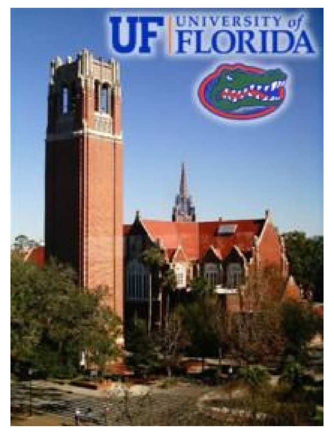


Classical representation of Quantum system at equilibrium

Sandipan Dutta and James Dufty

Department of Physics, University of Florida

Overview

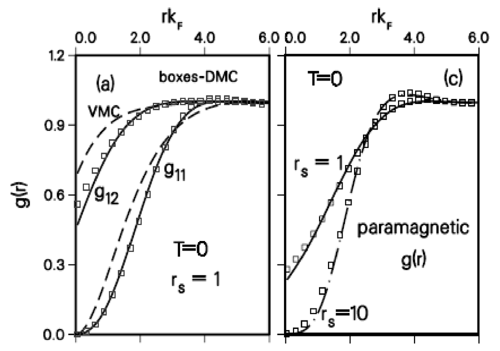
- **Use classical methods to describe quantum systems.**
- **Map the thermodynamics of the quantum system onto a classical system.**
- **Invert the map to solve for the thermodynamic parameters of the effective classical system.**
- **Exact Limits : ideal Fermi gas; RPA.**
- **Target systems: jellium,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

Some motivation

Previous phenomenological approach by Dharma-wardana (Int. J. Quant. Chem. 112, 53-64 (2011))

$$V(r)=\Phi^{(0)}(r)+\frac{e^2}{r}\left(1-e^{-r/\lambda_{cf}}\right)$$

$$T_c=\sqrt{T^2+T_{cf}^2}$$



Formulation of Effective Classical System

Quantum system	Classical system
Grand potential	
$\Omega(\beta\mid\mu)=-\beta^{-1}\ln\sum_N Tr_N\, e^{-\beta\left(K+\Phi-\int d\mathbf{r}\mu(\mathbf{r})\widehat{n}(\mathbf{r})\right)}$	$\Omega_c(\beta_c\mid\mu_c)=-\beta_c^{-1}\ln\sum_N\frac{1}{\lambda_c^{3N}N!}\int d\mathbf{q}_1..d\mathbf{q}_N e^{-\beta_c\left(\Phi_c-\int d\mathbf{r}\mu_c(\mathbf{r})\widehat{n}(\mathbf{r})\right)}$
Thermodynamic parameters/functions	
temperature $\beta=1/K_B T$	*effective temperature* β_c
local chemical potential $\mu(\mathbf{r})\equiv\mu-\phi_{ext}(\mathbf{r})$	*effective local chemical potential* $\mu_c(\mathbf{r})\equiv\mu-\phi_{c,ext}(\mathbf{r})$
pair potential $\phi(q_{ij})$	*effective pair potential* $\phi_c(q_{ij})$

The Map

$$\Omega_c(\beta_c\mid\mu_c)\equiv\Omega(\beta\mid\mu)$$

$$\frac{1}{\beta_c}\frac{\delta\Omega_c(\beta_c\mid\mu_c)}{\delta\phi_c(\mathbf{r},\mathbf{r}')}=\frac{1}{\beta}\frac{\delta\Omega(\beta\mid\mu)}{\delta\phi(\mathbf{r},\mathbf{r}')}\qquad\frac{\delta\Omega_c(\beta_c\mid\mu_c)}{\delta\mu_c(\mathbf{r})}\Big|_{\beta_c,\phi_c}\equiv\frac{\delta\Omega(\beta\mid\mu)}{\delta\mu(\mathbf{r})}\Big|_\beta$$

Interpretation of the map

$$p_c(\beta_c\mid\mu_c)\equiv p(\beta\mid\mu)$$

$$g_c(\mathbf{r},\mathbf{r}';\beta_c\mid\mu_c)\equiv g(\mathbf{r},\mathbf{r}';\beta\mid\mu)\qquad n_c(\mathbf{r};\beta_c\mid\mu_c)\equiv n(\mathbf{r};\beta\mid\mu)$$

Inversion of the Map

Effective pair potential

$$\beta_c\phi_c(\mathbf{r},\mathbf{r}',\beta_c|n_c,g_c)=-\ln(g_c(\mathbf{r},\mathbf{r}'))+\int d\mathbf{r}''\left(g_c(\mathbf{r},\mathbf{r}'')-1\right)n_c(\mathbf{r}'')c_c(\mathbf{r}'',\mathbf{r}')$$

$$(g_c(\mathbf{r},\mathbf{r}')-1)=c_c(\mathbf{r},\mathbf{r}')+\int d\mathbf{r}''\left(g_c(\mathbf{r},\mathbf{r}'')-1\right)n_c(\mathbf{r}'')c_c(\mathbf{r}'',\mathbf{r}')$$

Effective local chemical potential

$$\beta_c\mu_c(\mathbf{r},\beta_c|\rho_c,g_c)=-\ln(n_c(\mathbf{r})\lambda_c^3)-\int d\mathbf{r}''n_c(\mathbf{r}'')c_c(\mathbf{r},\mathbf{r}'')$$

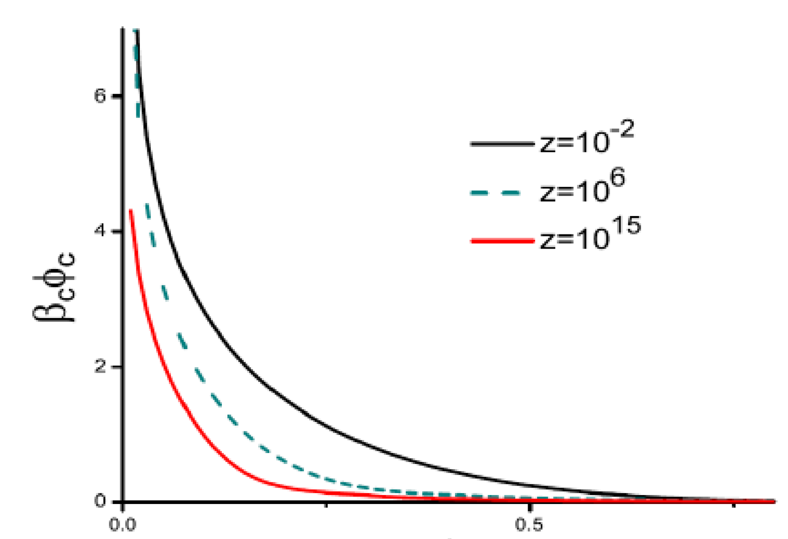
Effective temperature

$$\frac{\beta_c}{\beta}=\frac{n}{\beta p}\left(1-\frac{2\pi}{3}n\int_0^\infty drr^3\left(g(r)-1\right)\frac{d\beta_c\phi_c(r)}{dr}\right)$$

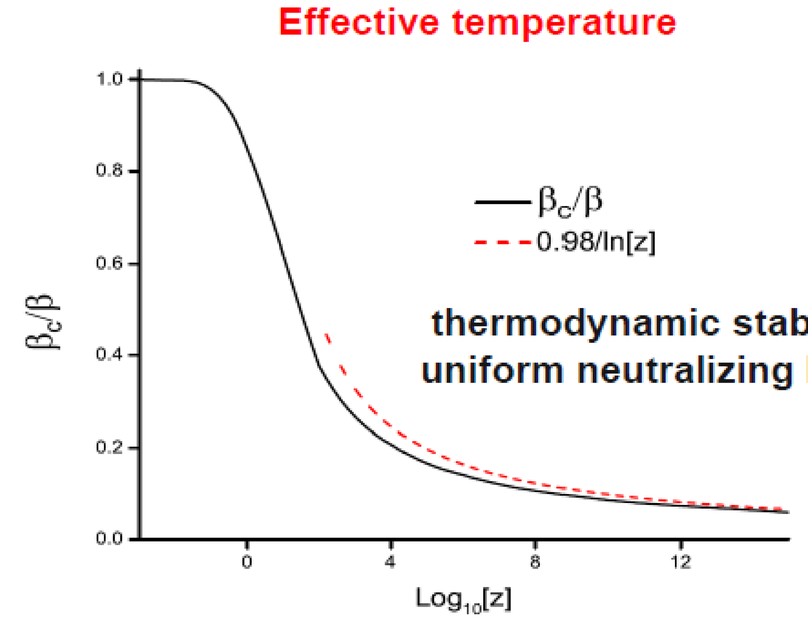
We replace all classical n_c, g_c by quantum n, g using the map

Ideal Fermi gas

Effective pair potential



Effective temperature



thermodynamic stability needs a uniform neutralizing background

Peculiarity of the thermodynamics

$$E_c=\frac{\partial\beta_c p_c V}{\partial\beta_c}\Big|_{z_c,V}\neq\langle H\rangle_c$$

$$E_c\overset{?}{=}E=\frac{\partial\beta pV}{\partial\beta}\Big|_{z,V}=\left\langle\widehat{H}\right\rangle=\frac{3}{2}pV$$

Internal Energy

$$E_c=\left(\frac{3}{2\beta_c}+n_c\frac{1}{2}\int d\mathbf{r}\frac{\partial\beta_c\phi_c(r)}{\partial\beta_{cl}}\Big|_{r,z_c}\left(g_c(r)-1\right)\right)=\frac{3}{2}p_cV$$

Uniform jellium:RPA limit

Construction of effective interaction

$$\beta_c\phi_c(\mathbf{r})=\left(\beta_c\phi_c(\mathbf{r})\right)^{(0)}+\Delta(\mathbf{r})$$

weak coupling limit:

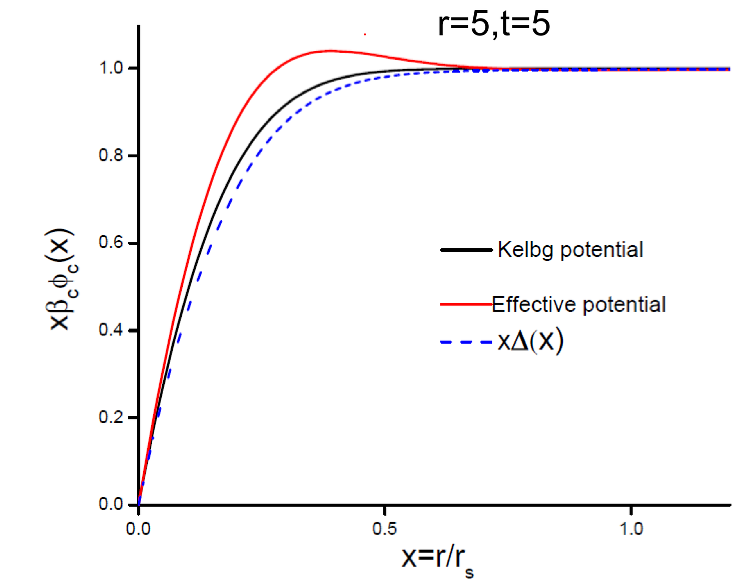
$$c(\mathbf{r})\rightarrow c^{RPA}(\mathbf{r})=-\beta_c\phi_c(\mathbf{r})=c^{(0)}(0)+\Delta^{RPA}(\mathbf{r})$$

$$\beta_c\phi_c(\mathbf{r})\simeq\left(\beta_c\phi_c(\mathbf{r})\right)^{(0)}-\left(c^{RPA}(\mathbf{r})-c^{(0)}(\mathbf{r})\right)$$

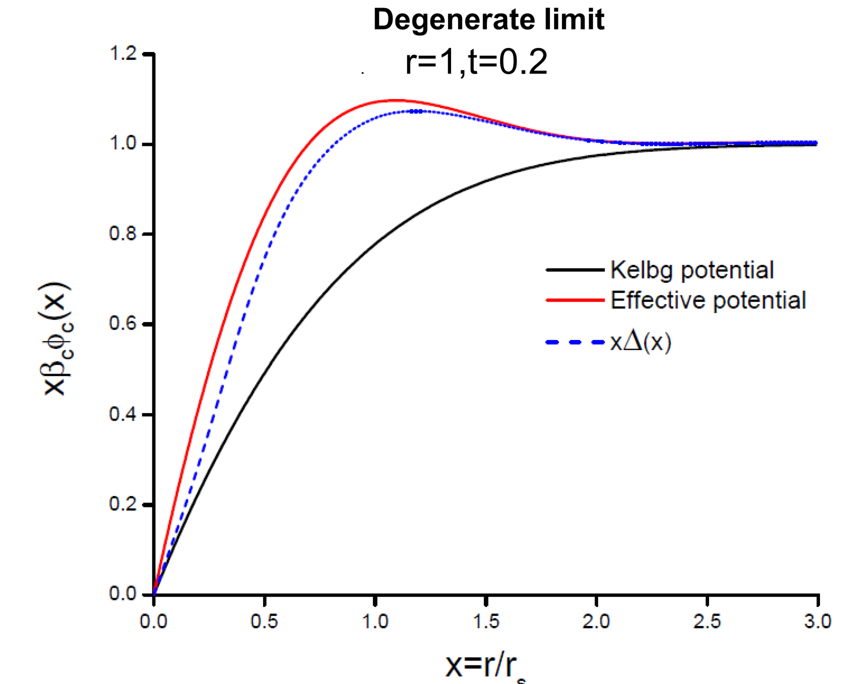
$$=-\ln(g^{(0)}(\mathbf{r}))+g^{(0)}(\mathbf{r})-1-c^{RPA}(\mathbf{r})$$

Weak Coupling, low density limit of the effective potential $\beta_c\phi_c(r)\underset{z<<1}{\rightarrow}$ Kelbg

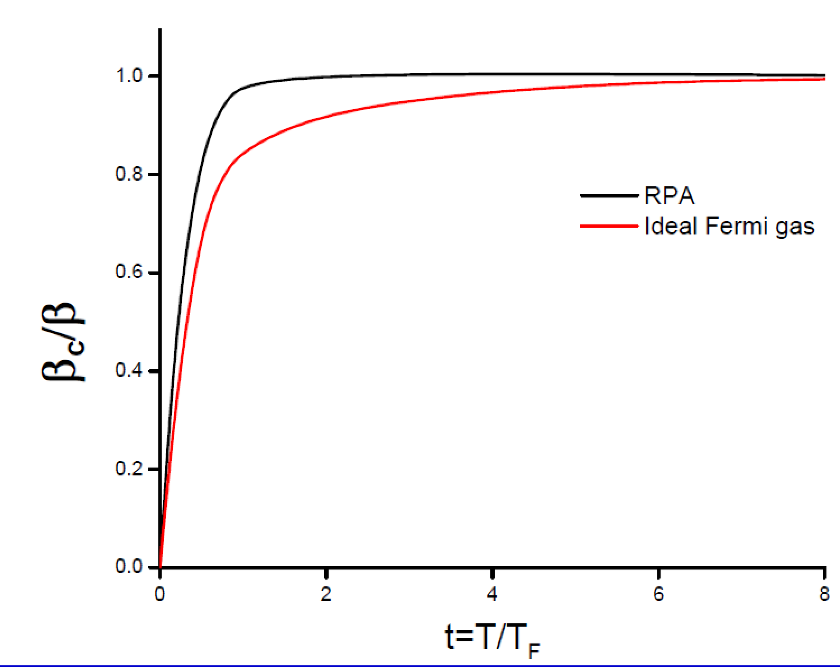
Non-degenerate limit
r=5,t=5



Degenerate limit
r=1,t=0.2



Effective temperature

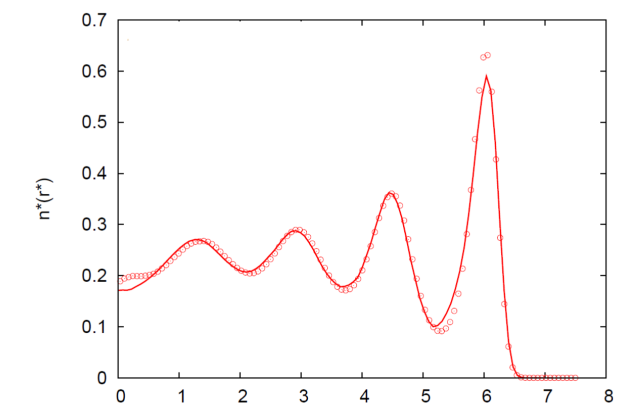


Confined systems

Density profile of confined systems using HNC approximation

$$ln\left(n_c(\mathbf{r})\lambda_c^3\right)=\beta_c\mu_c(\mathbf{r})+\int d\mathbf{r}'c_{RPA}(|\mathbf{r}-\mathbf{r}'|)n_c(\mathbf{r}')$$

Classical correlations showing shell formation ([4])



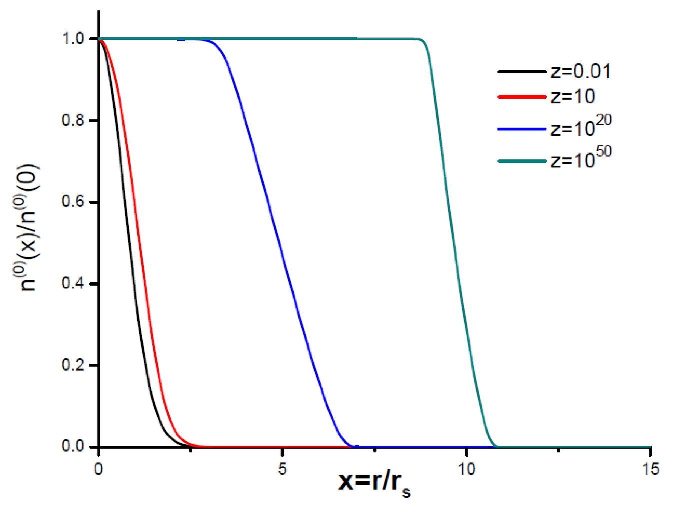
Under the assumption of uniform correlations and zeroth order in the map:

Approximate density profile

$$n(\mathbf{r})=n^{(0)}(\mathbf{r})\left(\frac{\beta_c^{(0)}}{\beta_c}\right)^{3/2}exp\left(\int d\mathbf{r}'\left(c_{RPA}(|\mathbf{r}-\mathbf{r}'|)n(\mathbf{r}')-c^{(0)}(|\mathbf{r}-\mathbf{r}'|)n^{(0)}(\mathbf{r}')\right)\right)$$

LDA (Thomas-Fermi)

$$n^{(0)}(\mathbf{r})=\int\frac{d\mathbf{k}}{(2\pi)^3}e^{-i\mathbf{k}\cdot\mathbf{r}}\left(e^{\beta(\epsilon_k-\mu^{(0)}(\mathbf{r}))}+1\right)^{-1}$$



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.
- Reference: Dufty and Dutta, Contrib. Plasma Phys., 2012 (in press)

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(2) A. V. Filinov, V. O. Golubnychiy, M. Bonitz, W. Ebeling, and J. W. Dufty, Phys. Rev. E 70, 046411 (2004)

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(4) J. Wrighton, J. W. Dufty, H. Kählert, and M. Bonitz, Phys. Rev. E 80, 066405, (2009)