Quantum-Mechanical Commentary on LED and OLED Device Properties

Prepared from supplied lecture notes [1] and Nakamura's Nobel Lecture [2]

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Abstract

This four-page note summarizes the essential quantum-mechanical and band-structure principles underlying the operation of inorganic LEDs (GaAs, GaN, InGaN), quantum-well structures, and organic LEDs. It condenses the longer commentary into a concise discussion emphasizing electronic structure, confinement, density-of-states effects, and radiative vs. non-radiative recombination mechanisms.

1 Band Structure and Optical Transitions

In direct-gap semiconductors, conduction-band and valence-band extrema occur at the same crystal momentum. Approximating these bands as parabolic,

$$E_c(\mathbf{k}) \approx E_{c0} + \frac{\hbar^2 k^2}{2m_e^*}, \qquad E_v(\mathbf{k}) \approx E_{v0} - \frac{\hbar^2 k^2}{2m_h^*},$$

the interband transition energy is

$$\hbar\omega = E_g + \frac{\hbar^2 k^2}{2m_r^*},$$

with reduced mass $m_r^{-1} = m_e^{-1} + m_h^{-1}$. This joint dispersion governs emission linewidth and temperature dependence.

The joint density of states (JDOS) for 3D parabolic bands scales as $\sqrt{E - E_g}$, so the spontaneous emission spectrum approximately follows

$$I(E) \propto \sqrt{E - E_g}\, e^{-E/k_B T},$$

producing thermal broadening and characteristic lineshapes observed in LEDs.

2 Confinement: Heterostructures and Quantum Wells

2.1 Double Heterostructure LEDs

The double heterostructure (DH), popularized in GaAs/AlGaAs devices, confines electrons and holes in a thin active layer with a smaller bandgap. This yields:

- **Higher carrier density** in the active region, increasing radiative recombination $R_{\text{rad}} = Bn^2$.
- **Reduced carrier leakage**, improving internal quantum efficiency (IQE).
- **Spatially overlapping wavefunctions**, enhancing optical transition strength.

2.2 Quantum Wells

In quantum wells only nanometers thick, motion in the growth direction is quantized, producing discrete subbands. The 2D JDOS becomes "step-like", sharpening spectral features unless disorder broadening dominates. Confinement also introduces a blue shift:

$$E_{e1} + E_{h1} \propto \frac{\hbar^2 \pi^2}{2} \left(\frac{1}{m_e^*} + \frac{1}{m_h^*} \right) \frac{1}{L^2}.$$

3 InGaN Quantum Wells: Localization and High Efficiency

Nakamura's Nobel Lecture [2] emphasizes a long-standing puzzle: InGaN LEDs remain highly efficient despite extremely high dislocation densities.

A widely accepted explanation is **carrier localization** arising from compositional fluctuations (Indium-rich regions) in $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys. These fluctuations create nanometer-scale potential minima that:

- Trap carriers or excitons, reducing diffusion to non-radiative dislocations.
- Create inhomogeneous broadening and Stokes shifts.
- Maintain high IQE even in imperfect crystals.

This mechanism underpins the remarkable performance of blue InGaN LEDs.

4 Recombination Rates and Efficiency

LED recombination dynamics are often captured by the

$$R = An + Bn^2 + Cn^3$$

model, where:

- A: Shockley–Read–Hall (trap-assisted, non-radiative),
- B: radiative band-to-band recombination,
- C: Auger recombination (three-particle, non-radiative).

The internal quantum efficiency is:

$$\text{IQE} = \frac{Bn^2}{An + Bn^2 + Cn^3}.$$

At moderate carrier densities, the Bn^2 term dominates, but at high density the Cn^3 Auger term causes **efficiency droop**, observed especially in high-power GaN LEDs [3, 4].

5 Polarization Fields in Wurtzite Nitrides

GaN and InGaN materials possess strong spontaneous and piezoelectric polarization fields. In strained quantum wells these fields tilt the bands (quantum-confined Stark effect), leading to:

- Reduced electron–hole overlap (larger radiative lifetime).
- Red-shifted emission.
- Lower efficiency if fields are too strong.

Modern device design uses barrier engineering or semi-polar orientations to mitigate these internal fields.

6 OLEDs: Molecular Picture

Unlike crystalline semiconductors, organic emitters exhibit localized molecular orbitals. The HOMO–LUMO gap determines emission colour, and excitons dominate recombination:

- Excitons can be singlet or triplet.
- Triplet harvesting via phosphorescent dopants or TADF increases efficiency.

- Transport is hopping-like rather than band-like.

Thus OLED physics is governed primarily by molecular electronic structure rather than extended band diagrams.

7 Conclusion

LED and OLED operation can be understood through a compact set of quantum-mechanical principles: band structures, density of states, quantum confinement, recombination kinetics, and disorder effects. InGaN localization and heterostructure engineering enable the high efficiencies that underpin modern solid-state lighting.

References

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[3] J. Iveland, L. Martinelli, J. Peretti, J. S. Speck, and C. Weisbuch. Direct measurement of auger electrons in an ingan led. *Phys. Rev. Lett.*, 110:177406, 2013.

[4] Y.-C. Shen, G. O. Mueller, S. Watanabe, N. Gardner, A. Munkholm, and M. Krames. Auger recombination in ingan. *Applied Physics Letters*, 91:141101, 2007.