Classical representation of Quantum system at equilibrium
Sandipan Dutta and James Dufty
Department of Physics, University of Florida

Overview
• Use classical methods to describe quantum systems.
• Map the thermodynamics of the quantum system onto a classical system.
• Invert the map to solve for the thermodynamic parameters of the effective classical system.
• Exact Limits: ideal Fermi gas; RPA.
• Target systems: jellium, confined charges, DFT.

Some motivation
Previous phenomenological approach by Dharmawardana (Int. J. Quant. Chem. 112, 53-64 (2011))

Formulation of Effective Classical System
Quantum system
\( \beta \langle \mathcal{H} \rangle \) = \(-\beta^2 \ln \sum \phi(x) e^{-\beta \mathcal{H}(x)} \)

Classical system
\( \Omega(\beta, \mu) = -\beta^2 \ln \sum \phi(x) e^{-\beta \mathcal{H}(x)} \)

Thermodynamic parameters/functions
- temperature \( T = \frac{\beta}{k_B} \)
- effective temperature \( T_e = \frac{\beta}{k_B} \)
- local chemical potential \( \mu(\alpha) = -\frac{d}{d\beta} \ln \Omega(\beta, \mu) \)
- effective local chemical potential \( \mu_e(\alpha) = -\frac{d}{d\beta} \ln \Omega(\beta, \mu) \)
- pair potential \( \phi(x) \)
- effective pair potential \( \phi_e(x) \)

Effective temperature
\( T_e = \frac{\beta}{k_B} \)

Effective pair potential
\( \beta \phi_e(r) \) = \( \beta \phi(r) \) + \( \Delta(r) \)

Effective temperature
\( \frac{\beta_e}{\beta} = \frac{n}{\beta} \left( \frac{1}{2} \right) \exp \left( \frac{1}{\beta} \int dr \phi_e(r) \right) \)

We replace all classical \( n, \phi_e \) by quantum \( n, \phi \) using the map

Ideal Fermi gas

Effective pair potential
\( \beta \phi_e(r) = \beta \phi(r) + \Delta(r) \)

Uniform jellium: RPA limit
Construction of effective interaction
\( \beta \phi_e(r) = \beta \phi(r) \) + \( \Delta (r) \)

Weak coupling limit:
\( e^{-\beta \phi(r)} \) \( \rightarrow \) \( e^{-\beta \phi(r)} \) \( = \) \( e^{\phi(r)} \) \( = \) \( e^{\phi(r)} \)

Degenerate limit:
\( \beta \phi_e(r) \) \( \rightarrow \) \( \beta \phi(r) \) \( \rightarrow \) \( \beta \phi(r) \)

LDA (Thomas-Fermi)

Density profile of confined systems using HNC approximation
\( \rho(r) = \frac{\rho^{(0)}(r)}{1 + \exp \left( \frac{\beta E_{\text{eff}}(r)}{k_B T_e} - 1 \right) \exp \left( \frac{1}{\beta} \int dr \phi_e(r) \right) \}

Under the assumption of uniform correlations and zeroth order in the map:

Approximate density profile
\( \rho(r) = \frac{\rho^{(0)}(r)}{1 + \exp \left( \frac{\beta E_{\text{eff}}(r)}{k_B T_e} - 1 \right) \exp \left( \frac{1}{\beta} \int dr \phi_e(r) \right) \}

Summary
• Defined a classical system that is exact for two limits: non-interacting and weakly interacting Fermi systems.
• Pair correlations for jellium can be calculated using the map and HNC at all temperatures.
• Density profile for confined charges can also be obtained from the map.

References: