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Classical Representation of a Quantum System at Equilibrium SANDIPAN DUTTA, JAMES DUFTY, University of Florida — A quantum system at equilibrium is represented by a corresponding classical system, chosen to reproduce the thermodynamic and structural properties. The objective is to develop a means for exploiting strong coupling classical methods (e.g., MD, integral equations, DFT) to describe quantum systems. The classical system has an effective temperature, local chemical potential, and pair interaction that are defined by requiring equivalence of the grand potential and its functional derivatives with respect to the external and pair potentials for the classical and quantum systems. Practical inversion of this mapping for the classical properties is effected via the hypernetted chain approximation, leading to representations as functionals of the quantum pair correlation function (similar in spirit to the approach of Dharma-wardana and Perrot [1]). The parameters of the classical system are determined such that ideal gas, weak coupling RPA, and strong coupling pair limits are preserved. The potential advantages of this approach are discussed. Research supported by US DOE Grant DE-SC0002139.

[1] M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. 84, 959 (2000).

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