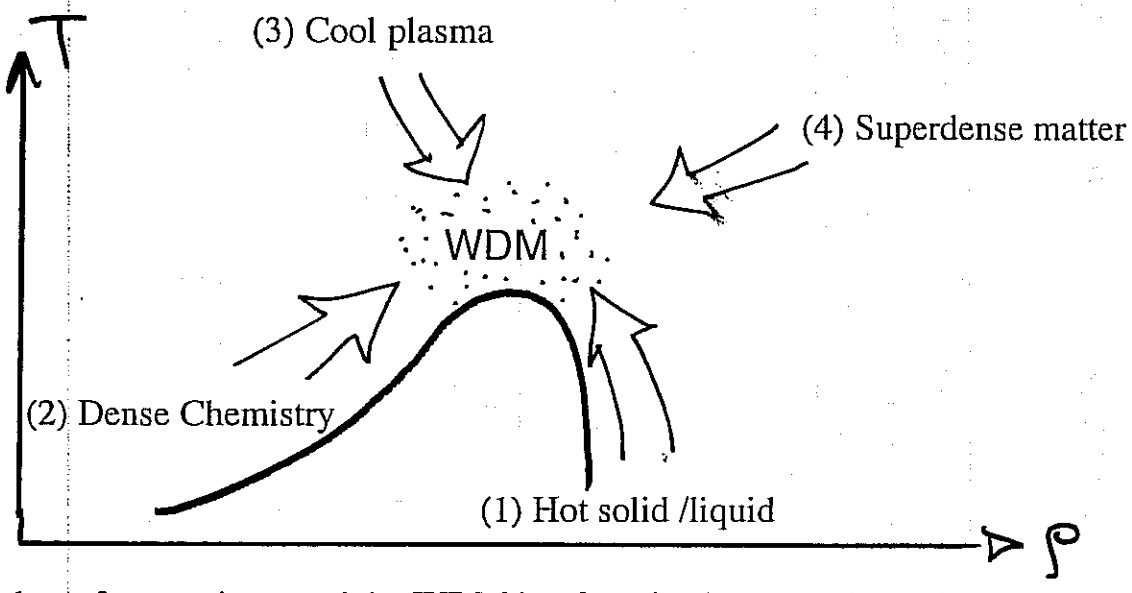
Lectures on Warm Dense Matter (Brief notes)

Richard More, participating guest, LBNL
Research collaborators:
UCB/LBNL - J. Wurtele
VNL/LBNL - F. Bieniosek, P. Ni and G. Logan
VNL/LLNL - J. Barnard, A. Friedman
SNLA - M. Desjarlais, T. Mattson, M. Knudson
LLNL - F. Graziani, J. Glosli, F. Streitz, L. Benedict, M. Surh
LANL - M. Murillo
UEC - H. Yoneda

PLAN FOR THE TALKS:

1.) WDM and Hot Solids
2.) WDM and Hot Dense Chemistry
3.) WDM and Cool Plasmas
4.) WDM and Superdense Matter
5.) Unknowns and Mysteries in WDM

WDM occupies the center of the (ρ, T) plane



At least for certain materials, WDM is a **barrier** between the regions.

(1) SOLID STATE	(2) DENSE CHEMISTRY	(3) LOW-T PLASMA	(4) DENSE MATTER
What's there?			
o Lattice of bonded atoms atomic vibration=sound waves o Some electrons free to move	o Free atoms and molecules molecular vibration, rot'n o ± ions, molec. ions	o Free electrons o Multicharge ions Weak long-range correlations	o Electron Fermi liquid weakly perturbed by ion cores
Equilibrium state			
Phonons - Planck function Electrons - Fermi-Dirac	o reaction equilibrium A + B <---> AB	Saha Ionization equilibrium Plasma wave modes Maxwellian e^-, ions photons?	Fermi-Dirac electrons, strongly correlated ions
Nonequilibrium			
Stress-strain; yield & flow Conduction (heat, current) Diffusion of lattice defects Temperatures for modes	% of reaction Nonlinear reaction kinetics Chain reactions, catalysis	T_e, T_i, T_R Strong currents or beams -> instabilities "Collective" damping	Supernova ignition shock (transient phenomena)
Difficulties:			
Bands ==> atomic levels ee interaction > level spacing	Pressure effect on molecules Clusters molecules --> fluid	$N\lambda^3$ is not large in WDM Coulomb log Λ --> 0 Onset of quantum effects Pressure effect on atoms	Superdense theory based on E_F >> (everything) Ion sphere model Both these fail for WDM

BARRIERS: ***Why do the main theories of matter fail at WDM conditions?***

1.) **Solid** ==> Liquid ==> expanding fluid
rising T

Electron energy-bands totally change .

Small band-gaps --> correlation is important --> problem for codes, theory

2.) **Dense chemistry** ==> Dense fluid
rising density

Pressure effect on molecules .

e.g., 2 N <--> N_2

have $[N]^2 / [N_2] = \text{const}/\lambda_a^3 \exp(-E_B/kT) = f(T)$

Then $[N]/[N_2] = f(T)/[N]$ falls with rising density ==> 100% molecules

Usually that's not the right answer at high density:

most solids don't contain molecules.

(Actually, nitrogen still has molecules in the solid state.)

3.) **Low-temperature plasmas** have two well-known problems:

At low T, usual plasma theory becomes invalid

$N\lambda_D^3$	falls to	≤ 1
$\log \Lambda$	falls to	≤ 0

More important, neutral atoms and molecules are dominant;
so plasma theory doesn't talk about what's really there.

4.) **Superdense matter** = Electron Fermi gas + (nuclei or + ion cores)

Theory & codes: E_F >> everything else
neutral ion spheres (high Γ ions)

need high density

QEOS, INFERNO give predictions for WDM, but QMD is more believable.

Unknown properties of matter in WDM regime:

Specific parameters:

$\boxed{\text{EOS}}$ { $p(\rho, T)$, $E(\rho, T)$ } --> [Sound-speed Specific heat]

Critical point ρ_c, T_c, p_c Two-phase boundary $T_{2\Phi}(\rho)$ vapor pressure $p_{vap}(T)$

Latent heat of evaporation $L(T)$ Liquid metal surface tension σ

loss of strength near melting [Viscosity of liquid]

Evaporation rate for dense gas -- "sticking coefficient α"

Electron thermionic emission -- Work function $\Phi(T)$

Electron-ion energy-exchange time τ_{ei} ==> nonequilibrium EOS? $p(\rho, T_e, T_i)$

o Electrical conductivity $\sigma(\rho, T)$ Thermal conductivity $\kappa(\rho, T)$

o AC dielectric function $\varepsilon(\rho, T, \omega)$ --> [X-ray absorption opacity]

o dE/dx for hot targets $L(\rho, T, E)$ (secondary electron yield)

Phenomena:

Metal-insulator transition. Other phase transition?

Rapid change of properties (= "transition") - gradual? rapid? sharp?

Plasma composition? (large molecules? Clusters? Negative ions?)

Magnetic properties? Mixed nuclear/atomic properties?

"Fancy properties": $g(r)$, $S(k)$, $S(k,\omega)$, $\varepsilon(k, \omega, \rho, T)$, ...

[These are directly observable in certain experiments]

NOT everything is equally unknown

Theoretical relations between parameters, some "exact", some are rough approximations

Comprehensive theoretical models give approximate values for some of the parameters

Applications

This list is probably incomplete - it omits things I didn't think of - and at the same time over-complete - it probably includes a number of applications that haven't happened or may never happen. No need to argue, only need to work hard to make the dreams come true.

1.) Applications of data for solids at high temperatures:

Electrical properties and hydro of early evaporation flow:

- Pulsed power technology
- fuses and detonators
- Switches for large currents
- Exploding wires as sources of radiation
- Hot wires as filaments, electron sources

Mechanical, chemical and optical properties:

- Laser machining, cutting, hardening ("laser peening")
- Hot work, control of microstructure, defense against oxydation
- Materials that resist high temperatures
  - Turbine blades
  - Confinement vessels for hot chemistry
  - Re-entry vehicles
  - Fusion reactor wall materials
    - Divertor strike-plate, limiter (scrape-off layer)
  - Diagnostic survival for fusion reactors
- Defense against laser weapons

Dreams or conjectures:

- Metal-insulator switching behavior in WDM
- High-temperature semiconductors
- High-current semiconductors

2.) Applications of WDM chemistry:

- Ultra-high temperature chemistry?
- Combustion science: droplets have high surface area.
- Radioisotope chemistry?
- Detonation of solid explosives - study individual molecules?

High-T semiconductors?

3.) Applications of low-T plasma science:

Exploding wires

Z-pinches, discharges

EUV source research

MFE - Edge plasmas, divertor, response to disruption

ICF Preheat dynamics of ICF targets

ICF - laser debris formation and damage to optics

Low-energy plasmas

MHD devices

Plasma processing

microplasmas in plasma displays

4.) Applications for data on super-dense mattter

Interpretation of shock-release experiments

Models for planetary interiors

Models for Impacts, explosions

Explosive forging and fabrication technology

APPROXIMATE OUTLINE OF LECTURES

1.) WDM and hot solid/liquid matter

Dulong-Petit law (high-T specific heats of solids)

$C_v \sim 3$ eV/eV-atom

Debye lattice specific heat

Gruneisen law (pressure of heated solid)

$p = p_o(\rho) + \gamma \rho \delta E_{thermal}$ γ = Gruneisen parameter

Lindemann law (melting temperature)

$T_{melt} = \alpha \Theta_D^2/\rho^{2/3}$ $\alpha \sim 0.5 A^{5/3}$

Boiling temperature $T_B \sim 1.7\text{-}2\, T_{melt}$

Latent heats:

Melting $L_m \sim kT_m$ per atom

Evaporation $L_B \sim 10\, kT_B$ per atom

Cohesive energy $\sim L_B$

Drude conductivity law

Surface tension σ versus cohesive energy

Deep ideas from solid-state physics

2.) WDM and hot dense chemistry

Van der Waals' gas law

VdW critical point

Comparison to H_2O EOS

Chemical equilibrium

Virial expansion (GCE statistical mechanics)

Pressure effect on molecules

3.) WDM and low-temperature plasmas

Plasma parameter $\boldsymbol{N}$

$\boldsymbol{N} = 4\pi/3\, n D^3 \sim T^{3/2} / n^{1/2}$

Coulomb logarithm $\log \Lambda$

Plasma coupling parameter Γ

$\Gamma = Z^2e^2/R_o kT$ $\boldsymbol{N} = 1/(3\Gamma)^{3/2}$

Drude (Spitzer) conductivity
Ellipsometry

4.) WDM and superdense matter

Fermi gas, Chandrasekhar EOS
Thomas-Fermi EOS (FMT)
QEOS
QM cell model

5.) WDM - unknowns and mysteries

Black glass
Electronegative plasmas
Localization and MI transition
Ionic materials at high T
Inner shell shell-crossing
Questions about WDM

R. More, Notes on lattice dynamics

Debye theory of monatomic solid

assume constant sound speed $\omega = c_s\, k$

density of phonon states per gram $g(\nu) = \dfrac{9}{AM_p \nu_D^3}\nu^2$

$$h\nu_D = \hbar\omega_D = k\Theta_D$$

Ion free energy:

$$\delta F_{ions} = \int_0^{\nu_D} g(\nu)\left\{\frac{h\nu}{2} + kT\log(1 - e^{-h\nu/kT})\right\} d\nu$$

Ion thermal vibration energy $u = \Theta_D/T$

$$\delta E_{ion} = \frac{9k\Theta_D}{8AM_p} + \frac{9k\Theta_D}{AM_p}\left(\frac{1}{u^3}\int_0^u \frac{x^3 dx}{e^x - 1}\right) \sim \frac{3kT}{AM_p}$$

Gruneisen pressure formula

$$\delta p_{ion}(T) = \gamma_s\ \rho\ \delta E_{ion}(T)$$

δp_{ion} = pressure of lattice vibrations (phonon gas)

$\gamma_s = \dfrac{\partial \log \Theta_D}{\partial \log \rho}$ Gruneisen parameter $\sim$ 0.5 to 2

Quantum theory of lattice dynamics

$$\bar{R} = \ell_1\bar{a}_1 + \ell_2\bar{a}_2 + \ell_3\bar{a}_3 + \delta\bar{R}$$

$$M\frac{d^2}{dt^2}\delta R_\alpha(\ell) = -\sum_{\beta,\ell'}\left[\frac{\partial^2\Phi}{\partial R_\alpha(\ell)\partial R_\beta(\ell')}\right]\delta R_\beta(\ell')$$

Lattice vibration normal modes in perfect crystal

$$\delta R_\alpha(\ell) = e_\alpha(k)\, e^{i\vec{k}\cdot\vec{R}(\ell)-i\omega t}$$

$$D_{\alpha\beta}(\vec{k}) \equiv \frac{1}{M}\sum_\ell \left[\frac{\partial^2\Phi}{\partial R_\alpha(\ell)\partial R_\beta(0)}\right] e^{i\vec{k}\cdot\vec{R}(\ell)}$$

$$\sum_\beta \left(D_{\alpha\beta}(k)-\omega^2\delta_{\alpha\beta}\right) e_\beta = 0$$

Phonon creation-annihilation operators

$$\delta R_\alpha(\ell) = \sum_{s=k,\lambda}\left(\frac{\hbar}{2MN\omega_s}\right)^{1/2} e_\alpha(s)\left\{a_s e^{ik\cdot R(\ell)} + a_s^+ e^{-ik\cdot R(\ell)}\right\}$$

$$\left[a_s^+, a_{s'}\right] = -\delta_{s,s'} \qquad\qquad H = \sum_s \hbar\omega_s\left[a_s^+ a_s + \tfrac{1}{2}\right]$$

$$\delta\dot{R}_\alpha(\ell) = \sum_{s=k,\lambda}\left(\frac{\hbar\omega_s}{2MN}\right)^{1/2} e_\alpha(s)\left\{-a_s e^{ik\cdot R(\ell)} + a_s^+ e^{-ik\cdot R(\ell)}\right\}$$

Photons and phonons are quite similar, perhaps we should underline the differences:

Photons -

constant speed of light
relativistic invariance
2 polarizations (spin = 1, mass = 0)

A is not observable (gauges)
nearly linear field equations

Phonons -

a natural rest frame
crystal symmetry group
3 polarizations
longitudinal and transverse
accoustic and optical phonons
δR is purely mechanical
nonlinear - "anharmonic"
Umklapp processes

Phonon second quantization is just ordinary quantum mechanics.

Thermodynamics:

First and second laws of thermodynamics: $dE = dQ - dW$

E = "Energy" function, "Heat" $dQ = T\,dS$, "Mechanical work" $dW = p\,dV$

2 basic independent variables, e.g., density ρ, temperature T

Energy	$E(S, V)$	$dE = T\,dS - p\,dV$
Helmholtz free energy	$F(T, V) = E - T\,S$	$dF = -S\,dT - p\,dV$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \qquad p = -\left(\frac{\partial F}{\partial V}\right)_T \qquad \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V$$

F = min for fixed N, T, V

Gibbs free energy	$G(T, p) = E - T\,S + p\,V$	$dG = -S\,dT + V\,dp$
Enthalpy	$H(S, p) = E + pV$	$dH = T\,dS + V\,dp$

Liquid-vapor thermodynamics:

Below the **critical temperature** T_{crit} there are two phases,
Thermal equilibrium ==> equal temperature
Mechanical equilibrium ==> equal pressure

$$p_{vap}(T) = p_{liq}(T) = \textbf{vapor pressure}$$

Evaporate/condense equilibrium ==> equal Gibbs free energy (per gram)

$$G_{vap}(p_s, T) = G_{liq}(p_s, T) \quad \text{<-- equivalent to Maxwell construction}$$

To convert liquid to vapor it is necessary to add the **latent heat** of vaporization

$$L(T) = \Delta E + p\Delta V = T\,(S_{vap} - S_{liq})$$

$\Delta G = \Delta E - T\Delta S + p\Delta V$ is zero when liquid changes to vapor.

Maxwell construction and two-phase fluids

Maxwell construction is equivalent to "equal T, equal p, equal G"

For a liquid-vapor mixture, volume V, energy E, and entropy S are linear combinations of liquid and vapor properties, which depend only on the temperature T.

x = liquid mass fraction

$$E(\text{mixture}) = x\,E_{liquid} + (1-x)\,E_{vapor}$$
$$S(\text{mixture}) = x\,S_{liquid} + (1-x)\,S_{vapor}$$
$$V(\text{mixture}) = x\,V_{liquid} + (1-x)\,V_{vapor}$$

The density $\rho_{mix} = 1/V_{mix}$ is not a linear combination.

Formula for sound speed in the 2-phase region:

$$\frac{1}{\rho^2 c_s^2} = \frac{x}{\rho_\ell^2 c_s^2[\ell]} + \frac{1-x}{\rho_g^2 c_s^2[g]}$$

$c_s[l]$, $c_s[g]$ are evaluated *just inside* the 2-phase boundary ≠ the values outside.

Clausius-Clapeyron equation is an exact thermodynamic relation:

$$\frac{dp_s}{dT} = \frac{(S_{vap} - S_{liq})}{(V_{vap} - V_{liq})}$$

==> Test for an EOS

Water - the critical point

Above the critical point, *no difference* between steam and water.

ρ_{crit} = **0.317 gm/cm³**

T_{crit} = **374.15 C = .05578 eV**

p_{crit} = **218.2 atm = 22.09 J/cm³**

E_{crit} = **2.032 kJoule/gram** (relative to liquid water)

S_{crit} = **4.435 J/g-C**

The critical density is about a third of the normal density of liquid water.

The critical temperature is above the normal boiling temperature (= 100 C)

$$\frac{p_c}{(n_c k T_c)} = 0.23394$$

Water is *not* an ideal gas at the critical point.

Van der Waals' gas law

pressure $$p = \frac{\rho kT}{AM_p(1-b\rho)} - a\rho^2$$

Energy/mass $$\varepsilon = \frac{3}{2}\frac{kT}{AM_p} - a\rho$$

Entropy/mass $$S = \frac{k}{AM_p}\log\left(AM_p\frac{1-b\rho}{\rho\lambda^3}\right)$$

Thermal deBroglie wavelength

Helmholtz free energy $$F = \varepsilon - TS$$

$$\lambda = \sqrt{\frac{h^2}{2\pi AM_p kT}}$$

Parameters a, b are determined by atomic mass A, solid density ρ_{sol}, critical temperature T_c.
The VdW EOS is unsatisfactory at or above solid density.

Critical-point parameters for Van der Waals' gas law:

Critical density, temperature $$\rho_c = \frac{1}{3b} \qquad kT_c = \frac{8a}{27b}AM_p$$

Critical pressure, energy/mass $$p_c = \frac{a}{27b^2} \qquad \varepsilon_c = \frac{a}{9b}$$

$$\frac{p_c}{(n_c kT_c)} = \frac{3}{8} = 0.3750$$

Note - VdW Energy is zero for cold, zero-density gas.

LTE neutral gas - virial expansion

$\beta = 1/kT$

N-atom classical partition function

$\lambda = \sqrt{h^2 / 2\pi mkT}$

$$Z_{(N)} = \frac{1}{N!} \int d^{3N}P_i \; d^{3N}R_i \; e^{-\beta H} = \frac{1}{N!} \frac{1}{\lambda^{3N}} \int d^{3N}R_i \prod_{(ij)} \left(1 + f_{ij}\right)$$

u(r) = interatomic potential, f = Mayer f-function:

$$e^{-\beta u\left(\left|\vec{R}_i - \vec{R}_j\right|\right)} \equiv 1 + f_{ij}$$

Then

$$\int d^{3N}R_i \prod_{(ij)} \left(1 + f_{ij}\right) = \sum_D N_D \; W_D$$

where

D = unlabeled N-atom bond-diagram
N_D = Number of diagrams of type D
W_D = integral of f's in diagram D

Resolve each bond diagram D into linked clusters Γ:

$$D = \sum_\Gamma \nu_\Gamma \Gamma = \nu_0 \Gamma_0 + \nu_1 \Gamma_1 + \ldots$$

$$W_D = \prod_\Gamma \left(V W_\Gamma\right)^{\nu_\Gamma}$$

Γ = Linked-cluster graph
ν_Γ = number of times that Γ appears in D ($\nu_\Gamma = 0, 1, 2, \ldots$)
n_Γ = number of atoms involved in Γ

$$W_\Gamma = \frac{1}{V} \int d^3R_1 \cdots d^3R_{n_\Gamma} \left[f_{ij} \cdots f_{kl}\right]$$

The number of N-atom diagrams of type D is

$$N_D = \frac{N!}{\prod_{\Gamma \in D} \left(\nu_\Gamma!\ S_\Gamma^{\nu_\Gamma} \right)}$$

where

$N!$ = total number of assignments of labels to D
$\nu_\Gamma!$ = correction for ν_Γ equivalent linked graphs Γ
S_Γ = number of symmetries of Γ,
correction for equivalent ways to label Γ

Then

$$Z_{(N)} = \frac{1}{\lambda^{3N}} \sum_D \prod_{\Gamma \in D} \frac{1}{\nu_\Gamma!} \left(\frac{VW_\Gamma}{S_\Gamma} \right)^{\nu_\Gamma}$$

this looks simple but the sum is constrained by $N = \sum_\Gamma n_\Gamma \nu_\Gamma$

Relax the constraint by using the Grand Canonical ensemble,

Adjust chemical potential μ to get the correct number density.

$$Q = \sum_{N=0}^{\infty} e^{\frac{\mu N}{kT}} Z_{(N)} = \sum_N \sum_D \prod_{\Gamma \in D} \left\{ \frac{1}{\nu_\Gamma!} \left(\frac{VW_\Gamma}{S_\Gamma \lambda^{3n_\Gamma}} e^{\beta \mu n_\Gamma} \right)^{\nu_\Gamma} \right\}$$

$$= \prod_\Gamma \sum_{\nu_\Gamma=0}^{\infty} \frac{1}{\nu_\Gamma!} \left(\frac{VW_\Gamma}{S_\Gamma} \frac{e^{\beta \mu n_\Gamma}}{\lambda^{3n_\Gamma}} \right)^{\nu_\Gamma}$$

$$= \prod_\Gamma \exp\left(\frac{VW_\Gamma}{S_\Gamma} \frac{e^{\beta \mu n_\Gamma}}{\lambda^{3n_\Gamma}} \right)$$

The point is that every possible diagram D is constructed automatically by multiplying together the linked clusters.

Thermodynamic functions are easily obtained, e.g.,

$$\frac{pV}{kT} = \log_e Q = \sum_\Gamma \frac{VW_\Gamma}{S_\Gamma}\left(\frac{e^{\beta\mu}}{\lambda^3}\right)^{n_\Gamma}$$

$$n = \frac{kT}{V}\frac{\partial}{\partial\mu}\log Q = \sum_\Gamma n_\Gamma \frac{W_\Gamma}{S_\Gamma}\left(\frac{e^{\beta\mu}}{\lambda^3}\right)^{n_\Gamma}$$

FIRST FEW LINKED CLUSTER GRAPHS:

Graph	n_Γ	S_Γ	W_Γ
Γ_0	1	1	$W_0 = 1$
Γ_1	2	2	$W_1 = \int f(r)d^3r$
Γ_2	3	2	$W_2 = W_1^2$
Γ_3	3	3!	$W_3 = \int f(r)f(r')f(r-r')\ d^3r\ d^3r'$

$$\frac{1}{\lambda^3}e^{\beta\mu} = n\left(1 - W_1 n + \tfrac{1}{2}(W_1^2 - W_3)n^2 + \ldots\right)$$

$$p = n\,kT\left(1 - \frac{W_1}{2}n - \frac{W_3}{3}n^2 + \ldots\right)$$

The expansion in powers of density is the **Virial expansion**.

Thomas-Fermi EOS

o A key paper on EOS of hot-dense matter:
Feynman, Metropolis & Teller, Phys. Rev., 1949

o FMT introduced the ***TF spherical-cell model***:
Nucleus plus Z electrons in a neutral cell of radius R_o
- Electrons --> semiclassical "Fermi gas"
- Aside from compression pdV work on the cell,
assume the neutral cells have no additional interaction.

o From today's viewpoint, the FMT theory
- remains the reference theory behind SESAME, QEOS
- defines our objectives:

Anything that goes beyond FMT is "interesting" WDM science

FMT is brilliant physics. (Feynman! Teller!)
The brilliance shows in several ways:

o A clear physical picture.
o Definite closed equations, worked out thoroughly.
[Many internal consistency checks] (alas, poor numerics!)
o Courage required because FMT strongly disagrees with
solid-state data.
oValid for superhigh density because it includes:
- Electron kinetic energies, Fermi statistics
- Electron-electron and electron-ion Coulomb energies
- Neutral cell describes strongly coupled ions (high Γ)
o Experiments and hindsight have justified the model.

However: FMT ignores molecules, negative ions, QM shell effects, and assumes everything is metallic at all ρ, T. FMT will not be enough for WDM.

TF Theory: atom in ion-sphere

R_o = Ion-sphere cell radius

Cell volume = V_{cell} = $4\pi/3\ R_o^3$ <-- set by density

Inside the atom, a self-consistent electrostatic potential:

$$\nabla^2 V = +4\pi e n(r)$$

Boundary conditions: $V(R_o) = 0$

$V(r) \dashrightarrow Ze/r$ near nucleus ($r = 0$)

The cell is electrically neutral (determines μ)

Electron number-density (inside atom) = n(r)

$$n(r) = \int \frac{2d^3p}{h^3} \frac{1}{e^{(p^2/2m - eV(r) - \mu)/kT} + 1} = c_1 (kT)^{3/2} F_{1/2}\left(-\frac{\mu + eV(r)}{kT}\right)$$

$$c_1 = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \qquad F_j(x) = \int_0^\infty \frac{y^j}{1+\exp(x+y)} dy$$

Electron pressure:

$$p = \frac{8kT}{3\sqrt{\pi}\lambda_e^3} F_{\frac{1}{2}}\left(-\frac{\mu + eV(R_o)}{kT}\right)$$

This is the pressure of the electron gas at the edge of the ion sphere

Free-energy density-functional for TF theory

$$\boxed{F[n(r)] = \int n(r) f(n(r),T)\, d^3r - e\int \frac{Ze}{r} n(r)\, d^3r + \frac{e^2}{2}\int \frac{n(r)n(r')}{|r-r'|}\, d^3r\, d^3r'}$$

$$f(n(r),T) = -kT\left\{\eta(r) + \frac{2}{3}\frac{F_{3/2}(\eta(r))}{F_{1/2}(\eta(r))}\right\}$$

$$n(r) = \alpha(kT)^{3/2} F_{\frac{1}{2}}(\eta(r)) \qquad \alpha = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$$

$$V(r) = \frac{Ze}{r} - e\int \frac{n(r')}{|r-r'|} d^3r'$$

Chemical potential:

$$\mu = \frac{\delta F}{\delta n(r)} = f(n(r),T) + n(r)\frac{\partial f}{\partial n} - eV(r)$$

Pressure

$$p = -\frac{\partial F}{\partial \Omega} \qquad p = n^2 \left.\frac{\partial f}{\partial n}\right]_{r=R_0}$$

The Thomas-Fermi cell-model gets the same pressure from three formulas: 1.) Thermodynamics, p = - dF/dV, 2.) the virial theorem 3pV = 2K - U, and 3.) a local stress tensor equivalent to the momentum flux across the cell boundary. As of today, the quantum generalizations of the TF cell model still do *not* have this remarkable self-consistency.

Thermodynamic properties:

Electron kinetic energy:

$$K = c_1 (kT)^{5/2} \int d^3r \; F_{3/2}\left(-\frac{\mu + eV(r)}{kT}\right)$$

Electron-nucleus interaction energy:

$$U_{en} = -\int d^3r \; \frac{Ze^2}{r} n(r)$$

Electron-electron interaction energy:

$$U_{ee} = \frac{e^2}{2} \int\int d^3r \; d^3r' \; \frac{n(r)n(r')}{|r - r'|}$$

Total energy (electrons and electron interaction with ion):

$$E = K + U_{en} + U_{ee}$$

Helmholtz free energy:

$$F = Z\mu - \frac{2}{3}K - U_{ee}$$

Entropy:

$$TS = \frac{5}{3}K - Z\mu + U_{en} + 2U_{ee}$$

Electron pressure p:

$$p = \frac{2}{3} c_1 (kT)^{5/2} \; F_{3/2}\left(-\frac{\mu}{kT}\right)$$

These energies obey the Virial theorem:

$$3pV_{cell} = 2K + U_{en} + U_{ee}$$

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