Nonequilibrium Electron Transport Through a Polymer Chain: Lattice Thermal Vibration

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By taking the scattering state method, we study non-equilibrium electron transport in static lattice relaxation method and adiabatic dynamical evolution method. We focus on the impact of temperature on lattice configuration and how temperature affects the non-equilibrium steady-state transport, and obtain some meaningful results.

I. Physical Process

- **The work is based on the scattering state operator method, which was brought forward by Hershfield:**

$$Z_{\text{noneq}} = Tre^{-\beta(\hat{H}-\hat{Y})} \to <\hat{A}> = \frac{Tr\hat{A}e^{-\beta(\hat{H}-\hat{Y})}}{Tre^{-\beta(\hat{H}-\hat{Y})}} \qquad Y = \mu_R \sum_{kR} \Psi_{kR}^{+}\Psi_{kR} + \mu_L \sum_{kL} \Psi_{kL}^{+}\Psi_{kL}$$

- **We can prove that scattering state operator satisfy Fermi distribution:**

$$<\Psi_{\alpha\kappa\sigma}^{+}\Psi_{\beta\kappa'\sigma'}> = f(\omega)\delta_{\alpha\beta}\delta_{\sigma\sigma'}\delta(\kappa-\kappa')$$

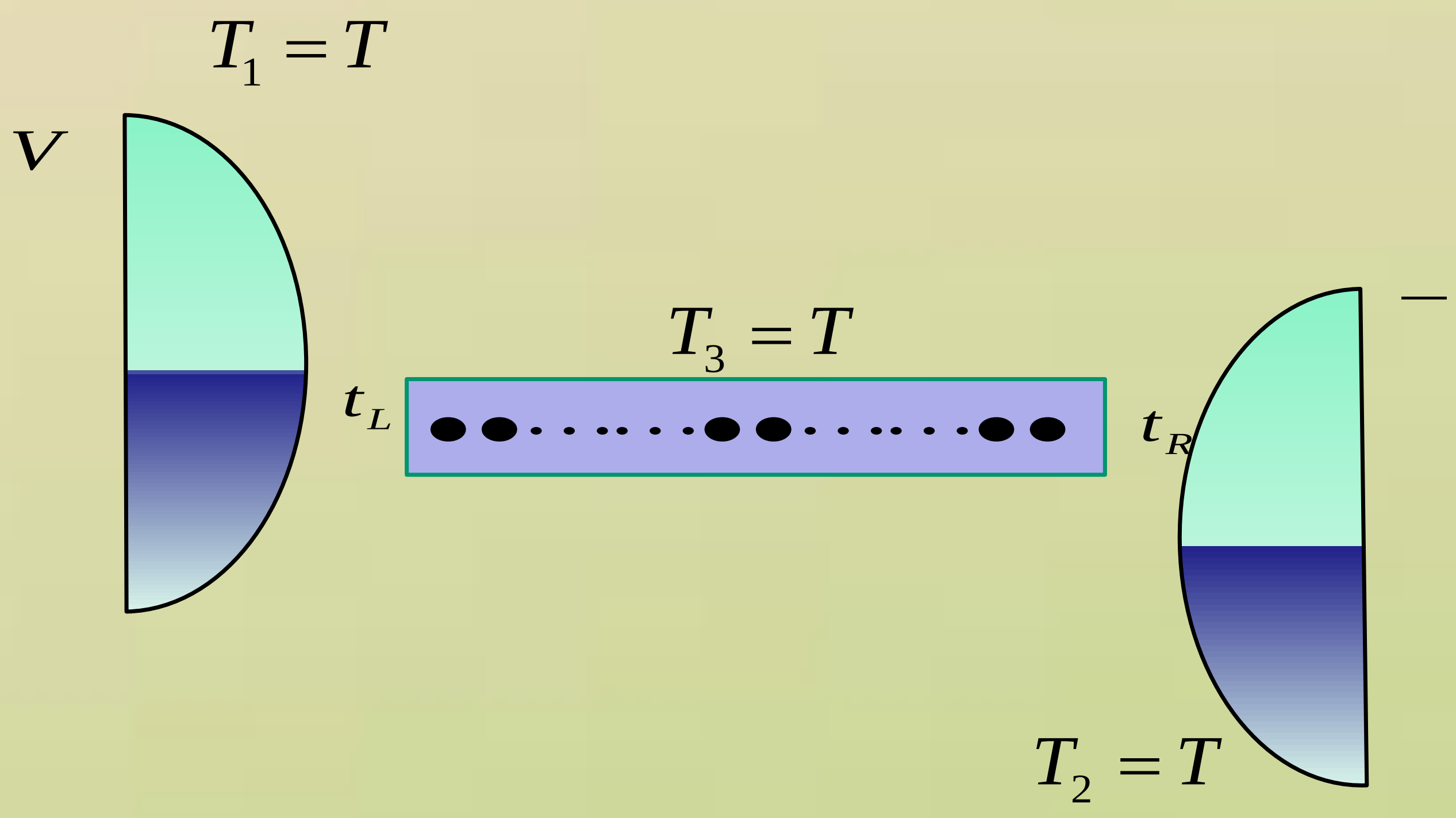
- **Without many-body interaction, the scattering state operator can be expanded within the one-particle basis:**

$$\Psi_{\alpha\kappa\sigma}^{+} = C_{\alpha\kappa\sigma}^{+} + \sum_{n=1}^{N}\gamma_n^{\alpha\kappa}d_{n\sigma}^{+} + \sum_{\beta\kappa'}\gamma_{\beta\kappa'}^{\alpha\kappa}C_{\beta\kappa'\sigma}^{+}$$

- **The lattice vibration equation is:**

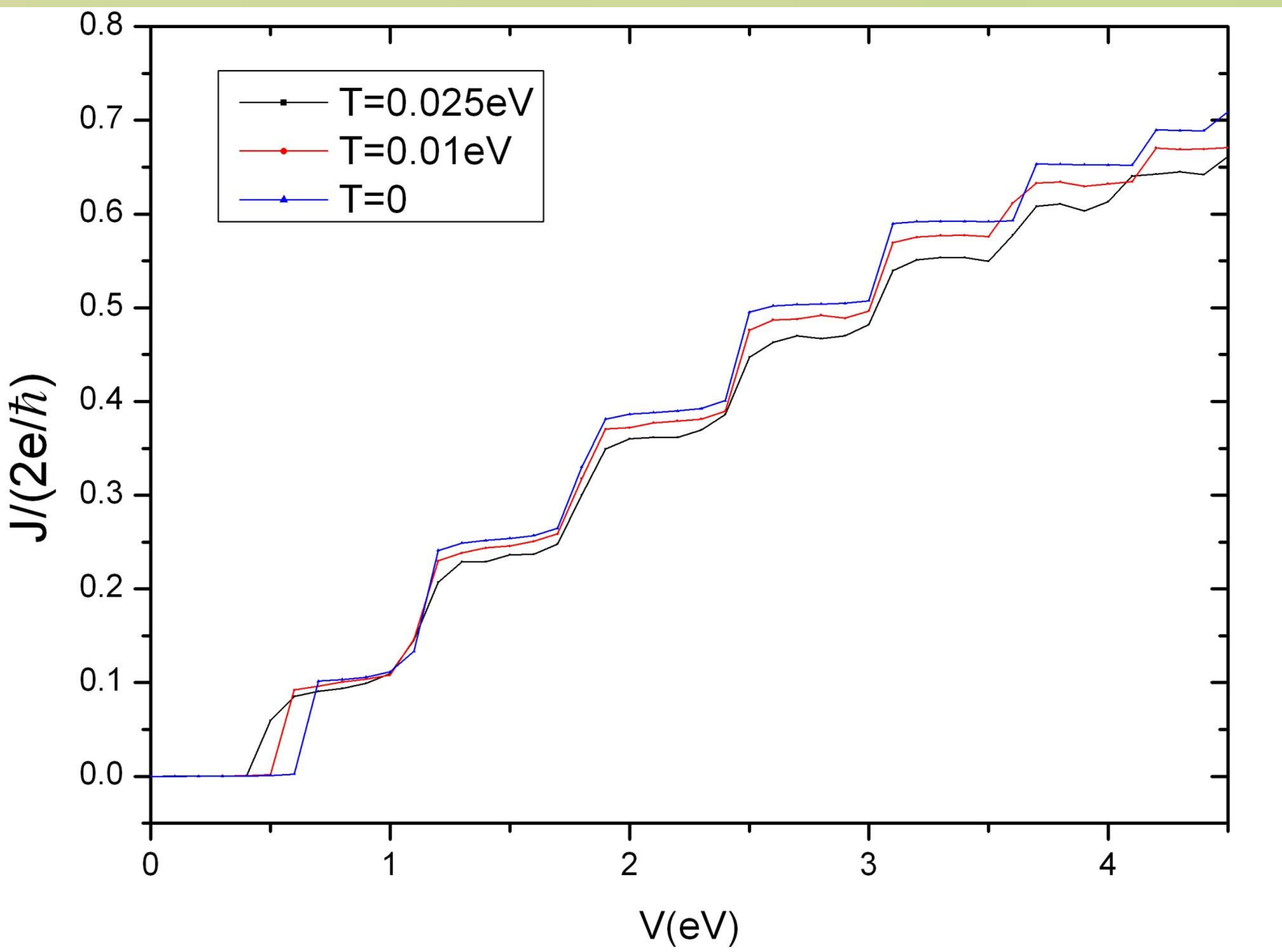
$$M\ddot{u}_n = -<\frac{\partial H}{\partial u_n}> - \eta_n\dot{u}_n$$

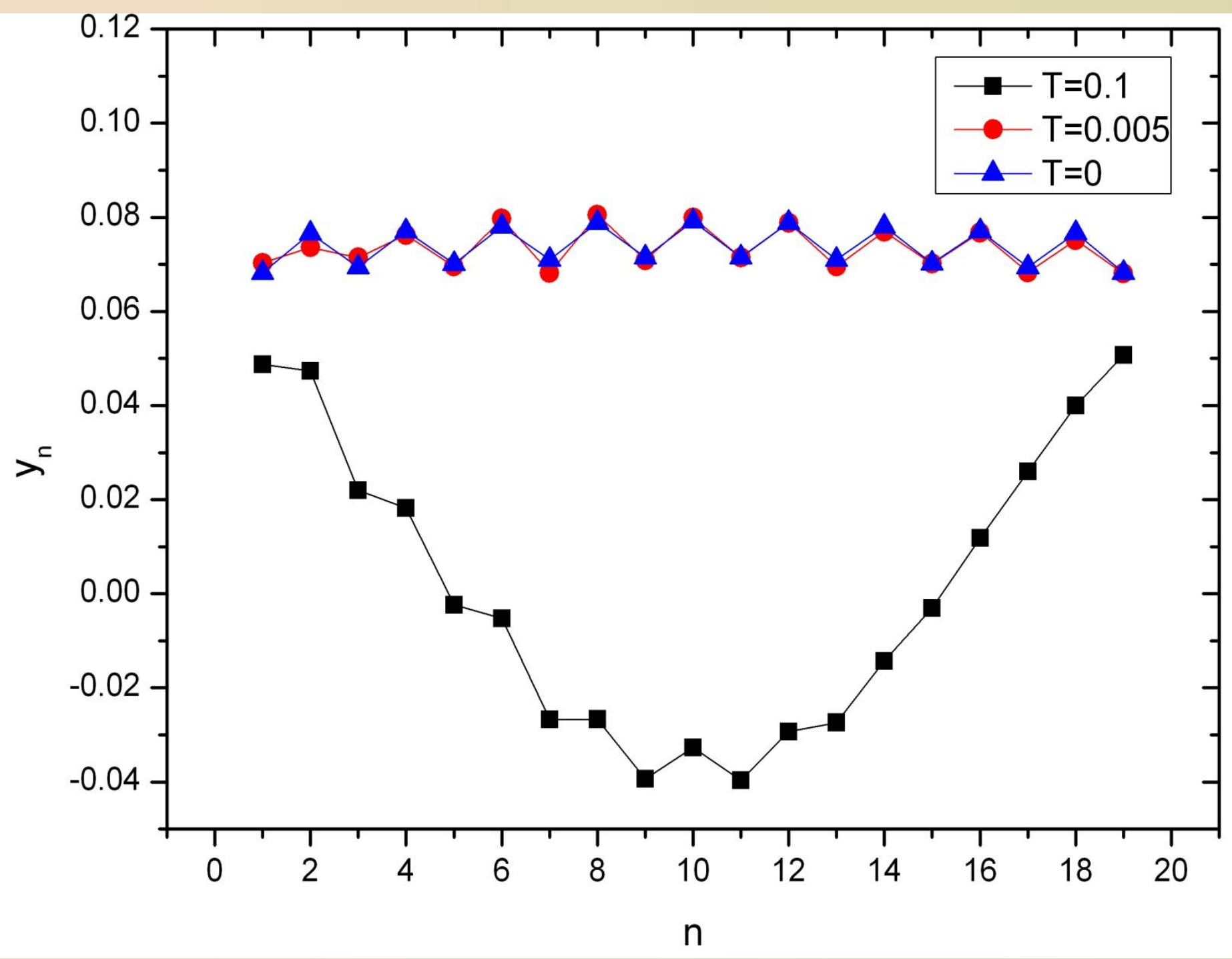
- **We choose Nose-Hover heat bath. The η satisfy the equation:** $\dot{\eta}_n = \frac{1}{{\tau_r}^2}(\frac{M}{T}{\dot{u}_n}^2 - 1)$



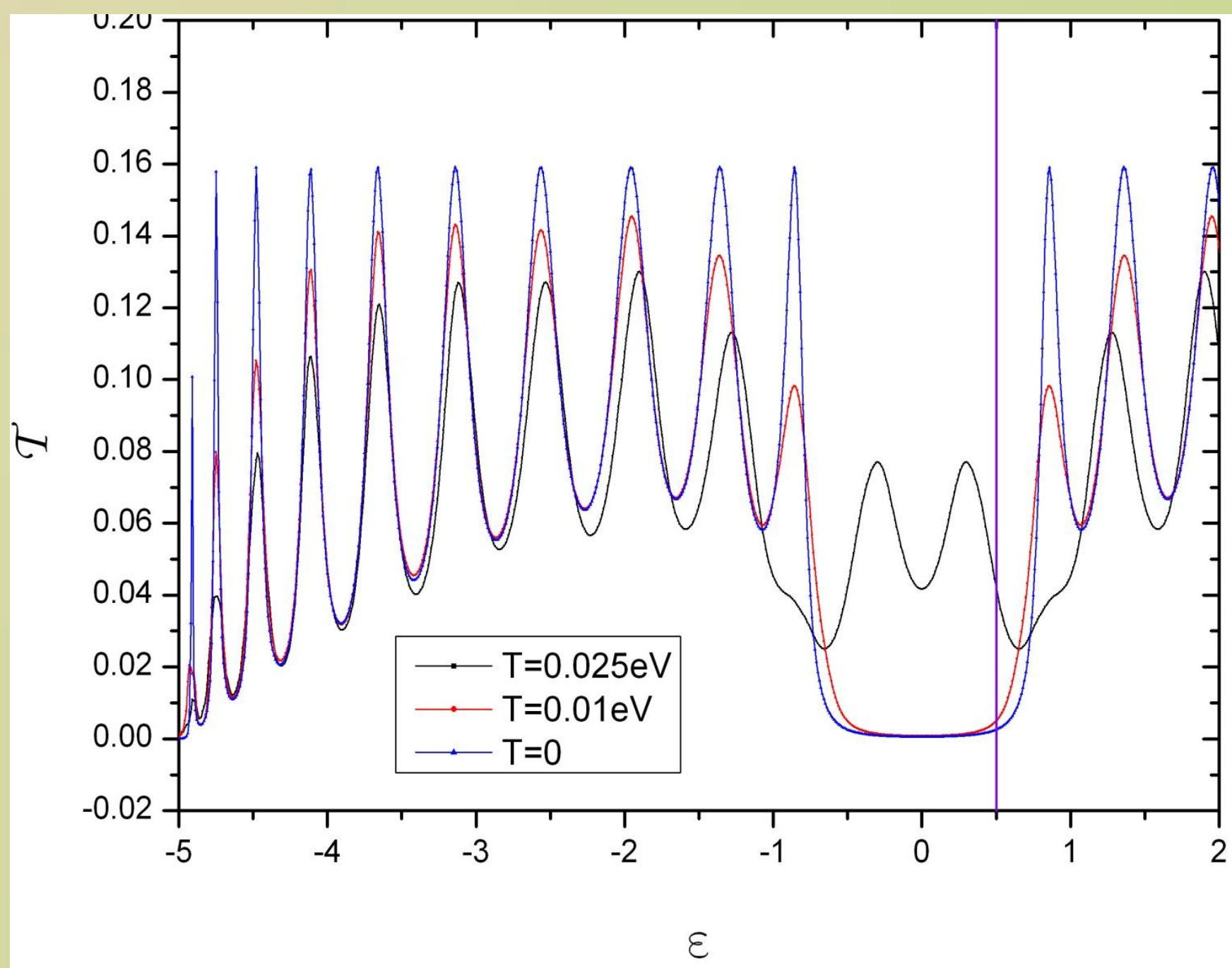
II. Main Results

- **Compare with different I-V curves for different temperature, we find that the high temperature will first emerge current at low voltage, while the higher temperature the smaller current at high voltage.**

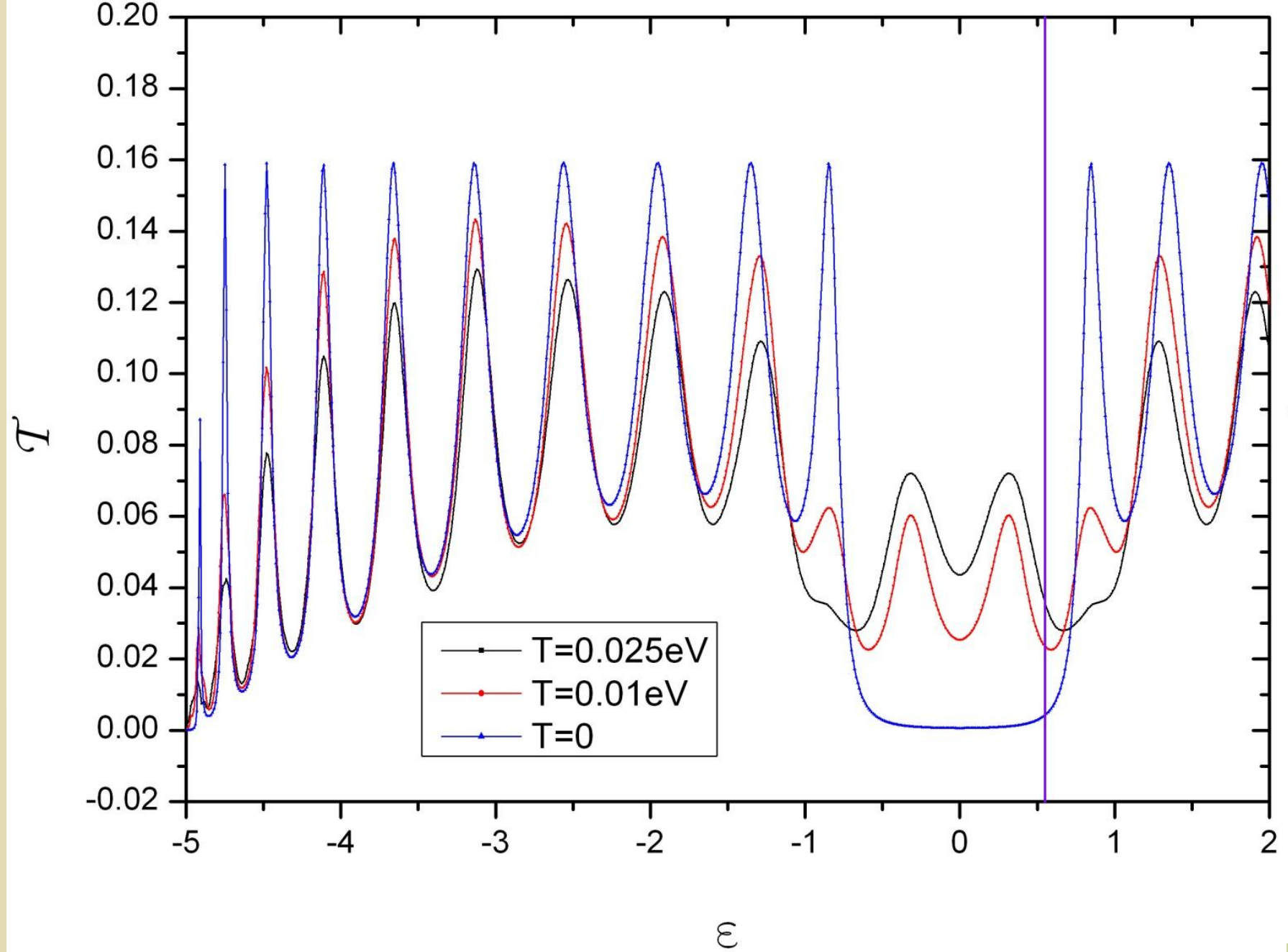




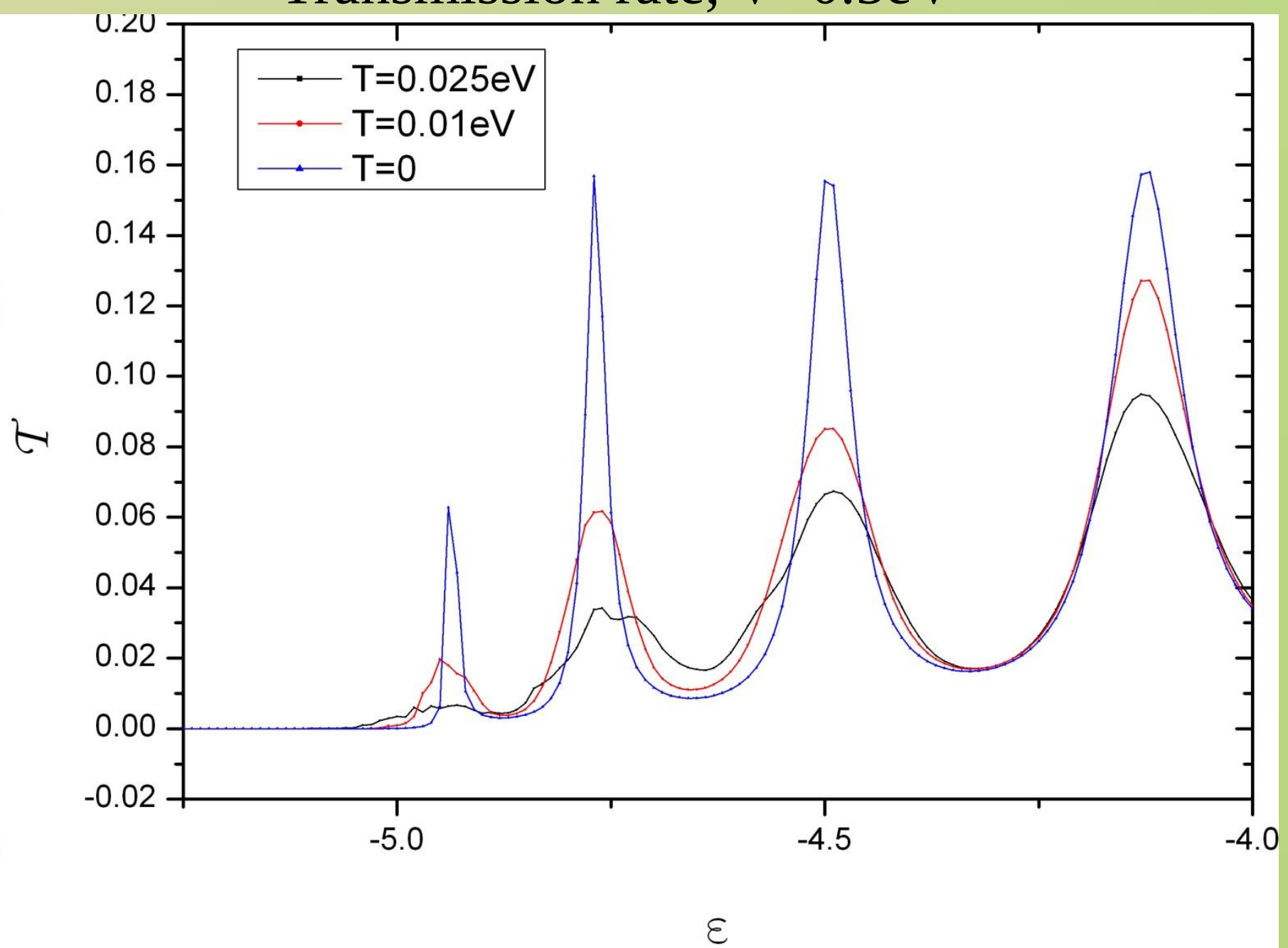
Lattice configuration for different T, V=0.55eV



Transmission rate, V=0.5eV



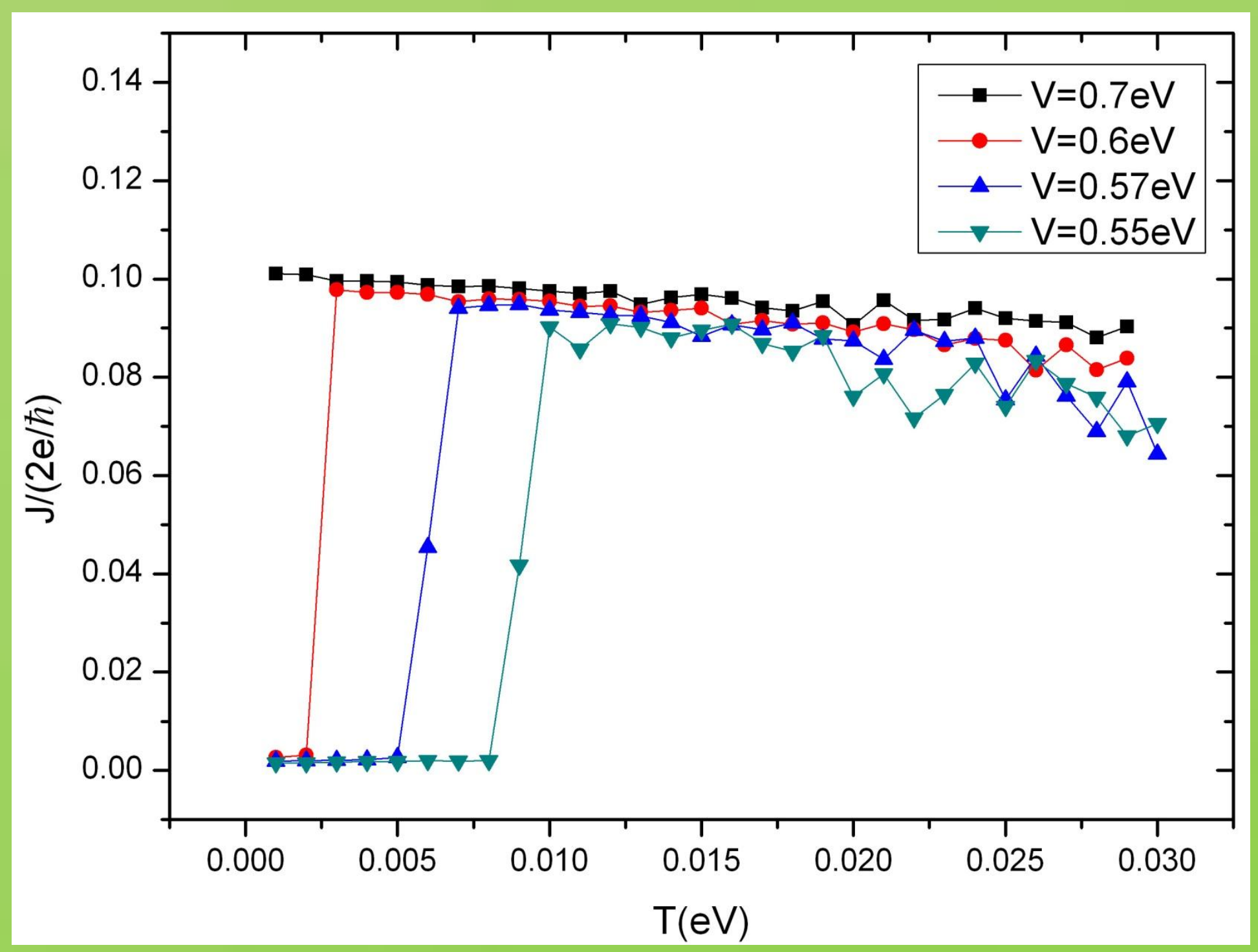
Transmission rate, V=0.55eV



Transmission rate, V=2.3eV

- **We find that as the temperature increases to a certain extent, it will produce soliton.**
- **From figures of transmission rate, we can see clearly the impact of temperature on soliton.**
- **What's more, we find that temperature makes the energy level broaden, that why the higher temperature the smaller current at high voltage.**

- **The current changes with temperature is as shown in the right figure. For low voltage such as 0.55eV and 0.57eV, when temperature is very low, there is no soliton, so the current is zero. As temperature increases, with soliton generation, the current is produced.**



III. Conclusion

As temperature increases, the energy level will broaden as function of temperature. As long as the temperature is high enough, the low voltage can also stimulate the solitons. In the same bias voltage, if soliton has been generated, the current will decay because the energy level broaden as the temperature gradually increased.