Derivation of Heat Flux in RNEMD Simulations

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Abstract

This document presents a simplified derivation of the heat flux formula within the context of Reverse Non-Equilibrium Molecular Dynamics (RNEMD) simulations and its relation to Fourier's law of heat conduction.

1 Introduction

Fourier's law of heat conduction is a fundamental principle which states that the heat flux J through a material is proportional to the negative temperature gradient within that material. In systems where establishing a temperature gradient is challenging, RNEMD simulations offer a way to calculate the heat flux by artificially creating a non-equilibrium state.

2 Derivation

Consider the RNEMD simulation approach, where kinetic energy is swapped between hot and cold regions rather than applying a direct temperature gradient. The total energy exchanged $\Delta\varepsilon$ over a simulation time step τ is analogous to heat transfer. The cross-sectional area A and the exchange frequency M represent the area through which heat flows and the rate of energy exchange, respectively.

The heat flux J_x can thus be expressed as the ratio of the energy exchanged to the product of the area, time step, and exchange frequency:

$$J_x = \frac{\Delta\varepsilon}{2AM\tau} \tag{1}$$

The factor of $\frac{1}{2}$ accounts for the periodic boundary conditions in the simulation, implying that the energy flows in both directions.

To relate this to Fourier's law, we define:

$$J = -k\nabla T \tag{2}$$

Where k is the thermal conductivity, and ∇T is the temperature gradient. In the RNEMD simulation, k can be derived by measuring J_x and using the known temperature difference to back-calculate k.

3 Conclusion

The RNEMD method provides a valuable tool for calculating heat flux and thermal conductivity in systems where direct measurement of temperature gradients is not feasible.