \dot{Q}_{dc} + \dot{Q}_{ac} + \alpha I_0^3 \sin^3(\omega t) \tag{57}$$

This means we have two extra heat equations to superimpose for finding our final solution.

$$\dot{Q}_{extra} = \alpha I_0^3 \sin^3(\omega t) = \alpha I_0^3 (\frac{3\sin\omega t - \sin 3\omega t}{4}) = \dot{Q}_\omega - \dot{Q}_{3\omega}. \tag{58}$$

We define

$$T_1 \equiv \alpha I_0^3 / K \tag{59}$$

The solution for these extra terms are:

$$T_{extra} = \frac{3T_1}{4\sqrt{1+\omega^2\tau_q^2}}\sin(\omega t + \tan^{-1}(\omega\tau_q)) - \frac{T_1}{4\sqrt{1+9\omega^2\tau_q^2}}\sin(3\omega t + \tan^{-1}(3\omega\tau_q)) \quad (60)$$

The first is larger and drops in magnitude slower than the second term when ω is increased. Therefore, in most cases, you will see a sine wave oscillating with ω in addition to a cosine wave oscillating with 2ω.