

DISTRIBUTION FUNCTION IN QUANTAL CUMULANT DYNAMICS

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In 1932, Wigner first opened a new field of quantum mechanics described in the phase space of position and momentum. He yielded the proper quantum mechanical marginal distribution function, which has the remarkable property that it can be used to calculate a class of quantum mechanical averages. However, the function cannot be considered a proper probability distribution, because it may take on negative values. For this reason the function has poor correspondence to classical distribution function, and then is sometimes called quasi-probabilities

Recently we derived the coupled equations of motion of cumulants, which we call the quantal cumulant dynamics (QCD) method, based on Heisenberg's equations of motion [1-3]. The key idea is to use a position shift operator acting on a potential operator and the expectation value of the shift operator can be evaluated using cumulant expansion techniques. In the present work, the same scheme is applied to evaluate the quantum distribution function. We analyze the properties of the positive definite distribution function and derive an approximate Liouville equation based on the QCD

[1] H. Miyachi, Y. Shigeta, and K. Hirao, Chem. Phys. Lett. **432**, 582 (2006).

[2] Y. Shigeta, H. Miyachi, and K. Hirao, J. Chem. Phys. **125**, 244102 (2006).

[3] Y. Shigeta, H. Miyachi, and K. Hirao, Chem. Phys. Lett. **443**, 414 (2007)