

Extending the Quantum Boundary Layer Method to Finite Confinement Potentials

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In quantum-confined systems, thermodynamic properties exhibit nontrivial size dependence due to the quantum nature of particles, a phenomenon known as the quantum size effect. The quantum boundary layer (QBL) framework relates the origin of QSE to the spatial non-uniformity of the quantum-mechanical density distribution even at equilibrium [1]. QBL method not only provides a deeper physical interpretation to QSEs, but also allows one to derive analytical expressions for statistical mechanical quantities that are beyond the conventional QSE corrections that appear in the literature [2,3]. In this paper, we extend this framework to systems with finite boundary potentials, beyond the idealized hard-wall confinement. We start by modeling the system as an infinite well with embedded finite potential regions and interpret thermally activated tunneling as an effective geometric modification of the accessible domain. To show the generality of the method, we demonstrate that it can be extended to different types of systems by applying the same approach to a linear (graded) potential well. We also show that, in certain physically relevant regimes of interest, the analytical framework yields a simple mathematical expression for the thermodynamics of a quantum finite well system. This extended QBL framework preserves the clarity of the original approach while incorporating quantum-tunneling of the particles, enabling analytical estimates of quantum size corrections without explicit spectral calculations.

References:

- [1] A. Sisman, Z.F. Ozturk and C. Firat, "Quantum boundary layer: a non-uniform density distribution of an ideal gas in thermodynamic equilibrium", *Phys. Lett. A*, 362 (1), 12-20, (2007).
- [2] A. Aydın and A. Sisman, "Quantum shape effects and novel thermodynamic behaviors at nanoscale", *Phys. Lett. A*, 383 (7), 655-665, (2019).
- [3] A. Aydın and A. Sisman, "Origin of the quantum shape effect", *Phys. Rev. E*, 108, 024105, (2023).