

Abstract Submitted
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Novel Approach in Statistical Physics for Accurate Multiscale Materials Investigation UDUZEI EDGAL, North Carolina Agricultural and Technical State University — This paper discusses a novel scheme recently developed by the author [(i)Edgal, U. F., J. Chem. Phys. **94**, 8179, 1991; (ii)Edgal, U. F. and Huber, D. L., J. Phys. Chem. B, **108**, 13777, 2004; (iii)Edgal, U. F. and Huber, D. L., accepted for publication in the journal “Physica A”, 2005] for **accurately** determining the free energy of arbitrary equilibrium classical and quantum (material) systems at arbitrary densities, temperatures, and interaction potentials. Nearest neighbor probability density functions are formulated. The scheme allows us avert the “sign” problem usually encountered in Fermion calculations. Extension to mixed systems, as well as a novel ensemble, the “Nearest Neighbor” ensemble, used to effect the computational component of the novel approach are briefly discussed.

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Uduzei Edgal
North Carolina Agricultural and Technical State University

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