Limitations of the BOLTZMANN TRANSPORT EQUATION

Approximations used in arriving at the BTE:

- Single particle description of a many-body system of carriers.
- Correlations between carriers are neglected.
- Semiclassical treatment of carriers as particles having well defined position and momentum, and which obey Newton's law.
- Simple model for binary collisions that occur instantaneously in time and are local in space.
- Statistical description of a many-particle system. This means that the BTE might break down if there are few carriers in the system.
- Limitations of the classical model, can be found by considering the Heisenberg uncertainty principle which states:

$$\Delta p \cdot \Delta x \geq \hbar$$

Now, if the spread in carrier energy is approximately k_BT (thermal carriers), then:

$$\Delta p \approx \sqrt{2m^* k_BT}$$

which gives:

$$\Delta x \geq \frac{\hbar}{\sqrt{2m^* k_BT}} = \lambda_B \quad (100 \div 200\text{Å in most common semicond.})$$

Thermal de Broglie wavelength, which gives the minimum distance where particles have wavelike properties.

Therefore, to treat particles as classical particles, we need to have potentials that vary slowly over distances comparable to λ_B. If the potential varies rapidly over these distances, then quantum-mechanical reflections occur at the barrier.

- Scattering mechanisms – Consider now the second uncertainty principle, which states that a carrier must stay long enough in a given state to have a well-defined energy. Mathematically this is expressed as:

$$\Delta E \cdot \Delta t \geq \hbar$$

Again, if $\Delta E \sim k_B T$, and if $\Delta \tau \sim \tau$, where τ is average time between scattering events, then

$$k_B T \tau \geq \hbar \Rightarrow \tau \geq \hbar / (k_B T)$$

The mean free path of a thermal carrier is then equal to:

$$l = v\tau \geq \frac{\hbar}{k_B T}\sqrt{\frac{2k_B T}{m^*}} = \frac{\hbar\sqrt{2}}{\sqrt{m^* k_B T}} = 2\frac{\hbar}{\sqrt{2m^* k_B T}} = 2\lambda_B$$

Therefore, for a carrier to have a well defined energy, the mean free path must be longer than the thermal de Broglie wavelength. This is not the case in heavy scattering regime.

- We can also estimate from the energy uncertainty, the operation frequency (limiting values):

$$\Delta E \cdot \Delta t \geq \hbar \Rightarrow \frac{1}{\Delta T} < \frac{\Delta E}{\hbar} \Rightarrow \omega = \frac{2\pi}{T} \leq 2\pi \frac{\Delta E}{\hbar} = \frac{\Delta E}{h}$$

Hence: $\omega \leq \frac{k_B T}{h} \approx 6 \times 10^{12}$ Hz at $T = 300$ K. This value is well below the operating frequency of today's state-of-the-art devices. This example suggests that BTE may still be applicable for future ultra-small devices if some of the quantum-mechanical corrections are accounted for.