

Quantum fluctuations sampling by means of classical molecular dynamics

*Alexandre Hernandes Barrozo
Universidade Estadual de Campinas*

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Resumo

We study a new method devised to sample the canonical ensemble [H. Dammak et al., Phys. Rev. Lett. 103, 190601 (2009)], which includes quantum fluctuations by means of classical Molecular Dynamics. This method is based on classical stochastic thermostats, except that it uses colored noise, instead of a white one. We show that, although we have excellent results for the harmonic oscillator case, problems arise while studying anharmonic potentials, in which the method sample distributions that are fundamentally incorrect. A suggestion about where is the problem is given, but no solutions until the moment.