Abstract

The formalism based on the Wigner function and the Moyal equation provides a natural bridge between classical and quantum descriptions of physical systems, enabling the use of the conceptual apparatus of statistical mechanics for the analysis of quantum phenomena. This work explores and develops entropic methods within the phase-space formalism of quantum theory to investigate the dynamics of so-called "small" systems where quantum effects play a fundamental role.

The central part of this work is the introduction of Wigner-Rényi entropy as a measure of non-classicality of quantum states in the phase-space representation. A rigorous relation between the one-half entropy (for Rényi index $\alpha = 1/2$) and the Kenfack-Życzkowski non-classicality parameter is established, providing a strict physical interpretation of this entropy. Furthermore, the universality of the Wigner-Rényi entropy family for characterizing topological phase transitions in two-dimensional Dirac materials is demonstrated using silicene as an example. A systematic analysis of the dynamics of a family of Schrödinger cat states – even, odd, and Yurke-Stoler states – interacting with a Gaussian potential barrier is performed. Numerical experiments employing the entropic measure of non-classicality allowed to identify the role of initial state symmetry in the scattering process. It is shown that potential parameters can be used to control the degree of non-classicality of quantum states.

In the subsequent sections of this work, the developed methods are applied to a problem in quantum biology – proton tunneling in the adenine-thymine base pair of DNA structure under electromagnetic radiation. Using an effective double-well potential model, phase-space entropic measures, and the Floquet state formalism, it is demonstrated that infrared radiation at a frequency of approximately 15 THz leads to resonant enhancement of tunneling. A correlation between increased non-classicality of the state, as measured by one-half Wigner-Rényi entropy, and enhanced tunneling capability, expressed through the dynamical transmission coefficient based on the Wigner function, is confirmed.

The theoretical results are supported by numerical calculations. A spectral split-operator method for time-independent as well as explicitly time-dependent potentials has been developed and implemented in C++. Moreover, the algorithms for transformation between the density matrix and the Wigner function based on shearing matrix decomposition were developed and applied to formulate an algorithm for solving the self-consistent Moyal-Poisson problem.

Keywords: Wigner-Rényi entropy, non-classicality of quantum states, Wigner function, Moyal equation, phase-space formalism, DNA tautomerization

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