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Correlations, Cluster Formation, and Phase Transitions in Dense Fermion Systems

Gerd Röpke, Rostock

Outline

- Part I: Quantum statistics and the method of Green functions, Coulomb systems
- Part II: Nuclear systems, correlations, bound states and in-medium effects, phase transitions, pairing and quartetting
- Part III: Nonequilibrium processes and cluster formation, freeze-out concept, heavy-ion collisions, fission, astrophysics, transport processes
- TI: Green functions and Feynman diagrams, partial summations, self-energy, polarization function, cluster decomposition
- TII: Separable potentials, bound and scattering states, Pauli blocking and shift of the binding energy

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Coulomb interaction

simple example of a Coulomb system: electrons, protons: fermions

Coulomb interaction: $V_{ab}(r) = \dfrac{e_a e_b}{4\pi\epsilon_0 |r_{ab}|}$

- single particle states $\{1\} = \{\mathbf{k}_1, \sigma_1, c_1\}$: {wave number (momentum), spin, species}
- occupation number representation: creation and annihilation operators,
  anticommutation relations

$$\{a_1, a_{1'}^+\}_+ = a_1 a_{1'}^+ + a_{1'}^+ a_1 = \delta_{11'} \qquad \{a_1, a_{1'}\}_+ = \{a_1^+, a_{1'}^+\}_+ = 0$$

Hamiltonian:

- kinetic energy $T = H^{(1)} = \sum_1 E_1 a_1^+ a_1 \quad \text{with} \quad E_1 = \dfrac{\hbar^2 k_1^2}{2m_1}$
- potential energy $V = H^{(2)} = \sum V_{12,1'2'} a_{1'}^+ a_{2'}^+ a_2 a_1$

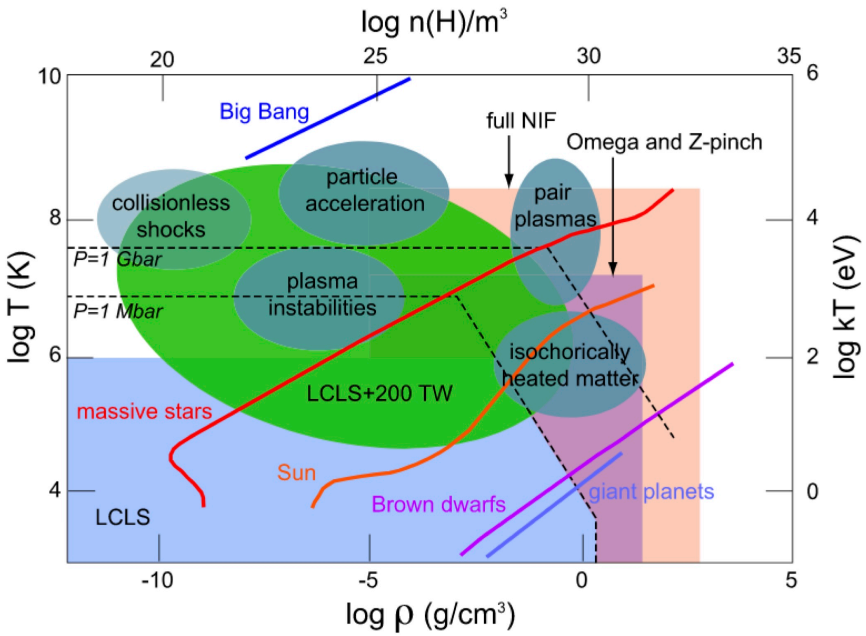
Fourier transform $V_{12,1'2'} = \dfrac{e_1 e_2}{\epsilon_0 \Omega |k_1 - k_1'|^2} \delta_{k_1+k_2,k_1'+k_2'} \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} \delta_{c_1 c_1'} \delta_{c_2 c_2'}$

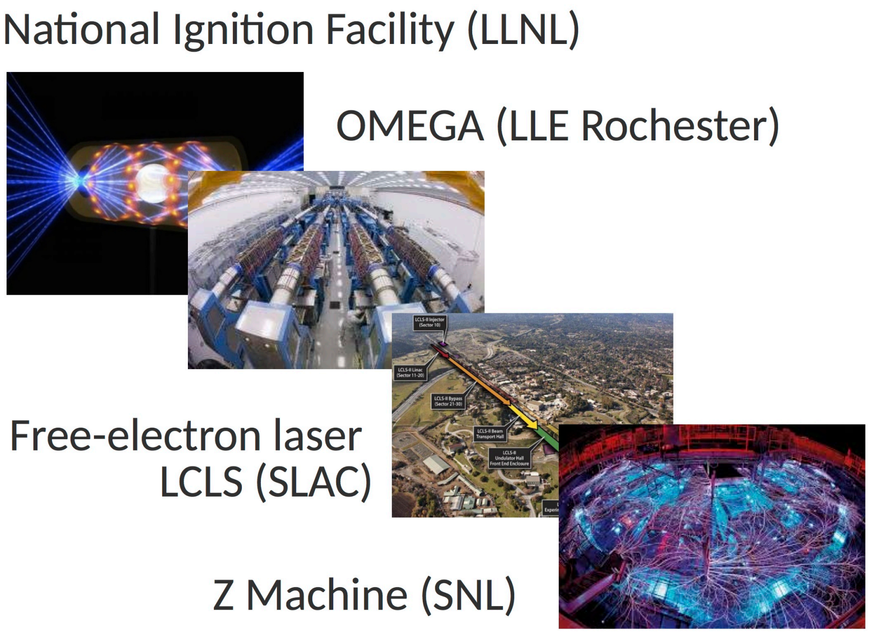
Ω: volume

Coulomb systems

- Electrons, protons: fermions, Coulomb interaction
- Bound state: H atom, partially ionized plasma, ionization degree
- Other elements, compounds,…, condensed matter, metals…
- Pseudopotentials, polarisation potentials, van der Waals potentials
- Electron-hole plasma in semiconductors: exciton as bound state
- High density of atoms: electrons become delocalized, liquid metal, bound states disappear, liquid metal phase transition
- Warm dense matter (WDM)

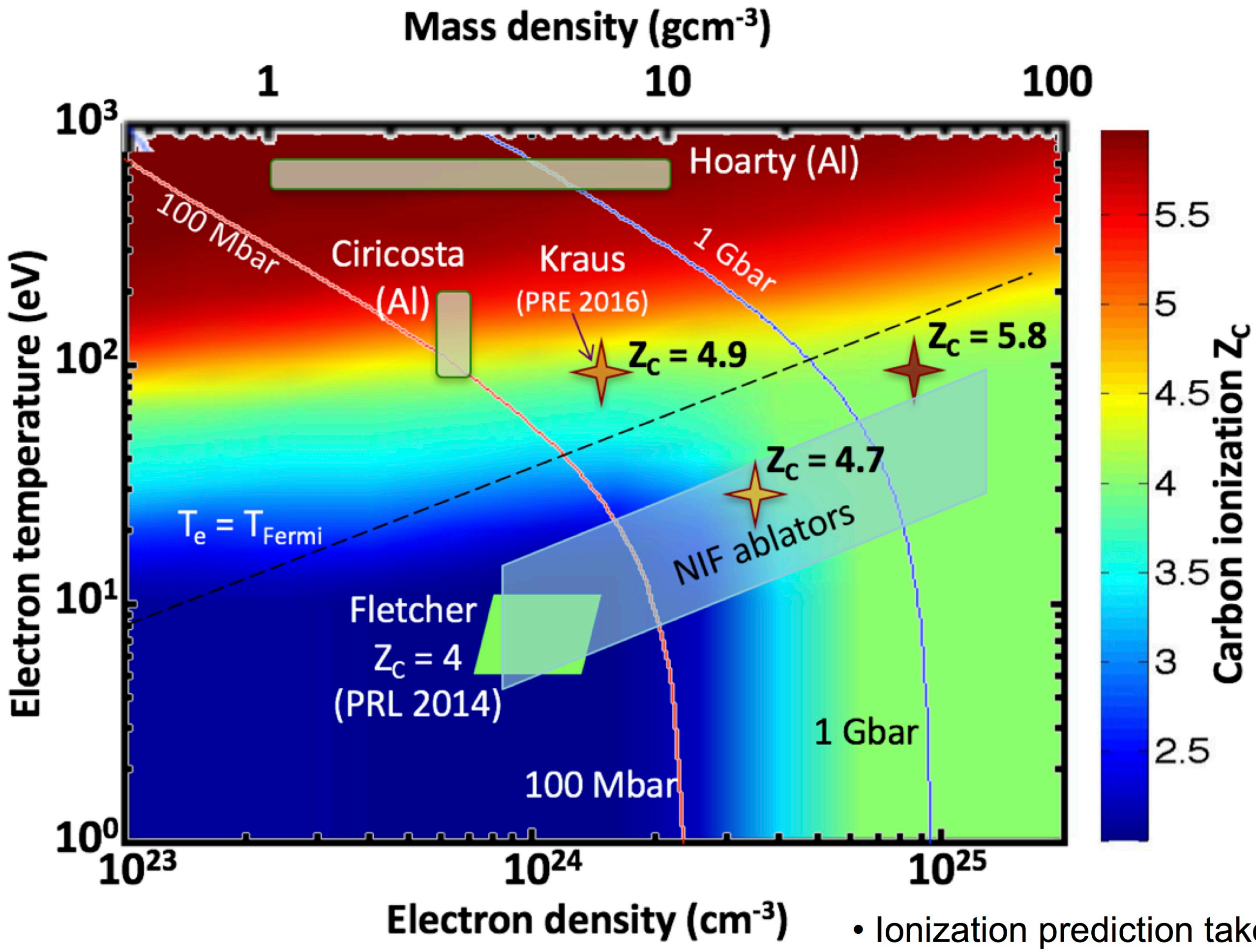
WDM facilities / US

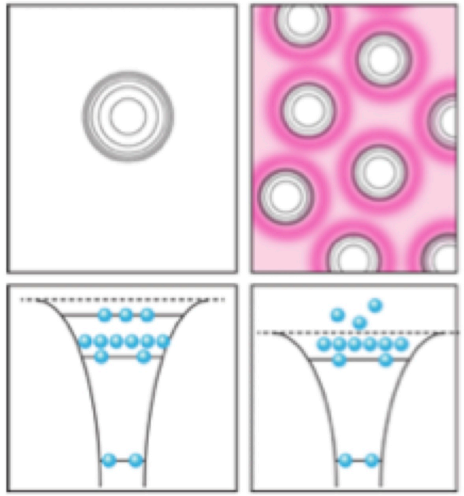




- experimental facilities have access to a broad range of temperatures and densities
- design and interpretation of data often relies on equation of state (EOS), material and transport properties such as opacity, electrical conductivity, and ionization degree

NIF XRTS experiments find higher carbon K-shell ionization than predicted by widely used IPD models (Stewart & Pyatt, OPAL)





NIF data point

Hoarty et al., PRL **110**, 265003 (2013)

Ciricosta et al., PRL **109,** 065002 (2012)

Fletcher et al., PRL **112**, 145004 (2014)

Kraus et al., PRE **94**, 011202(R) (2016)
[C. Lin et al., PRE 96, 013202 (2017)]

- Ionization prediction taken from OPAL

Rogers et al., APJ **456**, 902 (1996)

Preliminary, from Tilo Döppner et al., LLNL

Nuclear systems

- baryons: neutrons, protons,…(strange particles)
- Bound states: nuclei (deuteron ^2H, triton ^3H, helion ^3He, alpha ^4He,…)
- Interaction potentials (Bonn, Paris, Reid, Argonne, Nijmegen ,..),
  fitted to empirical data (bound states, scattering phase shifts,…)
- Heavy ion collisions, astrophysics
- High density matter: nuclei are dissolved, phase transition to nuclear matter
- More fundamental: QCD, leptons, quarks, bound states: hadrons
- High density of hadrons: hadrons are dissolved, phase transition to quark matter (deconfinement, quark-gluon plasma)

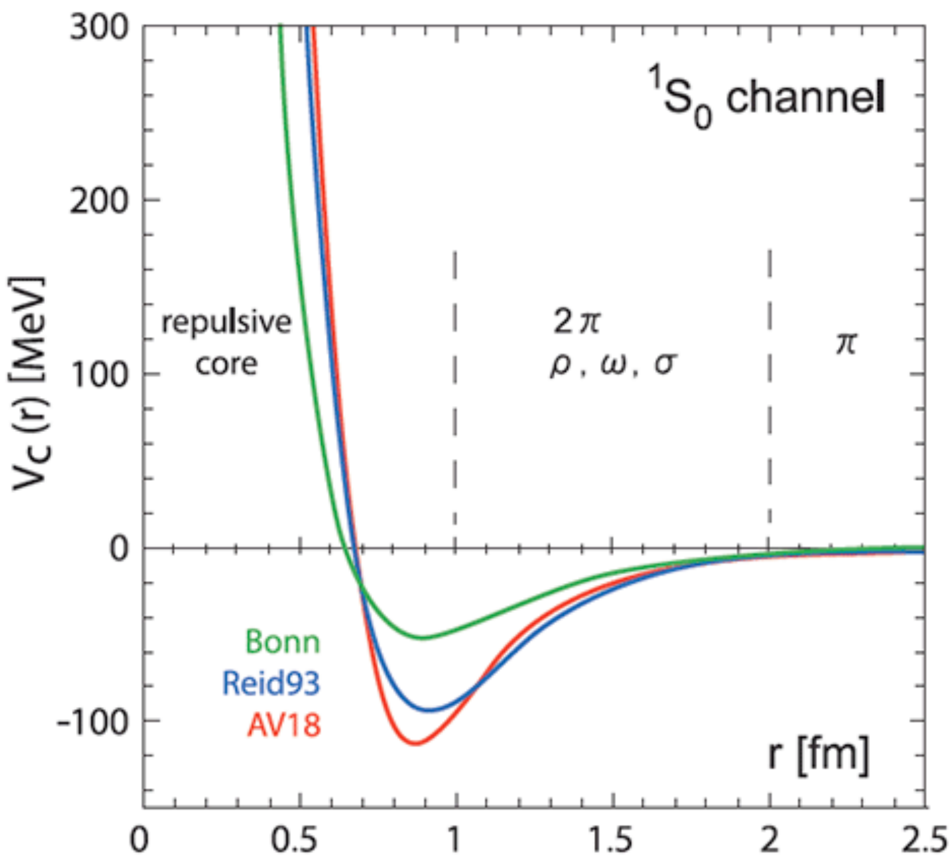
nucleon-nucleon interaction potential

- Effective potentials
  (like atom-atom potential)
  binding energies, scattering

- non-local, energy-dependent?
  QCD?

- microscopic calculations
  (AMD, FMD)

- single-particle descriptions:
  Thomas-Fermi approximation
  shell model
  density functional theory (DFT)



Separable interaction (Yamaguchi)

$$V^{\rm sep}(p,p') = -\lambda/\Omega w(p) w(p')$$

Exact solution in closed form, including scattering states.
Theorem of Ernst, Shakin and Thaler: each potential can be represented as a sum of separable potentials.

- **general form:**

$$V_\alpha(p,p') = \sum_{i,j=1}^{N} w_{\alpha i}(p)\lambda_{\alpha ij} w_{\alpha j}(p') \qquad \text{uncoupled}$$

and

$$V_\alpha^{LL'}(p,p') = \sum_{i,j=1}^{N} w_{\alpha i}^{L}(p)\lambda_{\alpha ij} w_{\alpha j}^{L'}(p') \qquad \text{coupled}$$

PEST (Paris),
BEST (Bonn),
...

p, p' in- and outgoing relative momentum
α ... channel
N ... rank
$\lambda_{\alpha ij}$. coupling parameter
L, L' orbital angular momentum

D. J. Ernst, C. M. Shakin, R. M. Thaler, Phys. Rev. C **8**, 46 (1973).

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.

- QED and QCD are fundamental theories

- Question: macroscopic properties (equations of state, transport coefficients, reaction rates, etc.) from microscopic description (Hamiltonian, Lagrangian)

Statistical operator

eigenstates of the system, probabilities: $\rho = \sum_n |n\rangle w_n \langle n| = e^{-S_i}$

averages $\langle A \rangle = \mathrm{Tr}\,\{\varrho\, A\}$

- New concept in physics: (information) entropy $\langle S \rangle = -\langle \ln \varrho \rangle$

- New principle: extremum of entropy at given boundary conditions (information):

  normalization $\langle 1 \rangle = 1$, conserved quantities $\langle H \rangle = U$ $\quad \langle \hat{N}_c \rangle = N_c = n_c \Omega$

  $\delta[\langle S \rangle - \lambda_0 \langle 1 \rangle - \lambda_c \langle \hat{N}_c \rangle - \lambda_T \langle H \rangle] = 0$ $\quad \hat{N}_c = \sum_{\bar{1}} a_{\bar{1}}^{+} a_{\bar{1}}$

- grand canonical distribution $\varrho = \dfrac{\mathrm{e}^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{\mathrm{e}^{-\beta(H-\mu N)}\right\}}$

- Elimination of Lagrange multipliers $n_c = \dfrac{1}{\Omega} N_c(T, \mu_c), \qquad u = \dfrac{1}{\Omega} U(T, \mu_c)$

equation of state

$$S = S^{(0)} + S^{(1)} + S^{(2)} + \dots$$
$$= \ln Z(T, \Omega, \mu) + \sum_k s_k^{(1)} c_k^{+} c_k + \sum_{k_1 k_2, k_1' k_2'} s^{(2)}_{k_1 k_2, k_1' k_2'} c^{+}_{k_1} c^{+}_{k_2} c_{k_2'} c_{k_1'} + \dots$$

partition function

$$Z(T, \Omega, \mu) = \mathrm{Tr}\left\{\mathrm{e}^{-\left(S^{(1)} + S^{(2)}\right)}\right\}$$

Gibbs-Duhem equation $U - k_B T S - \mu N = -k_B T \ln Z(T, \Omega, \mu) = -p\Omega$

Thermodynamics

equation of state $n_B = n_B(T, \mu)$ (species B)

equation of state $\mu = \mu(T, n_B)$

thermodynamic potential to T, n_B: free energy density

$$f(T, n_B) = \frac{F(T,V,N_B)}{V} = f(T, n_0) + \int_{n_0}^{n_B} \mu(T, n')\, dn'$$

thermodynamic relations (Gibbs-Duhem):

$$F + pV = G = \mu N$$

equation of state: pressure $p(T, n_B) = n_B \mu(T, n_B) - f(T, n_B)$

consistency

Virial expansions

- short-range interaction $p^{\rm sr}(T,n) = b_1^{\rm sr}(T)n + b_2^{\rm sr}(T)n^2 + b_3^{\rm sr}(T)n^3 + \dots.$

second virial coefficient: classical limit $b_2^{\rm sr}(T) = k_B T \int d^3r\, \left(e^{-V(r)/k_BT} - 1\right)$

- Coulomb systems: long-range Coulomb interaction

$$k_BT\int_0^\infty 4\pi r^2 dr (e^{-V(r)/k_BT}-1) \approx -\int_0^\infty 4\pi r^2 dr \frac{e_a e_b}{4\pi\epsilon_0 r} \to \infty$$

- Debye potential $V^D(r) = \frac{e_1 e_2}{4\pi\varepsilon_0} \cdot \frac{\mathrm{e}^{-\kappa r}}{r}$, screening parameter $\kappa^2 = \sum_c \frac{e_c^2 n_c}{\varepsilon_0 k_B T}$

virial expansion $\beta p = n - \frac{\kappa^3}{12\pi} + \dots = n - \frac{1}{12\pi}\left(\frac{e^2}{\epsilon_0 k_B T}\right)^{3/2} n^{3/2} + \dots$

- Hydrogen bound states: internal partition function

$$\sigma_H = 2\sum_s s^2 e^{-\beta E_s} = 2\sum_s s^2 e^{1/(2T_{\rm Ha}s^2)} = 2\sum_s s^2\left[1 + \frac{1}{2T_{\rm Ha}s^2} + \frac{1}{8T_{\rm Ha}^2 s^4} + \dots\right]$$

Planck-Larkin-Brillouin internal partition function $\sigma_H^{\rm PLB} = 2\sum_s s^2\left[e^{-\beta E_s} - 1 - \frac{1}{2T_{\rm Ha}s^2}\right]$

Phase transitions

thermodynamic stability

$$\left.\frac{\partial p}{\partial v}\right|_T < 0$$

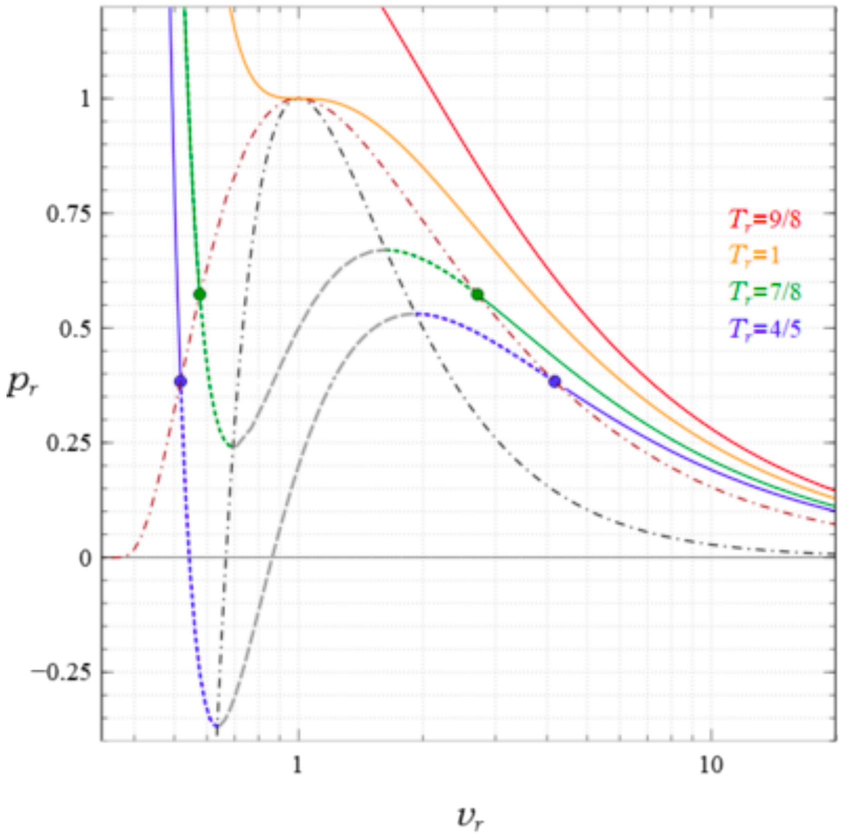
model:
Van der Waals equation of state

$$p = \frac{k_B T}{v - b} - \frac{a}{v^2}$$

volume per particle $\quad v = 1/n = \Omega/N$

b: excluded volume

reduced form $\quad p_r = \frac{8T_r}{3v_r - 1} - \frac{3}{v_r^2}$



phase transition:
critical point,
spinodal decomposition
Maxwell construction

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.

- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)

- Convergence of perturbation expansions, analytical behavior

- Bound/free state contribution? Ionization degree?

Ideal Fermi gas (neutrons)

equation of state (EoS): (T = 0)

nonrelativistic $E_k = \frac{\hbar^2}{2m_n} k^2$

$$N_n = (2s+1) \sum_k f_n(E_k); \quad n_n = \frac{2}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk = \frac{1}{3\pi^2} k_F^3$$

$$k_F = (3\pi^2 n_n)^{1/3}$$

chemical potential $\mu(n_n) = E_{k_F} = \frac{\hbar^2}{2m_n}(3\pi^2)^{2/3} n_n^{2/3}$

free energy density $f(n_n) = \frac{\hbar^2}{2m_n}(3\pi^2)^{2/3} \frac{3}{5} n_n^{5/3}$

“ab initio” calculations vs. analytic expressions

Strongly interacting quantum systems

equation of state (EoS)

density

$$n(T,\mu) = \frac{1}{\mathrm{Vol}} \int d^3r \langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r})\rangle$$

transport coefficients: electrical, thermal,…

electrical conductivity: Kubo

$$\sigma(T,\mu) = \frac{e^2\beta}{3m^2\mathrm{Vol}} \int_{-\infty}^{0} dt e^{\epsilon t} \int_0^1 d\lambda \langle \mathbf{P}\cdot\mathbf{P}(t+i\hbar\beta\lambda)\rangle$$

electron total momentum $\mathbf{P} = \sum_k \hbar\,\mathbf{k}\, a_k^\dagger a_k$

Fermi function

$$\mathrm{Tr}\{\rho\,\psi^\dagger(1',t')\,\psi(1,t)\} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\frac{i}{\hbar}\omega(t'-t)} f(\omega) A(1,1';\omega)$$

statistical operator, $T = 1/\beta,\ \mu$

spectral function, see below

Green’s functions:
perturbation theory,
partial summations
quasiparticle, screening

limiting cases

DFT-MD simulations
Exchange-correlation
functional

electron-ion interaction

PIMC simulations
sign problem
limited particle number

uniform electron gas

Perturbation expansion for calculation of mean values

- expanding the exponential functions of operators

$$e^{A+B} = e^{A}\left(1 + \int_0^1 d\tau\, e^{-\tau A} B e^{\tau(A+B)}\right)$$

Dyson series

$$e^{A+B} = e^{A} + \int_0^1 d\tau\, e^{(1-\tau)A} B\, e^{\tau A} + \int_0^1 d\tau \int_0^{\tau} d\tau_1\, e^{(1-\tau)A} B\, e^{(\tau-\tau_1)A} B\, e^{\tau_1 A} + \ldots.$$

- for single-particle operator $S^{(1)} = \sum_k s_k n_k$

Sandwich expression

$$e^{S^{(1)}} c_k^{+} e^{-S^{(1)}} = e^{s_k} c_k^{+}$$
$$e^{S^{(1)}} c_k e^{-S^{(1)}} = e^{-s_k} c_k$$

- Wick's theorem

$$\mathrm{Tr}\left\{\varrho^0 A_1 A_2 \cdots A_s\right\} = \sum_{\substack{\text{all pairings} \\ \mathfrak{p} = (\{i,j\}\ldots\{k,l\})}} (-1)^{\mathfrak{p}} \prod_{\substack{\text{all pairs} \\ \{i,j\} \text{ in } \mathfrak{p}}} \langle A_i A_j \rangle$$

for $\varrho^0 = e^{-\left(S^{(0)}+S^{(1)}\right)}$

$S^{(1)} = \sum_k s_k^{(1)} c_k^{+} c_k$

$A_1 A_2 A_3 A_4$: (pairs 1–2, 3–4)	$(+1) \cdot \langle A_1 A_2 \rangle \cdot \langle A_3 A_4 \rangle$	[$\mathfrak{p}$ even]
$A_1 A_2 A_3 A_4$: (pairs 1–3, 2–4)	$(-1) \cdot \langle A_1 A_3 \rangle \cdot \langle A_2 A_4 \rangle$	[$\mathfrak{p}$ odd]
$A_1 A_2 A_3 A_4$: (pairs 1–4, 2–3)	$(+1) \cdot \langle A_1 A_4 \rangle \cdot \langle A_2 A_3 \rangle$	[$\mathfrak{p}$ even]

$$\left\langle a_i^{+} a_j \right\rangle = \delta_{ij} \frac{1}{e^{\beta(E_i-\mu)} + 1} = \delta_{ij} f_i$$
$$\left\langle a_i a_j^{+} \right\rangle = \delta_{ij} \frac{1}{e^{-\beta(E_i-\mu)} + 1} = \delta_{ij} (1 - f_i)$$

Thermodynamic Green's functions

correlation functions of a_1, a_1^+ with $\varrho = \frac{\mathrm{e}^{-\beta(H-\mu N)}}{\mathrm{Tr}\left\{\mathrm{e}^{-\beta(H-\mu N)}\right\}} = \mathrm{e}^{-S}$

tau-dependence $A(\tau) = \mathrm{e}^{\tau(H-\mu N)} A \mathrm{e}^{-\tau(H-\mu N)}$

define $G_1\left(1\tau_1, 1'\tau_{1'}\right) = -\mathrm{Tr}\left\{\varrho \mathrm{T}\left[a_1(\tau_1) a_{1'}^+(\tau_{1'})\right]\right\} = \begin{cases} -\mathrm{Tr}\left\{\varrho a_1(\tau_1) a_{1'}^+(\tau_{1'})\right\} & \text{for } \tau_{1'} < \tau_1 \\ \mathrm{Tr}\left\{\varrho a_{1'}^+(\tau_{1'}) a_1(\tau_1)\right\} & \text{for } \tau_1 < \tau_{1'} \end{cases}$

- thermodynamic equilibrium $G_1\left(1\tau_1, 1'\tau_{1'}\right) = G_1\left(1\tau_1 - \tau_{1'}, 1'0\right) = G_1\left(1\tau, 1'0\right) \equiv G_1\left(11', \tau\right)$

- Kubo-Martin-Schwinger condition $G_1\left(11', \beta - \tau\right) = -G_1\left(11', -\tau\right)$

quasi-periodicity, Fourier expansion $G_1\left(11', \tau\right) = \frac{1}{\beta} \sum_\nu G_1\left(11', iz_\nu\right) \mathrm{e}^{-iz_\nu \tau}$

- Matsubara frequencies $z_\nu = \frac{\pi \nu}{\beta}, \quad \nu = \pm 1, \pm 3, \ldots \text{ for fermions}$

inverse transformation $G_1(11', iz_\nu) = \int_0^\beta \mathrm{d}\tau\, G_1\left(11', \tau\right) \mathrm{e}^{iz_\nu \tau}$

Spectral functions

with the eigenstates of the grand canonical operator $(H-\mu N)|n\rangle = \epsilon_n |n\rangle$

define the single-particle spectral density

$$I_1(11',\omega) = 2\pi \frac{1}{Z} \sum_{m,n} \delta(\epsilon_n - \epsilon_m - \omega)\, \mathrm{e}^{-\beta\epsilon_n} \langle n| a^+_{1'} |m\rangle \langle m| a_1 |n\rangle$$

It is the Fourier transform of

$$\langle a^+_{1'} a_1(\tau)\rangle = G^<_1(11',\tau) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} I_1(11',\omega')\, \mathrm{e}^{-\omega'\tau}$$

$$\langle a_1(\tau) a^+_{1'}\rangle = -G^>_1(11',\tau) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \mathrm{e}^{\beta\omega'} I_1(11',\omega')\, \mathrm{e}^{-\omega'\tau}$$

and is connected with the Matsubara Green's function

$$G_1(11',iz_\nu) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \left(1+\mathrm{e}^{\beta\omega'}\right) \frac{I_1(11',\omega')}{iz_\nu - \omega'}$$

Analytical continuation into the whole complex z-plane

$$G_1(11',z) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \frac{A_1(11',\omega')}{z-\omega'}$$

with the spectral function $A_1(11',\omega) = \left(1+\mathrm{e}^{\beta\omega}\right) I_1(11',\omega)$

Cauchy-type integral,
branch cut at the real axis

$$\begin{aligned} G_1(11',\omega - i\varepsilon) - G_1(11',\omega + i\varepsilon) &= 2i\mathrm{Im}\left\{G_1(11',\omega - i\varepsilon)\right\} \\ &= iA_1(11',\omega) \quad . \end{aligned}$$

1. We calculate $G_1(11', iz_\nu)$. An appropriate perturbation theory for doing so will be given later.
2. $G_1(11', z)$ is the analytic continuation of the MATSUBARA GREEN's function into the complex z-plane.
3. We compute the spectral function $A_1(11', \omega)$ via

$$A_1\left(11', \omega\right) = 2\mathrm{Im}\left\{G_1\left(11', \omega - i\varepsilon\right)\right\} . \tag{2.2.13}$$

4. From the spectral function we calculate the spectral density $I_1(11', \omega)$:

$$I_1\left(11', \omega\right) = \frac{A_1\left(11', \omega\right)}{1 + \mathrm{e}^{\beta\omega}} . \tag{2.2.14}$$

5. The correlation functions are obtained by integration, for example through (2.2.3):

$$\left\langle a_{1'}^{+} a_1(\tau)\right\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} I_1\left(11', \omega\right) \mathrm{e}^{-\omega\tau} . \tag{2.2.15}$$

6. Equations of state ($f(\omega) = \frac{1}{\mathrm{e}^{\beta\omega}+1}$):

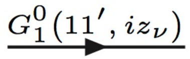
$$\text{e.g.} \quad n(\beta, \mu) = \frac{1}{\Omega} \sum_1 \langle a_1^{+} a_1 \rangle = \int \frac{\mathrm{d}\omega}{2\pi} f(\omega) A_1(11, \omega) . \tag{2.2.16}$$

7. Thermodynamic potential (contains all equilibrium properties):

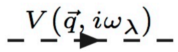
$$\text{e.g.} \quad J(T, \Omega, \mu) = -p(T, \mu)\,\Omega = -\int_{-\infty}^{\mu} \mathrm{d}\mu'\, n\left(\mu', T\right) \Omega . \tag{2.2.17}$$

Feynman diagrams

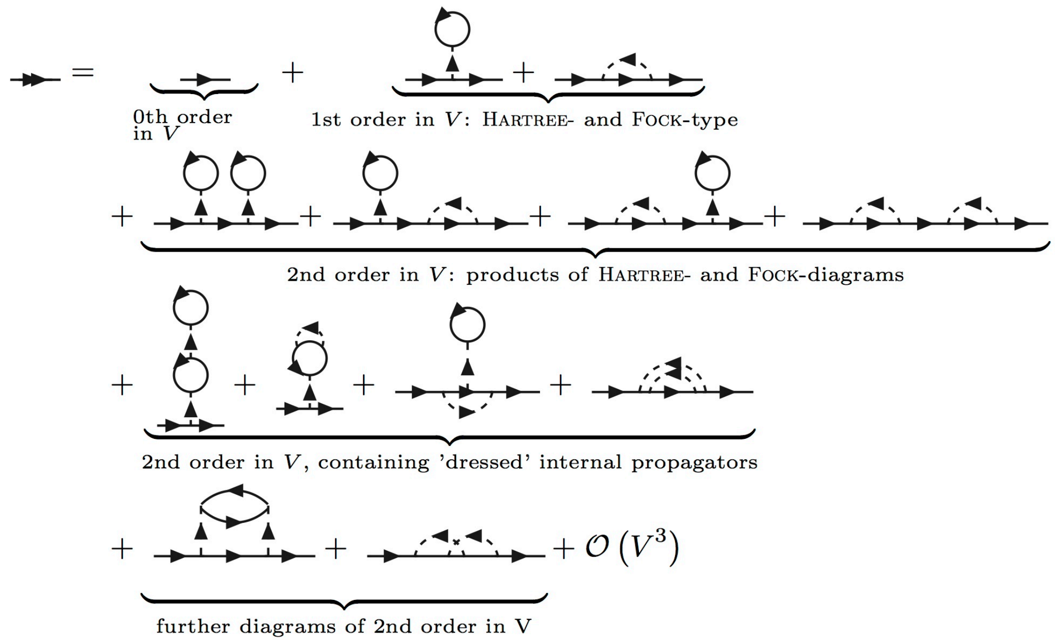
Diagrammatic representation of the perturbative series for the Green's functions

elements: free propagator 

$$G_1^0\left(11', iz_\nu\right) = \frac{\delta_{11'}}{iz_\nu - \epsilon_1}$$

interaction 

$$V\left(\vec{q}\right) = \frac{1}{\Omega}\int \mathrm{d}^3 r\, \mathrm{e}^{i\vec{q}\vec{r}} V\left(\vec{r}\right)$$

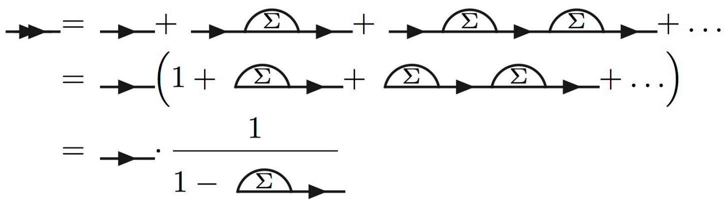
G_1: 

rules
to represent
all contributions
of perturbation theory
by diagrams,
evaluate the
frequency summation.

Partial summations

- Dyson equation and self-energy

$$G_1(1, iz_\nu) = \frac{1}{iz_\nu - \epsilon_1 - \Sigma_1(1, iz_\nu)}$$

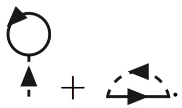


$$= G_1^0(1, iz_\nu)\,\frac{1}{1 - \Sigma_1(1, iz_\nu)\,G_1^0(1, iz_\nu)}$$

$$= \frac{1}{G_1^0(1, iz_\nu)^{-1} - \Sigma_1(1, iz_\nu)}$$

- Hartree-Fock

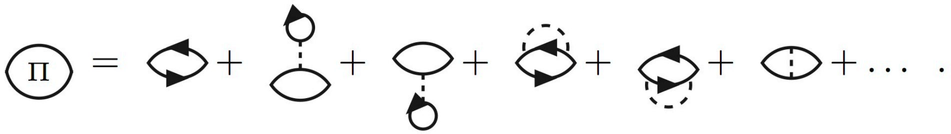
$$\Sigma_1^{\mathrm{HF}}(1, iz_\nu) =$$



$$\int \frac{d^3k'}{(2\pi)^3}\left((2s+1)V(0) - V\left(\vec{k}' - \vec{k}\right)\right) f(\epsilon_{k'})$$

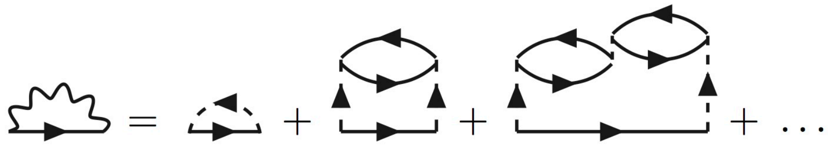
$$A_1(1,\omega) = \lim_{\varepsilon \searrow 0} 2\,\frac{\mathrm{Im}\{\Sigma_1(1, \omega - i\varepsilon)\}}{[\omega - \epsilon_1 - \mathrm{Re}\{\Sigma_1(1, \omega - i\varepsilon)\}]^2 + [\mathrm{Im}\{\Sigma_1(1, \omega - i\varepsilon)\} - \varepsilon]^2}$$

- screening $$V_{ab}^s(q, iz_\mu) = \frac{V_{ab}(q)}{1 - \sum_c V_{cc}(q)\Pi_{cc}(q, iz_\mu)} \equiv \frac{V_{ab}(q)}{\varepsilon(q, iz_\mu)}$$



polarization function

$$\Sigma_1^{\mathrm{MW}}(1, iz_\nu) =$$

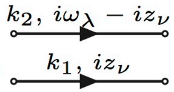


- Debye potential $V^D(r) = \frac{e_1 e_2}{4\pi\varepsilon_0} \cdot \frac{e^{-\kappa r}}{r}$ screening parameter $\kappa^2 = \sum_c \frac{e_c^2 n_c}{\varepsilon_0 k_B T}$

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.
- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)
- Convergence of perturbation expansions, analytical behavior
- Bound/free state contribution? Ionization degree?

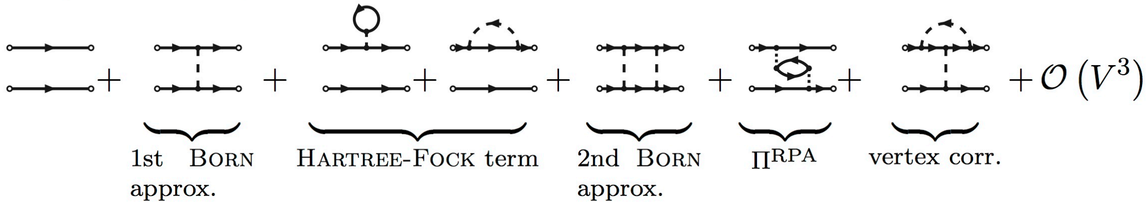
Bethe-Salpeter equation

Free two-particle propagator $G_2^0\left(12,1'2',i\omega_\lambda\right) =$ 

$= \dfrac{1-f\left(\epsilon_1\right)-f\left(\epsilon_2\right)}{i\omega_\lambda-\epsilon_1-\epsilon_2}\delta_{11'}\delta_{22'}$

Full two-particle propagator

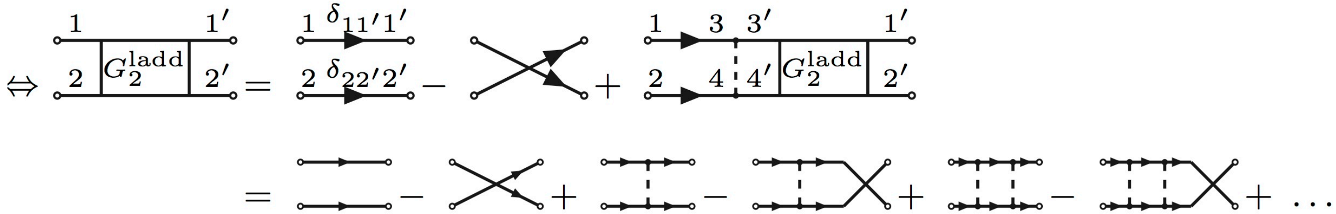
$G_2\left(12,1'2',i\omega_\lambda\right) =$



Bethe-Salpeter equation

$$G_2^{\text{ladd.}}\left(12,1'2',i\omega_\lambda\right) = G_2^0\left(12,1'2',i\omega_\lambda\right) + \sum_{\substack{34\\3'4'}} G_2^0\left(12,34,i\omega_\lambda\right)V\left(34,3'4'\right)G_2^{\text{ladd.}}\left(3'4',1'2',i\omega_\lambda\right)$$

Ladder summation

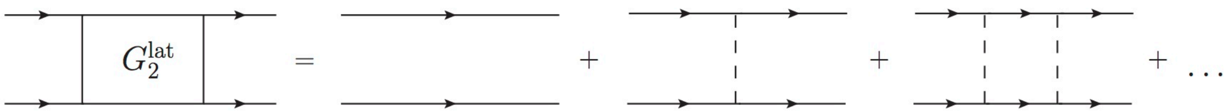


Solution low-density limit $G_2^{\text{ladd.}}\left(12,1'2',i\omega_\lambda\right) = \sum_{nP}\psi_{nP}(12)\dfrac{1}{i\omega_\lambda - E_{nP}+\mu_{12}}\psi_{nP}^*(1'2')$

Schroedinger equation $\left(E_1+E_2-E_{nP}\right)\psi_{nP}(12)+\sum_{1'2'}V\left(12,1'2'\right)\psi_{nP}\left(1'2'\right)=0$

Beth-Uhlenbeck formula

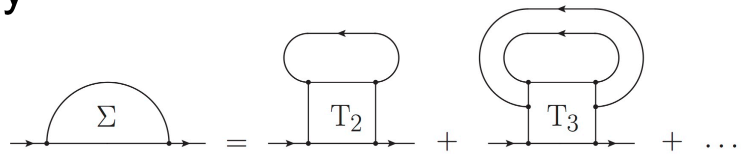
Two-particle correlations



cluster propagator

$$\langle \nu, \mathbf{P}|G_2(z)|\nu', \mathbf{P}'\rangle = \frac{1}{z - E^0_{\nu,P}} \delta_{\nu\nu'} \delta_{\mathbf{P},\mathbf{P}'}$$

cluster decomposition of the self-energy



Beth-Uhlenbeck formula: second virial coefficient (f_2)

$$n_B^{\mathrm{BU}}(\beta,\mu) = \frac{1}{\Omega_0}\sum_{\mathbf{p}} f_p^0 + \frac{2}{\Omega_0}\sum_{\alpha,\mathbf{P}}\int_{-\infty}^{\infty}\frac{dE_{\mathrm{rel}}}{\pi} f_2\left(E_{\mathrm{rel}} + \frac{P^2}{4m}\right) D^{\mathrm{BU}}_{\alpha,\mathbf{P}}(E_{\mathrm{rel}}),$$

$$D^{\mathrm{BU}}_{\alpha,\mathbf{P}}(E_{\mathrm{rel}}) = g_\alpha \left(\sum_\nu \pi\delta(E_{\mathrm{rel}} - E^0_{\alpha\nu,\mathbf{P}}) + \frac{\partial}{\partial E_{\mathrm{rel}}}\delta_{\alpha,\mathbf{P}}(E_{\mathrm{rel}})\right)$$

degeneracy bound states scattering phase shifts

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.
- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)
- Convergence of perturbation expansions, analytical behavior
- Bound/free state contribution? Ionization degree?

Quasiparticle concept

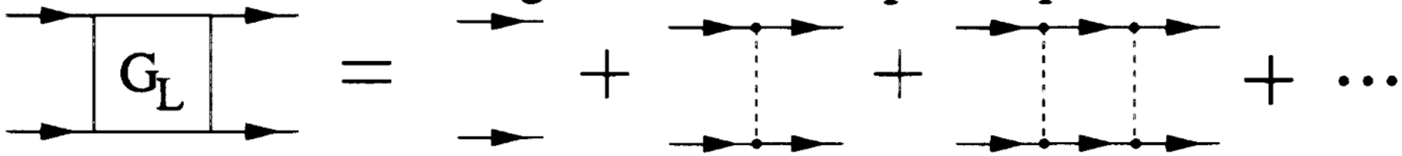
- **Expansion for small Im $\Sigma(1, \omega + i\eta)$**

$$A(1,\omega) \approx \frac{2\pi\delta(\omega - E^{\text{quasi}}(1))}{1 - \frac{\text{d}}{\text{d}z}\text{Re }\Sigma(1,z)|_{z=E^{\text{quasi}}-\mu_1}} - 2\text{Im }\Sigma(1,\omega+i\eta)\frac{\text{d}}{\text{d}\omega}\frac{P}{\omega+\mu_1-E^{\text{quasi}}(1)}$$

quasiparticle energy $E^{\text{quasi}}(1) = E(1) + \text{Re }\Sigma(1,\omega)|_{\omega=E^{\text{quasi}}}$

- **chemical picture: bound states $\hat{=}$ new species**

summation of ladder diagrams, Bethe-Salpeter equation



In-medium Schroedinger equation

Consistent treatment of the two-particle problem:
in-medium wave equation

$$\frac{p^2}{2m_e}\psi_n(p)+\sum_q V(q)\psi_n(p+q)-E_n\psi_n(p)=\sum_q V(q)\left[\psi_n(p+q)f_e(p)-\psi_n(p)f_e(p+q)\right]$$

Pauli blocking, Fock self-energy shift

V-> V_{screened}: dynamical screening, dynamical self-energy

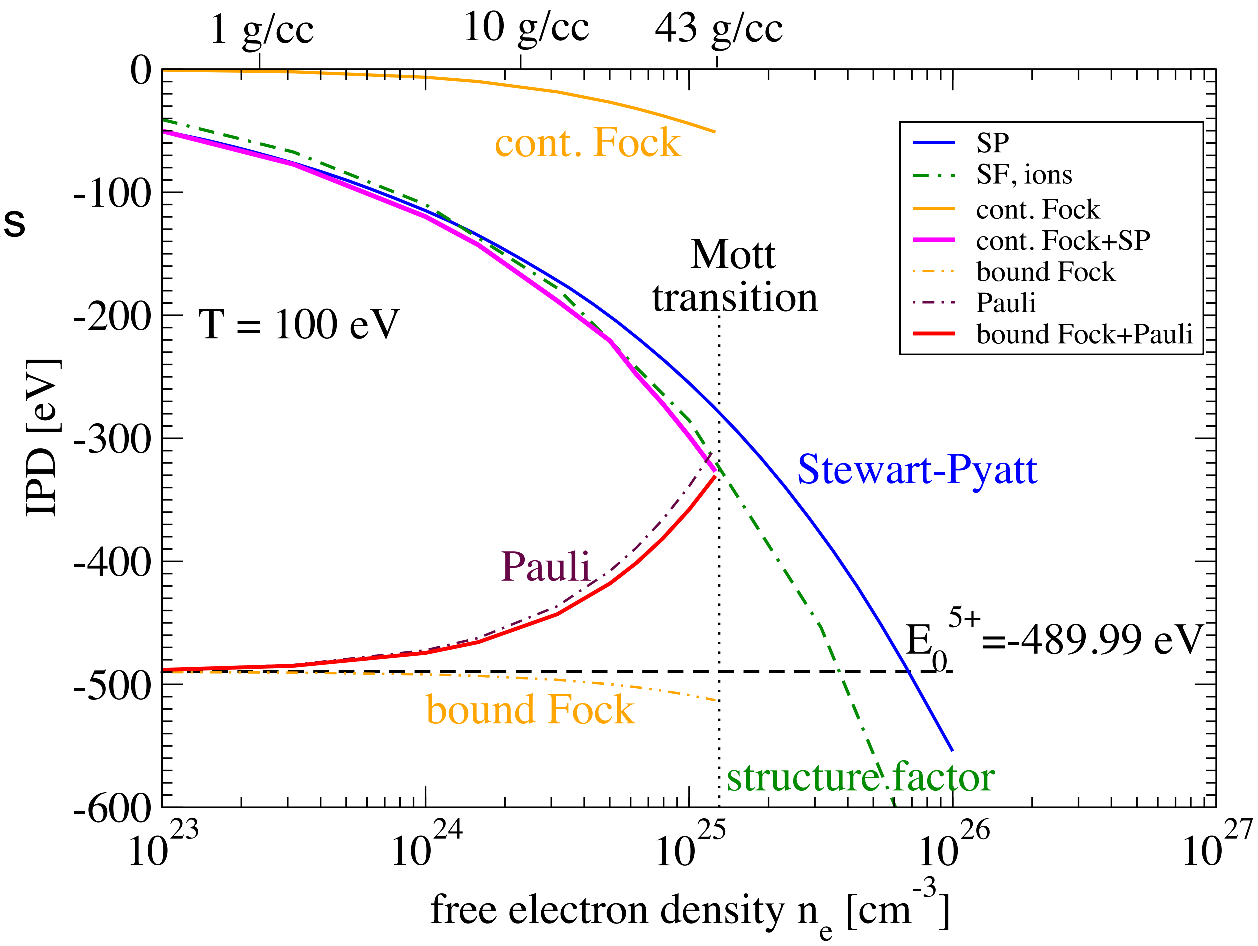
R. Zimmermann, K. Kilimann, W. D. Kraeft, D. Kremp and G. Röpke
Phys. Stat. sol. (b) **90**, 175 (1978)

W.-D. Kraeft, D. Kremp, W. Ebeling, G.R.
Quantum Statistics of Charged Particle Systems,
Akademie-Verlag, Berlin 1986

Ionization potential depression

Pauli blocking
in degenerate plasmas
at extreme densities

Carbon



G. R., D. Blaschke, T. Döppner, C. Lin, W.-D. Kraeft, R. Redmer, H. Reinholz
Phys. Rev. E **99**, 033201 (2019)

Quasiparticle approach

The total density as well as the DoS are given by the spectral function A,

$$n_e^{\rm total}(T,\mu_e,\mu_a) = \frac{1}{\Omega}\sum_1 \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\hat{f}_e(\omega)A_e(1,\omega) = \int_{-\infty}^{\infty} d\omega \hat{f}_e(\omega)D_e(\omega)$$

$$A_e(1,\omega) \approx \frac{2\pi\,\delta(\omega - E_e^{\rm quasi}(1))}{1-\frac{d}{dz}{\rm Re}\,\Sigma_e(1,z)|_{z=E_e^{\rm quasi}-\mu_e}} - 2{\rm Im}\,\Sigma_e(1,\omega+i0)\frac{d}{d\omega}\frac{\mathcal{P}}{\omega+\mu_e-E_e^{\rm quasi}(1)}$$

- quasiparticle concept

$$E^{\rm quasi}(1) = p_1^2/(2m) + {\rm Re}\Sigma(1,\omega)|_{\omega=E^{\rm quasi}(1)}$$

- generalized Beth-Uhlenbeck formula (quasiparticles)

$$n_e^{\rm total}(T,\mu_e,\mu_a) = \frac{1}{\Omega}\sum_1 f_e(E^{\rm quasi}(1))$$

$$+\frac{1}{\Lambda^3}\sum_{i,\gamma} Z_i e^{\beta\mu_i}\left[\sum_\nu^{\rm bound}(e^{-\beta E_{i,\gamma,\nu}}-1)+\frac{\beta}{\pi}\int_0^\infty dE e^{-\beta E}\left\{\delta_{i,\gamma}(E)-\frac{1}{2}\sin[2\delta_{i,\gamma}(E)]\right\}\right]$$

In-medium Schrödinger equation for $E_{i,\gamma,\nu}(T,\mu)$, $\delta_{i,\gamma}(T,\mu)$, channel (spin…) γ

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.
- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)
- Convergence of perturbation expansions, analytical behavior
- Bound/free state contribution? Ionization degree?
- Avoid double counting

Mott effect

increasing density, T fixed: more atoms (H), molecules (H_2), decreasing ionization degree

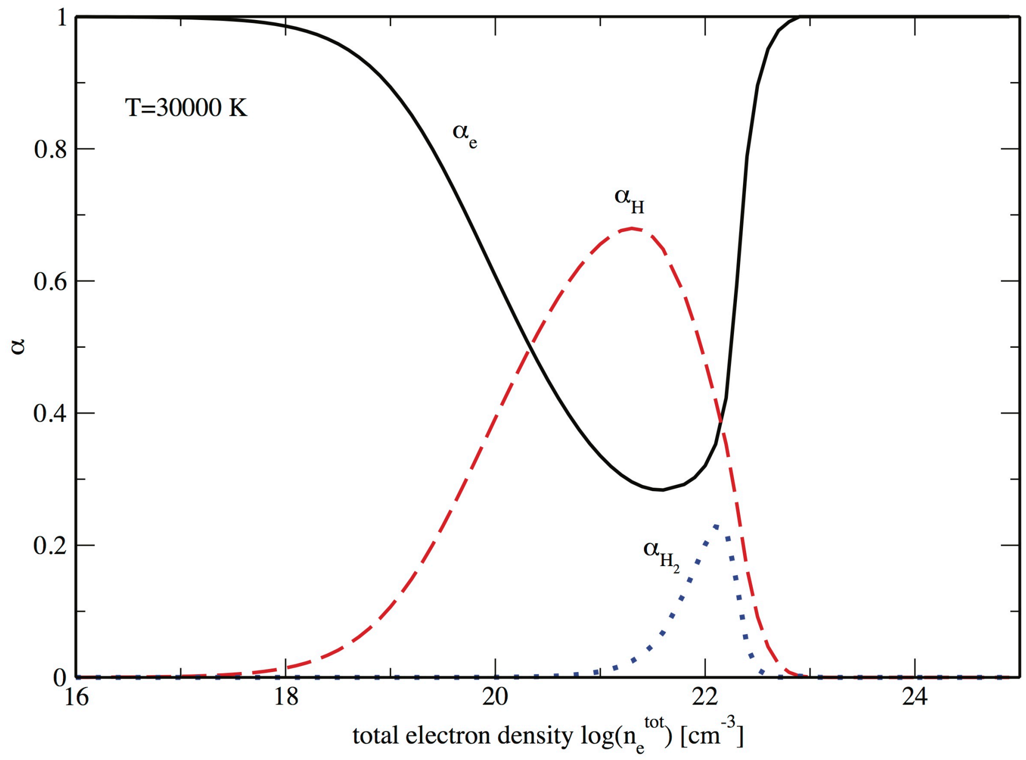
medium modifications

Debye screening

$$\mu_e = \mu_e^{\mathrm{id}} + \Delta_e$$

$$\Delta_e = \Delta_p = -\kappa e^2/2$$

$$\kappa^2 = \left(\frac{4\pi \sum_i n_i e_i^2}{k_B T}\right)$$



neutral bound states unshifted – at the Mott density merging with the continuum

Homogeneous (uniform) electron gas

specific mean potential energy $v = V/N$

virial expansion

$$\kappa^2 = \frac{ne^2}{\epsilon_0 k_B T}, \qquad \lambda^2 = \frac{\hbar^2}{m k_B T}, \qquad \tau = \frac{e^2\sqrt{m}}{4\pi\epsilon_0\sqrt{k_B T}\hbar}.$$

$$v(T,n) = v_0(T)n^{1/2} + v_1(T)n\ln\left(\kappa^2\lambda^2\right) + v_2(T)n + v_3(T)n^{3/2}\ln\left(\kappa^2\lambda^2\right) + v_4(T)n^{3/2} + \mathcal{O}(n^2\ln(n))$$

$$\begin{aligned}
v_0(T) &= -\frac{\sqrt{\pi}}{T^{1/2}}, \qquad v_1(T) = -\frac{\pi}{2T^2}, \\
v_2(T) &= -\frac{\pi}{T}\left[\frac{1}{2} - \frac{\sqrt{\pi}}{2}(1+\ln(2))\frac{1}{T^{1/2}} + \left(\frac{C}{2} + \ln(3) - \frac{1}{3} + \frac{\pi^2}{24}\right)\frac{1}{T}\right. \\
&\quad \left. -\sqrt{\pi}\sum_{m=4}^{\infty}\frac{m}{2^m\Gamma(m/2+1)}\left(\frac{-1}{T^{1/2}}\right)^{m-1}\left[2\zeta(m-2) - (1-4/2^m)\zeta(m-1)\right]\right], \\
v_3(T) &= -\frac{3\pi^{3/2}}{2T^{7/2}}.
\end{aligned}$$

(atomic units)

fourth virial coefficient? $v_4(T)$

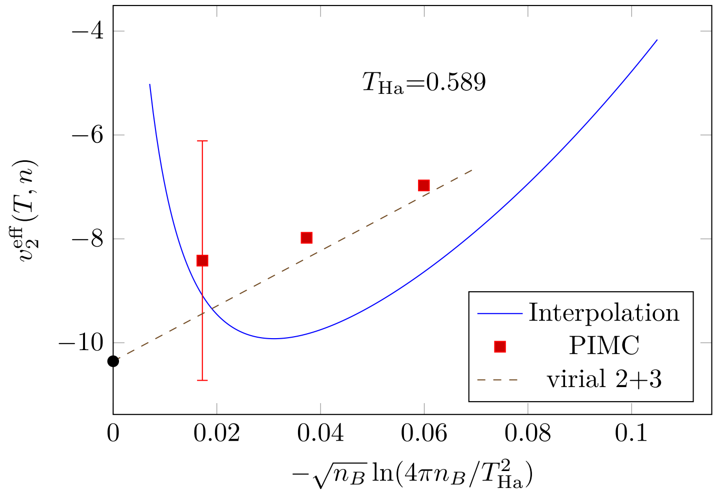
analytical expressions from perturbation theory

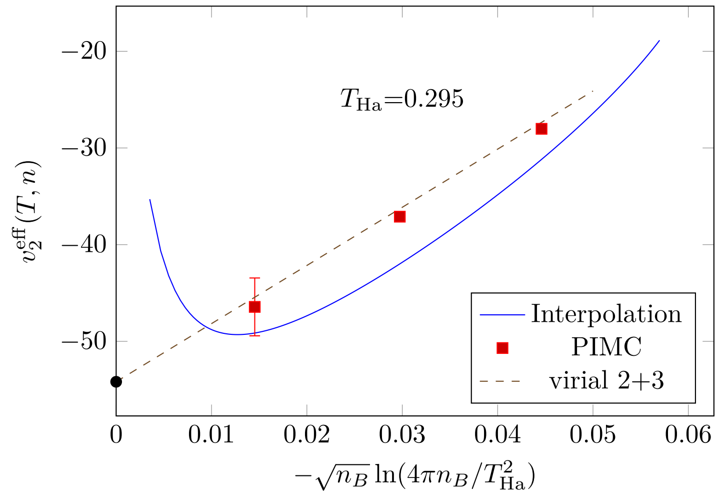
Virial plots for isotherms

reduced thermodynamic functions:
subtraction of known terms

$$v_2^{\rm eff}(T,n) = \left[v(T,n) - v_0(T) n_{\rm B}^{1/2} - v_1(T) n_{\rm B} \ln\left(\frac{4\pi n_{\rm B}}{T_{\rm Ha}^2}\right)\right] / n_{\rm B}$$

- isotherms from PIMC simulations





- interpolation formula (S.Groth et al., Phys. Rev. Lett. **119**, 135001 (2017))
- virial expansion $v_2^{\rm eff}(T,n) = v_2(T) + v_3(T) n_{\rm B}^{1/2} \ln(4\pi n_{\rm B}/T_{\rm Ha}^2) + \mathcal{O}[n^{1/2}].$

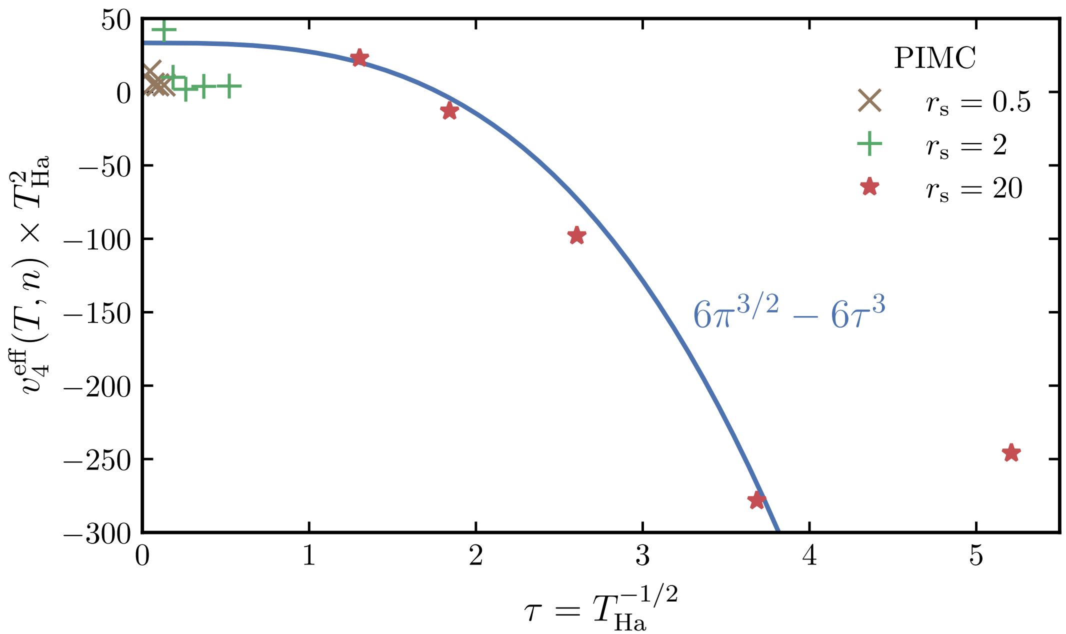
G.R., T.Dornheim, J Vorberger, D.Blaschke, B.Mahato, Phys. Rev. E **109**, 025202 (2024)

Fourth virial coefficient

extraction of the fourth virial coefficient

$$\Delta v_3^{\rm red}(T,n) = \left[v^{\rm PIMC} - v^{(1)}(T,n) - v_2(T)n - v_3(T)n^{3/2}\ln\left(\frac{4\pi n}{T^2}\right)\right]\frac{T}{\pi n}.$$

$$v_4^{\rm eff}(T,n) = \Delta v_3^{\rm red}(T,n)\,\frac{\pi}{T n^{1/2}} = v_4(T) + \mathcal{O}(n^{1/2}\ln(n))$$



Interpolation formulas:

G.R., T. Dornheim, J. Vorberger, D. Blaschke, B. Mahato, Phys. Rev. E **109**, 025202 (2024)

Fourth virial coefficient of interest for helioseismology

Dielectric function

Response of matter to electric fields: permittivity, dielectric function

Transverse part – longitudinal part refraction index

absorption coefficient

Maxwell's equations, μ = 1,

$$\alpha(\omega) = \frac{\omega}{c\,n(\omega)} \operatorname{Im} \varepsilon(\omega)$$

$$k = \left(n(\omega) + i\frac{c}{2\omega}\alpha(\omega)\right)\frac{\omega}{c} = \sqrt{\varepsilon(\omega)}\frac{\omega}{c}$$

$$n(\omega) = \frac{1}{\sqrt{2}}\sqrt{\operatorname{Re}\varepsilon(\omega) + |\varepsilon(\omega)|}$$

$$\lim_{k\to 0} \epsilon_t(\vec{k},\omega) = \left(n(\omega) + \tfrac{ic}{2\omega}\alpha(\omega)\right)^2$$

optical information: reflection, absorption

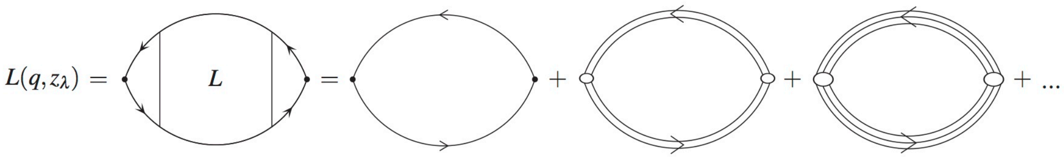
Optical (dynamic) conductivity, dynamical collision frequency

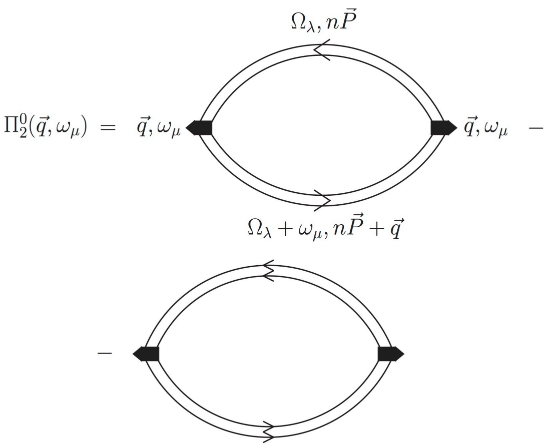
$$\epsilon(\vec{k},\omega) = 1 + \frac{i}{\epsilon_0\omega}\sigma(\vec{k},\omega) = 1 - \frac{\omega_{\rm pl}^2}{\omega(\omega - i\nu(\vec{k},\omega))}$$

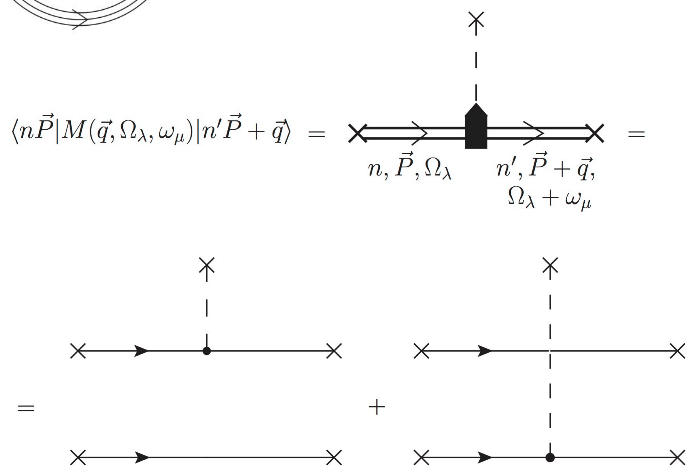
dynamical structurfactor (Thomson scattering)

$$S(\vec{k},\omega) = \frac{1}{\pi\,V(k)}\,\frac{1}{\mathrm{e}^{-\beta\hbar\omega}-1}\,\operatorname{Im}\epsilon_l^{-1}(\vec{k},\omega)$$

Cluster decomposition of the polarization function







$$M_{\nu\nu'}(\mathbf{q}) = \langle \nu, \mathbf{P}| M(\mathbf{q}, z_\lambda, z_\mu)|\nu', \mathbf{P}+\mathbf{q}\rangle = \sum_{\mathbf{p}_1,\mathbf{p}_2} \psi^*_{\nu,\mathbf{P}}(p_1,p_2)[\psi_{\nu',\mathbf{P}+\mathbf{q}}(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2)+\psi_{\nu',\mathbf{P}+\mathbf{q}}(\mathbf{p}_1,\mathbf{p}_2+\mathbf{q})]$$

dipole matrix element

$$\Pi_2^0(\mathbf{q}, z) = \sum_{n,n',P} |M_{n,n'}(\mathbf{q})|^2 \, \frac{g(E^0_{n,\mathbf{P}}) - g(E^0_{n,\mathbf{P}+\mathbf{q}})}{z + E^0_{n,\mathbf{P}} - E^0_{n',\mathbf{P}+\mathbf{q}}}$$

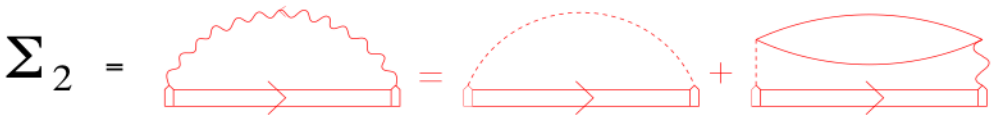
unperturbed energies $E^0_{n,P}$

Doppler broadening

Polarization function: bound state contribution

Modification of two-particle states due to self-energy:

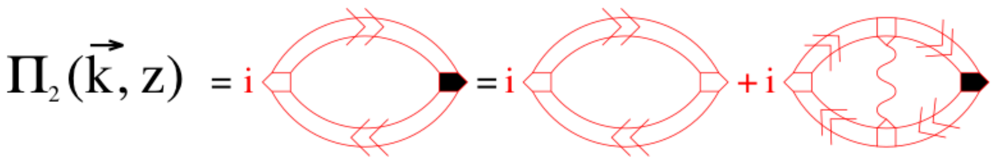
screened Born approximation



wavy line: dynamically screened Coulomb interaction, $\epsilon(\vec{q}, \omega)$

strong collisions: T matrix (instead of an empirical cut-off)

polarization function



modified bound state wave function (coupling to the entire plasma, collective effects)

Problems

- Potentials are in general four-point functions, dynamical, energy dependent, non-local, three-body contributions, etc.
- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)
- Convergence of perturbation expansions, analytical behavior
- Bound/free state contribution? Ionization degree?
- Avoid double counting
- But: exact results in limiting cases, benchmarks for simulations

Virial expansions

short-range interaction

$$p^{\rm sr}(T,n) = b_1^{\rm sr}(T)n + b_2^{\rm sr}(T)n^2 + b_3^{\rm sr}(T)n^3 + \dots .$$

second virial coefficient: classical limit $b_2^{\rm sr}(T) = k_B T \int d^3r \left(e^{-V(r)/k_BT} - 1\right)$

Coulomb systems: long-range Coulomb interaction

$$F(T,\Omega,N) = \Omega k_B T \left\{ n \ln n + [\ln(\Lambda^3) - 1]n \right.$$
$$-A_0(T)n^{3/2} - A_1(T)n^2 \ln n - A_2(T)n^2$$
$$\left. -A_3(T)n^{5/2} \ln n - A_4(T)n^{5/2} + \mathcal{O}(n^3 \ln n) \right\}$$

Debye $A_0(T) = \kappa^3/(12\pi n^{3/2})$ screening parameter $\kappa^2 \;=\; ne^2/(\epsilon_0 k_B T)$

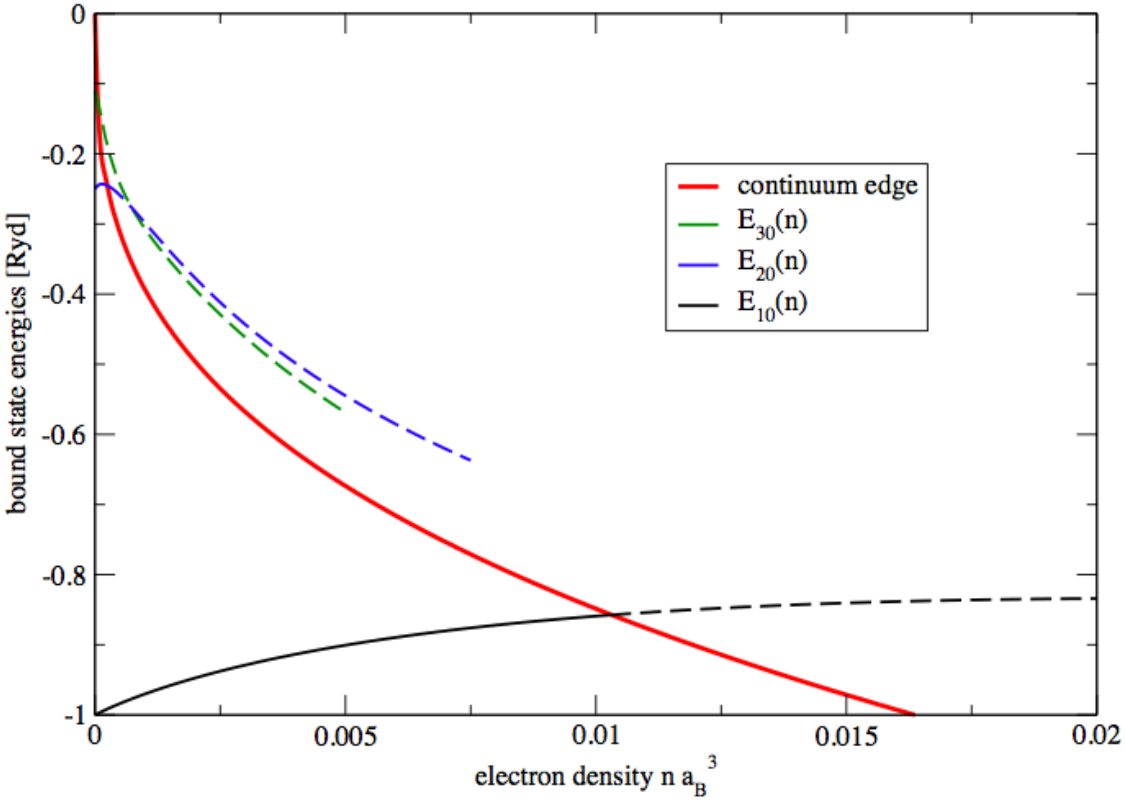
second virial coefficient $A_2(T) = 2\pi\lambda^3 K(\xi) + \frac{\pi}{3}\left(\frac{e^2}{4\pi\epsilon_0 k_B T}\right)^3 \ln(\kappa\lambda/n^{1/2})$

thermal wave length $\lambda^2 = \hbar^2/(mk_BT)$ $\xi = -e^2/(4\pi\epsilon_0 k_B T\lambda) = ({\rm Hartree}/k_BT)^{1/2}$

W.-D. Kraeft, D. Kremp, W. Ebeling, G.R., *Quantum Statistics of Charged Particle Systems,* 1986

Shift of binding energies

$$\lim_{n\to 0}\Delta E_{10}^{\rm PF} = \frac{n}{2}\sum_q \frac{4\pi e^2}{q^2}\phi_{10}(q)[\phi_{10}(0)-\phi_{10}(q)] = 32\pi n' - 20\pi n' = 12\pi n'$$



H-Plasma:
Shift of the ground state and two excited states, Pauli-Fock-approximation, T=0

$$\lim_{n\to 0}\Delta E_{20}^{\rm PF} = 48\pi n'$$

$$\lim_{n\to 0}\Delta E_{30}^{\rm PF} = 108\pi n'$$

W. Ebeling, W.D. Kraeft, G.R.
Bound States in Coulomb Systems
Contr. Plasma Phys. **52**, 7 (2012)

$$\Delta E^{\rm Fock}(p=0) = -\sum_q V(q) f_e(q) = -\frac{4p_F}{\pi} = -4\left(\frac{3n'}{\pi}\right)^{1/3}$$

Pauli blocking and Mott effect

Two different fermions (a,b: proton,neutron) form a bound state (c: deuteron).

$$c_q = \sum_p F(q,p) a_p b_{q-p}$$

Is the bound state a boson? Commutator relation

$$\left[c_q, c_{q'}^+\right]_- = \sum_{p,p'} F(q,p) F^*(q',p') \left[a_p b_{q-p}, b_{q'-p'}^+ a_{p'}^+\right]_-$$

$$\underline{a_p b_{q-p} b_{q'-p'}^+ a_{p'}^+} + a_p b_{q'-p'}^+ b_{q-p} a_{p'}^+ - a_p b_{q'-p'}^+ b_{q-p} a_{p'}^+ - b_{q'-p'}^+ a_p b_{q-p} a_{p'}^+$$

$$+ b_{q'-p'}^+ a_p b_{q-p} a_{p'}^+ + b_{q'-p'}^+ a_p a_{p'}^+ b_{q-p} - b_{q'-p'}^+ a_p a_{p'}^+ b_{q-p} \underline{- b_{q'-p'}^+ a_{p'}^+ a_p b_{q-p}}$$

$$= a_p a_{p'}^+ \delta_{q-p,q'-p'} - b_{q'-p'}^+ b_{q-p} \delta_{p,p'} = \left(\delta_{p,p'} - a_{p'}^+ a_p\right) \delta_{q-p,q'-p'} - b_{q'-p'}^+ b_{q-p} \delta_{p,p'}$$

$$\left[c_q, c_{q'}^+\right]_- = \sum_{p,p'} F(q,p) F^*(q',p') \left[\left(\delta_{p,p'} - a_{p'}^+ a_p\right) \delta_{q-p,q'-p'} - b_{q'-p'}^+ b_{q-p} \delta_{p,p'}\right]$$

$$= \sum_p F(q,p) F^*(q,p) \delta_{q,q'} - \sum_{p,p'} F(q,p) F^*(q',p') \left[\left(a_{p'}^+ a_p\right) \delta_{q-p,q'-p'} + \left(b_{q'-p'}^+ b_{q-p}\right) \delta_{p,p'}\right]$$

averaging

$$\left\langle \left[c_q, c_{q'}^+\right]_- \right\rangle = \delta_{q,q'} \left[1 - \sum_p F(q,p) F^*(q,p) \left(\left\langle a_p^+ a_p \right\rangle + \left\langle b_{q-p}^+ b_{q-p} \right\rangle\right)\right]$$

Fermionic substructure: phase space occupation, “excluded volume”

Optical Properties

$$\epsilon(\mathbf{k},\omega) = 1 + \frac{1}{\epsilon_0 k^2}\Pi(\mathbf{k},\omega) \qquad \Pi(\mathbf{k},\omega) = \Pi_1(\mathbf{k},\omega) + \Pi_2(\mathbf{k},\omega) + \ldots$$

- polarization function $\Pi(\mathbf{k},\omega)$ from many-body theory using cluster decomposition

  $\Pi_1(\mathbf{k},\omega)$ - single-particle contribution[1]

  $\Pi_2(\mathbf{k},\omega)$ - two-particle contributions (bound states) [2]

- optical information: refraction index & absorption coefficient

  $\Pi_1(\mathbf{k},\omega)$ - bremsstrahlung [1,3], $\Pi_2(\mathbf{k},\omega)$ - spectral line profiles [2]

$$\lim_{k\to 0} \epsilon(\mathbf{k},\omega) = \left(n(\omega) + \frac{ic}{2\omega}\alpha(\omega) \right)^2$$

- dynamical structure factor [1] $\rightarrow$ Thomson scattering

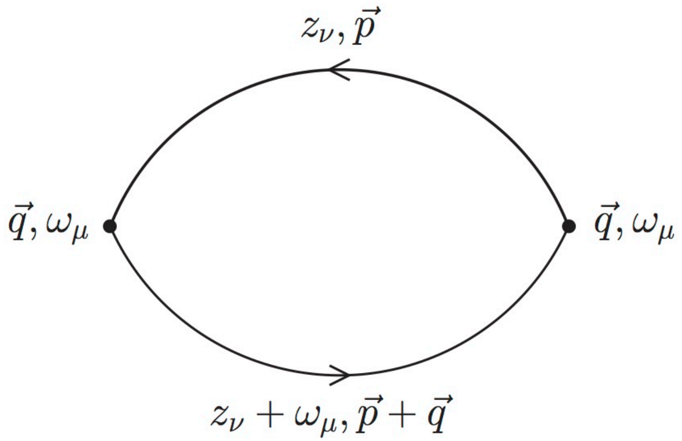
$$S(\mathbf{k},\omega) = \frac{1}{\pi V(k)} \frac{1}{\mathrm{e}^{-\beta\hbar\omega} - 1} \mathrm{Im}\epsilon_l^{-1}(\mathbf{k},\omega)$$

[1] Reinholz, Ann. de Phys. (2005); [2] Omar et al. PRE 2007; [3] Wierling et al. PoP (2001); Fortmann et al. HEDP

Noninteracting Fermi-gas

polarization loop

$$L(\vec{q},\omega_\mu) \approx \Pi_1^0(\vec{q},\omega_\mu) \ =$$



$$L_0(\mathbf{q}, z) = g_\nu \int \frac{d^3p}{(2\pi)^3} \frac{f^0_{\mathbf{p}} - f^0_{\mathbf{p+q}}}{z + \epsilon^0_{\mathbf{p}} - \epsilon^0_{\mathbf{p+q}}}$$

$$S_0(\mathbf{q}, \omega) = \frac{1}{e^{\beta\omega} - 1} g_\nu \int \frac{d^3p}{(2\pi)^3} \left(f^0_{\mathbf{p}} - f^0_{\mathbf{p+q}}\right) \delta(\omega + \epsilon^0_{\mathbf{p}} - \epsilon^0_{\mathbf{p+q}})$$

isothermal compressibility

$$\kappa^{(0)}_{\text{iso}}(T, \mu) = \frac{\beta}{n_B^2} g_\nu \int \frac{d^3p}{(2\pi)^3} f^0_p (1 - f^0_p)$$

$$n_B^{(0)}(\beta, \mu) = \frac{1}{\Omega_0} \sum_p \frac{1}{e^{\beta(\epsilon^0_p - \mu)} + 1} = \frac{1}{\Omega_0} \sum_p f^0_p = \frac{N}{\Omega_0}$$

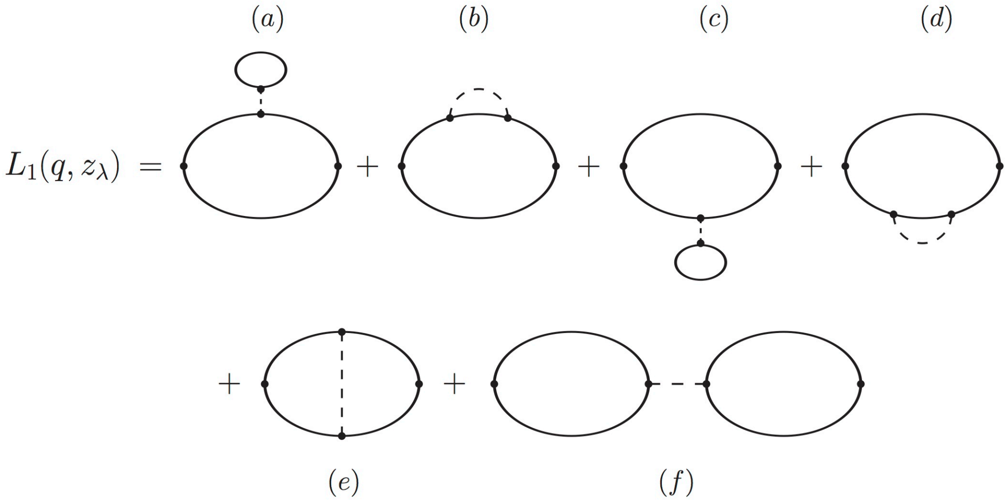
Quasiparticle approximation

Hartree-Fock approximation

$$\epsilon_p^{\rm HF} = \epsilon_p^0 + \sum_k V(\mathbf{p},\mathbf{k};\mathbf{p},\mathbf{k})_{\rm ex} f(\epsilon_k^{\rm HF})$$

$$n_B^{\rm HF}(\beta,\mu) = g_\nu \int \frac{d^3p}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_p^{\rm HF}-\mu)}+1}$$

$$\frac{\partial \mu^{\rm HF}}{\partial n_B}\Big|_T = \left\{ \frac{g_\nu}{2\pi^2} \int_0^\infty p^2 dp f_p^{\rm HF}(1-f_p^{\rm HF})\beta \left[1-\beta\int \frac{d^3k}{(2\pi)^3} V(\mathbf{p},;\mathbf{p},\mathbf{k})_{\rm ex} f_k^{\rm HF}(1-f_k^{\rm HF})\right]\right\}^{-1}$$



$$\kappa_{\rm iso}^{(1)}(T,\mu) = \frac{\beta}{n_B^2} g_\nu \int \frac{d^3p}{(2\pi)^3} f_p^{\rm HF}(1-f_p^{\rm HF}) \left[1-\beta\int \frac{d^3k}{(2\pi)^3} V(\mathbf{p},\mathbf{k};\mathbf{p},\mathbf{k})_{\rm ex} f_k^{\rm HF}(1-f_k^{\rm HF})\right]$$

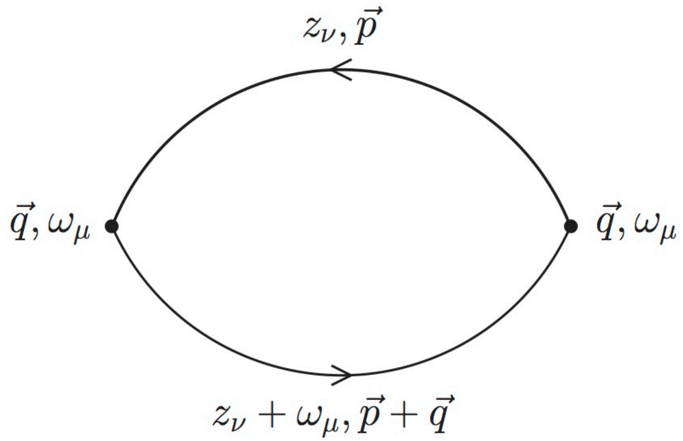
Polarization function

the polarization tensor describes the relation
between the induced electrical current or charge densities
and the total vector or scalar potential, respectively

$$\epsilon_{\text{long}}(\vec{k},\omega) = 1 - \frac{1}{\epsilon_0 k^2}\Pi_{\text{long}}(\vec{k},\omega)$$

Lowest order (0), RPA polarization loop

$$L(\vec{q},\omega_\mu) \approx \Pi_1^0(\vec{q},\omega_\mu) =$$



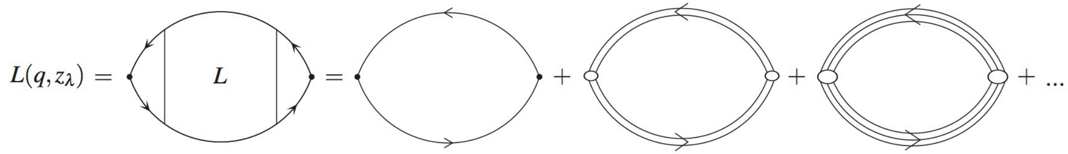
$$L_0(\mathbf{q}, z) = g_\nu \int \frac{d^3p}{(2\pi)^3} \frac{f^0_{\mathbf{p}} - f^0_{\mathbf{p+q}}}{z + \epsilon^0_{\mathbf{p}} - \epsilon^0_{\mathbf{p+q}}}$$

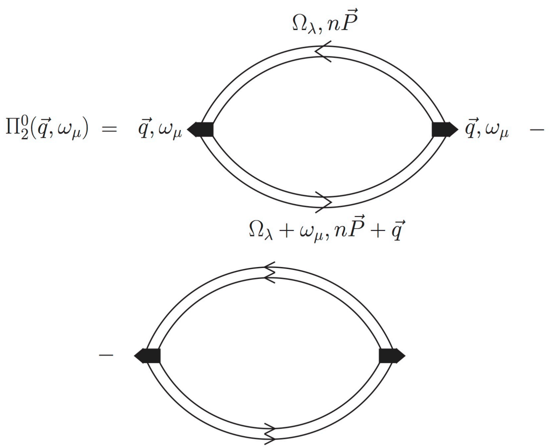
No line spectra, higher order perturbation theory?

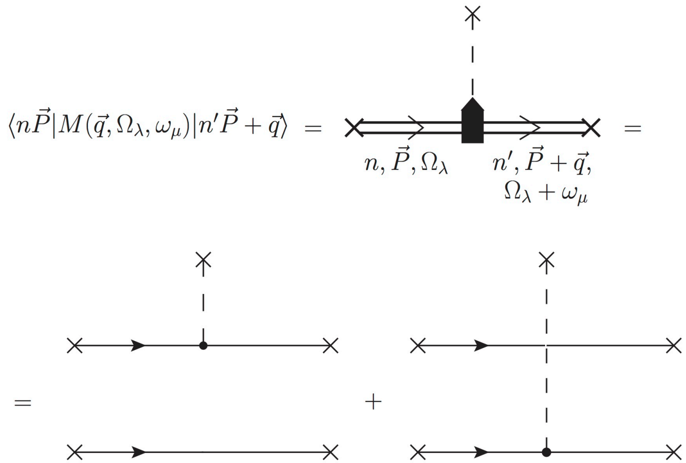
$$\epsilon(\vec{k},\omega) = 1 - \frac{1}{\epsilon_0 k^2}\left(\Pi_1(\vec{k},\omega) + \Pi_2(\vec{k},\omega) + \ldots\right)$$

cluster expansion of polarization function:
contributions of free electrons $\mathbf{\Pi_1}$ und bound states $\mathbf{\Pi_2}$

Cluster decomposition of the polarization function







$$M_{\nu\nu'}(\mathbf{q}) = \langle \nu, \mathbf{P}|M(\mathbf{q}, z_\lambda, z_\mu)|\nu', \mathbf{P} + \mathbf{q}\rangle = \sum_{\mathbf{p}_1, \mathbf{p}_2} \psi^*_{\nu, \mathbf{P}}(p_1, p_2)[\psi_{\nu', \mathbf{P}+\mathbf{q}}(\mathbf{p}_1 + \mathbf{q}, \mathbf{p}_2) + \psi_{\nu', \mathbf{P}+\mathbf{q}}(\mathbf{p}_1, \mathbf{p}_2 + \mathbf{q})]$$

$$\kappa_{\rm iso}^{\rm (BU)}(T, \mu_n, \mu_p) = \frac{\beta}{\Omega_0 n_B^2} \left\{ \sum_{\mathbf{p}} f_p^0 (1 - f_p^0) + \sum_{\alpha, \mathbf{P}} \int_{-\infty}^{\infty} \frac{dE}{\pi} f_2\left(E + \frac{P^2}{4m}\right) \left[1 + f_2\left(E + \frac{P^2}{4m}\right)\right] D_{\alpha, \mathbf{P}}(E) \right\}$$

Quantum electrodynamics

Lagrangian

$$\mathcal{L}(x) = \bar{\psi}(x)\left(i\hbar c\gamma^\mu\partial_\mu - mc^2\right)\psi(x) - \frac{\epsilon_0}{4}c^2 F_{\mu\nu}(x)F^{\mu\nu}(x) - j_\mu(x)A^\mu(x)$$

field strength tensor $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$

4-vector fermion current density $j^\mu(x) = ec\bar{\psi}(x)\gamma^\mu\psi(x) = (c\rho(x), \vec{J}(x))$

Nonrelativistic limit: Hamiltonian, photons

$$\begin{aligned} H &= \sum_{c,p} E_c(\vec{p})a^\dagger_{c,p}a_{c,p} + \sum_{k\lambda}\hbar\omega_k a^\dagger_{k\lambda}a_{-k\lambda} \\ &\quad -\sum_{k\lambda}\vec{j}_k\cdot\vec{\epsilon}_{k\lambda}\left(\frac{\hbar\Omega}{2\epsilon_0\omega_k}\right)^{1/2}(a^\dagger_{-k\lambda}+a_{k\lambda}) + \frac{1}{2}\sum_{cd,pp'k}V_{cd}(k)a^\dagger_{c,p-k}a^\dagger_{d,p'+k}a_{d,p'}a_{c,p} \end{aligned}$$

$$\vec{j}_k = \frac{1}{\Omega}\sum_{c,p}\frac{e_c}{m_c}\hbar\vec{p}\,n^c_{p,k}$$

H. Reinholz, Ann. Phys. (Paris) **30**, 1 (2005)

Fermi's golden rule

Coulomb interaction

Hamiltonian

$$H = \sum_{1} E(1) a_1^\dagger a_1 + \sum_{121'2'} V(12,1'2') a_1^\dagger a_2^\dagger a_{2'} a_{1'}$$

$\{1\} = \{\vec{p}_1, \sigma_1, c_1\}$: {momentum, spin, species}

$E(1) \; = \; p_1^2/2m_1$: kinetic energy

$$V(12,1'2') \; = \; e_1 e_2 \hbar^2/(\epsilon_0 \Omega) |\vec{p}_1 \; - \; \vec{p}_2|^{-2} \delta_{p_1+p_2, p_1'+p_2'}$$

Coulomb interaction

Examples: Hydrogen atom
Partially ionized (hydrogen) plasmas
excited semiconductors, metals,…
electrolytes….
dusty plasmas……

Pseudopotentials, polarisation potentials, van der Waals potentials

Beth-Uhlenbeck formula

yields, partial densities

$$Y_{A,Z}^{(0)} \propto n_{A,Z}^{(0)} = g_{A,Z}\left(\frac{2\pi\hbar^2}{Am\lambda_T^{(0)}}\right)^{-3/2} e^{(B_{A,Z}+(A-Z)\lambda_n^{(0)}+Z\lambda_p^{(0)})/\lambda_T^{(0)}}$$

intrinsic partition function

$$R_{A,Z}^{\gamma}(\lambda_T) = 1 + \sum_i^{\text{exc}} \frac{g_{A,Z,i}}{g_{A,Z}} e^{-E_{A,Z,i}/\lambda_T}$$

Inclusion of scattering states: Beth-Uhlenbeck formula: deuteron

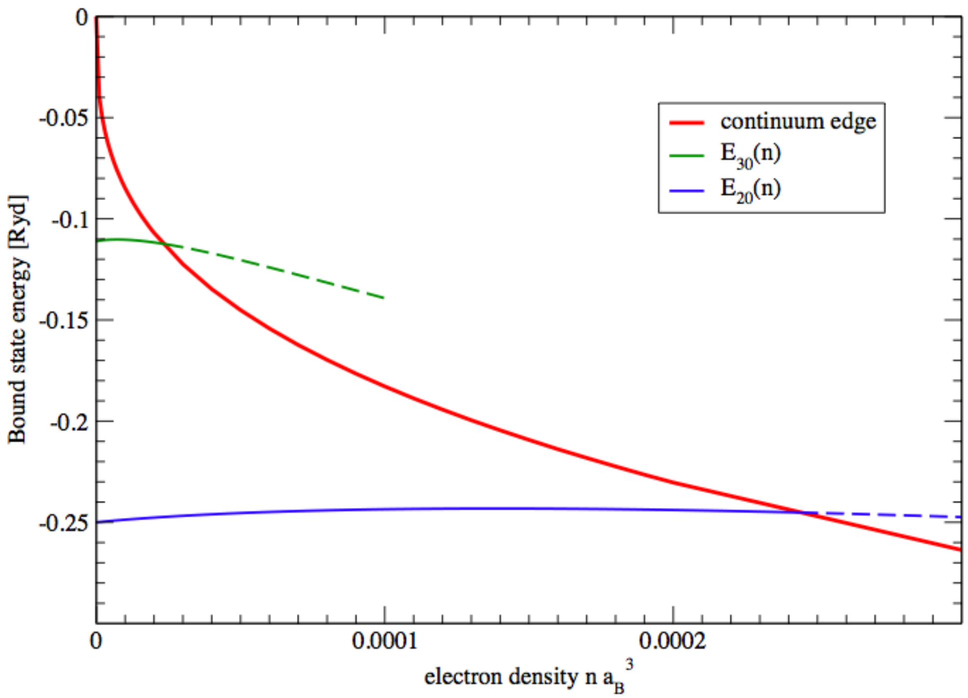
$$R_d^{\text{vir}}(\lambda_T) = 1 - e^{-E_d^{\text{thresh}}/\lambda_T} + e^{-E_d^{\text{thresh}}/\lambda_T}\frac{1}{\pi\lambda_T}\int_0^{\infty} dE e^{-E/\lambda_T}\delta_d(E)$$

effective binding energy: ^{4}H

$$R_{4,1}^{\text{vir}}(\lambda_T) = e^{-E_{t,n}^{\text{eff}}(\lambda_T,0)/\lambda_T + E_{4,1}^{\text{thresh}}/\lambda_T}$$

Shift of binding energies

$$\lim_{n\to 0} \Delta E_{10}^{\rm PF} = \frac{n}{2}\sum_{\tilde{}} \frac{4\pi e^2}{q^2}\phi_{10}(q)[\phi_{10}(0)-\phi_{10}(q)] = 32\pi n' - 20\pi n' = 12\pi n'$$



H-Plasma:
Shift of the ground state and two excited states, Pauli-Fock-approximation, T=0

$$\lim_{n\to 0} \Delta E_{20}^{\rm PF} = 48\pi n'$$

$$\lim_{n\to 0} \Delta E_{30}^{\rm PF} = 108\pi n'$$

$$\Delta E^{\rm Fock}(p=0) = -\sum_q V(q) f_e(q) = -\frac{4p_F}{\pi} = -4\left(\frac{3n'}{\pi}\right)^{1/3}$$

W. Ebeling, W.D. Kraeft, G.R.
Bound States in Coulomb Systems
Contr. Plasma Phys. **52**, 7 (2012)

Many-particle theory

$$n_\tau^{\rm tot}(T,\mu_n,\mu_p) = \frac{1}{\Omega}\sum_{p_1,\sigma_1}\int\frac{d\omega}{2\pi}\frac{1}{e^{(\omega-\mu_\tau)/T}+1}S_\tau(1,\omega)$$

Spectral function S (or A)

- Dyson equation and self energy (homogeneous system)

$$G(1,iz_\nu) = \frac{1}{iz_\nu - E(1) - \Sigma(1,iz_\nu)}$$

- Evaluation of $\Sigma(1,iz_\nu)$:
  perturbation expansion, diagram representation

$$A(1,\omega) = \frac{2{\rm Im}\,\Sigma(1,\omega+i0)}{[\omega - E(1) - {\rm Re}\,\Sigma(1,\omega)]^2 + [{\rm Im}\,\Sigma(1,\omega+i0)]^2}$$

approximation for self energy $\longrightarrow$ approximation for equilibrium correlation functions

alternatively: simulations, path integral methods

Equations of state

many-particle system, temperature T, volume Ω, particle number N, density $n=N/\Omega$
thermodynamic potential: Free energy $F(T,\Omega,N)$

pressure $$p(T,n) = \left(\frac{\partial}{\partial\Omega} F(T,\Omega,N)\right)\Big|_{T,N}$$

mean potential energy $$V(T,\Omega,N) = e^2 \frac{\partial}{\partial(e^2)} F(T,\Omega,N)$$

quantum statistical approach: grand canonical ensemble

statistical operator, $T = 1/\beta,\ \mu$ chemical potential/T

$$\rho(\beta,\mu) = \frac{1}{Z_{g.c.}} e^{-\beta H + \mu N} \qquad Z_{g.c.} = \mathrm{Tr}\, e^{-\beta H + \mu N} \qquad p\Omega = -k_B T\ \ln Z_{g.c.}$$

density $n(T,\mu) = \frac{1}{\mathrm{Vol}} \int d^3r \langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r})\rangle$

Fermi function

$$\mathrm{Tr}\{\rho\, \psi^\dagger(1',t')\, \psi(1,t)\} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\frac{i}{\hbar}\omega(t'-t)} f(\omega) A(1,1';\omega)$$

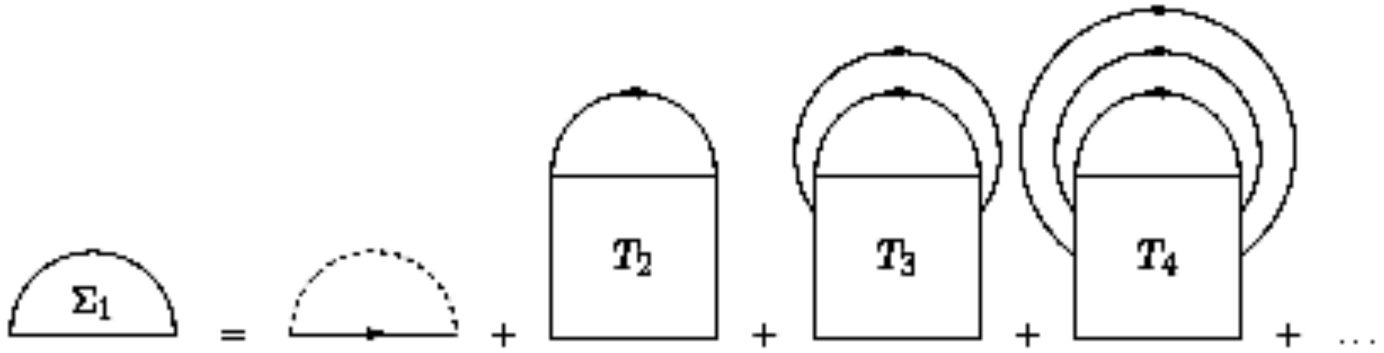
spectral function

Correlation function

Green's function method

path integral Monte Carlo (PIMC) simulations

Cluster decomposition of the self-energy



T-matrices: bound states, scattering states
Including clusters like new components
chemical picture,
mass action law, nuclear statistical equilibrium (NSE)

Mean potential energy

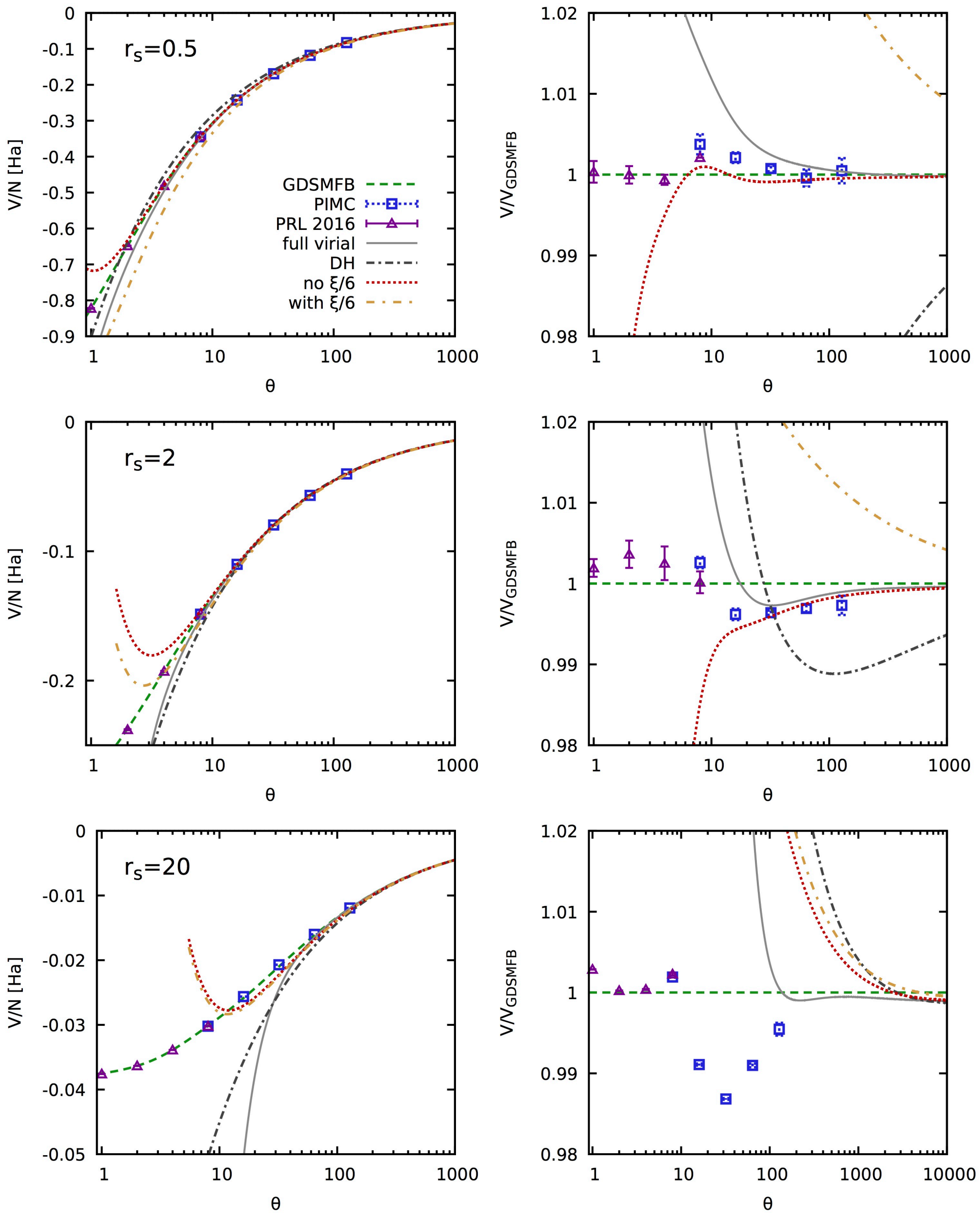
$$\frac{V}{Nk_BT} = -\frac{\kappa^3}{8\pi n} - 2\pi n\lambda^3\left[-\frac{\xi}{4} - \frac{\sqrt{\pi}}{4}\xi^2(1+\ln 2)\right.$$
$$\left. - \frac{\xi^3}{2}\left(\ln\kappa\lambda + \frac{C}{2} + \ln 3 - \frac{1}{3} - \frac{\pi^2}{24}\right)\right].$$

$$\frac{V}{N\,k_BT} = \frac{V_1}{N\,k_BT} + \frac{V_2}{N\,k_BT}$$

Exact results, not debated:
Debye, logarithmic ξ^3-term

$$\frac{V_1}{N\,k_BT} = -\frac{\kappa^3}{8\pi n} + \pi n\lambda^3\xi^3\ln(\kappa\lambda)$$

$$v^{\mathrm{red}} = \frac{\Delta v}{\pi n\lambda^3\xi\,k_BT} = \left[\frac{V}{N\,k_BT} - \frac{V_1}{N\,k_BT}\right]\frac{1}{\pi n\lambda^3\xi}$$



T. Dornheim et al., High Energy Density Physics **45**, 101015 (2022)

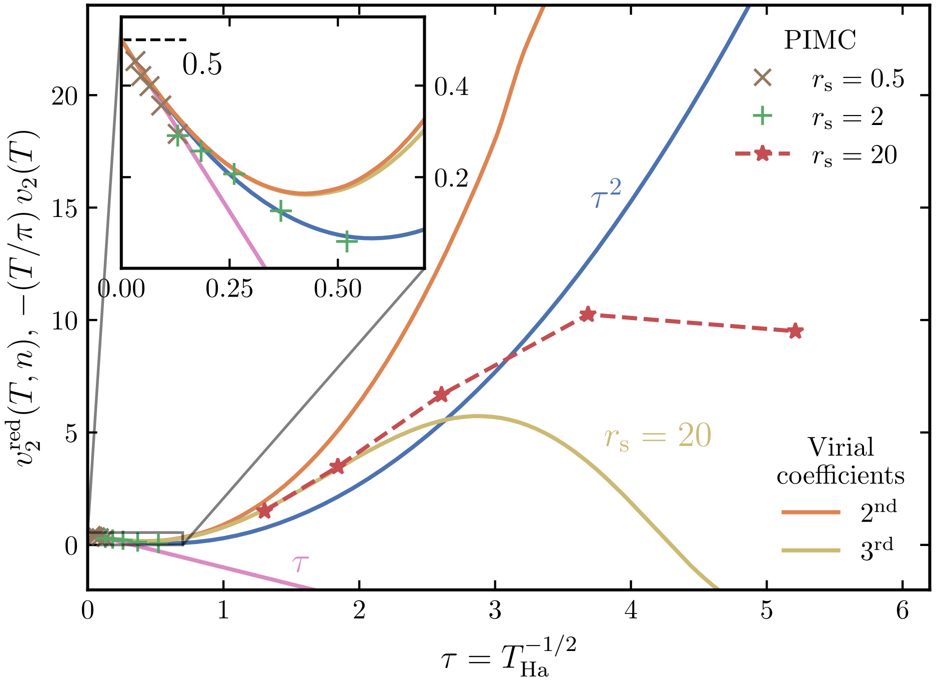
Virial plot

extraction of the second virial coefficient

$$v^{(1)}(T,n) = -\frac{\sqrt{\pi}}{T^{1/2}}n^{1/2} - \frac{\pi}{2T^2}n\ln\left(\frac{4\pi n}{T^2}\right)$$

$$v_2^{\mathrm{red}}(T,n) = \left[v^{\mathrm{PIMC}} - v^{(1)}(T,n)\right]\frac{-T}{\pi n} = \frac{-T}{\pi}v_2(T) + \mathcal{O}(n^{1/2}\ln(n))$$

$$= \frac{1}{2} - \frac{\sqrt{\pi}}{2}(1+\ln(2))\tau + \left(\frac{C}{2} + \ln(3) - \frac{1}{3} + \frac{\pi^2}{24}\right)\tau^2 + \mathcal{O}(\tau^3) + \mathcal{O}(n^{1/2}\ln(n))$$



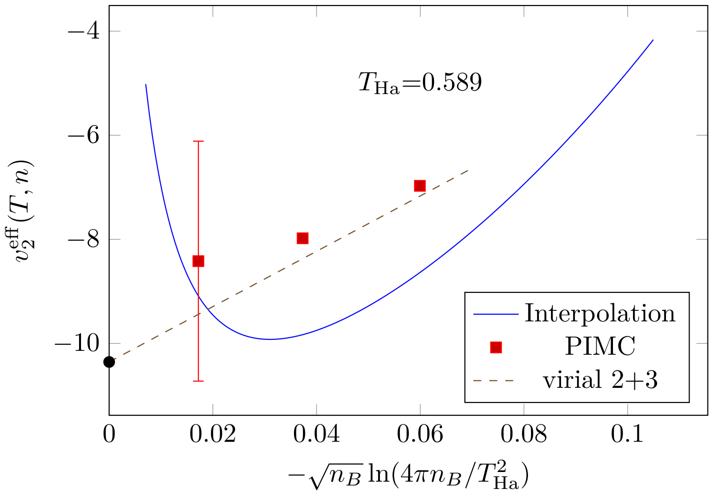
G.R., Contrib. Plasma Phys. **63**, e202300002 (2023)

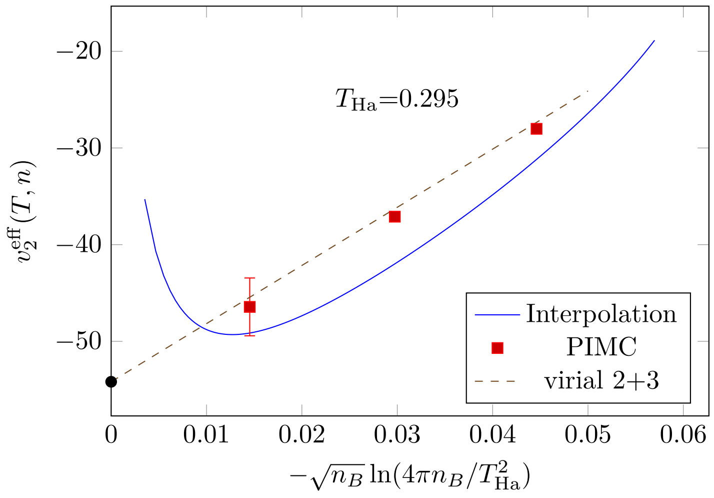
Virial plots for isotherms

$$v_2^{\mathrm{eff}}(T,n) = \Big[v(T,n) - v_0(T)n_{\mathrm{B}}^{1/2} - v_1(T)n_{\mathrm{B}}\ln\left(\frac{4\pi n_{\mathrm{B}}}{T_{\mathrm{Ha}}^2}\right)\Big]/n_{\mathrm{B}}$$

$$v_2^{\mathrm{eff}}(T,n) = v_2(T) + v_3(T)n_{\mathrm{B}}^{1/2}\ln(4\pi n_{\mathrm{B}}/T_{\mathrm{Ha}}^2) + \mathcal{O}[n^{1/2}].$$

Isotherms for T_{Ha} = 0.589 and 0.295: PIMC simulations





Interpolation formula for the free energy (S.Groth et al., Phys. Rev. Lett. **119**, 135001 (2017))

$$f_{\mathrm{XC}}^{\mathrm{GDSMFB}}(r_S,\Theta) = -\frac{1}{r_s}\frac{a(\Theta)+b(\Theta)\sqrt{r_s}+c(\Theta)r_s}{1+d(\Theta)\sqrt{r_s}+e(\Theta)r_s},$$

$$v(r_s,\Theta) = 2f_{\mathrm{XC}}(r_s,\Theta) + r_s\frac{\partial f_{\mathrm{XC}}(r_s,\Theta)}{\partial r_s}\Big|_\Theta .$$

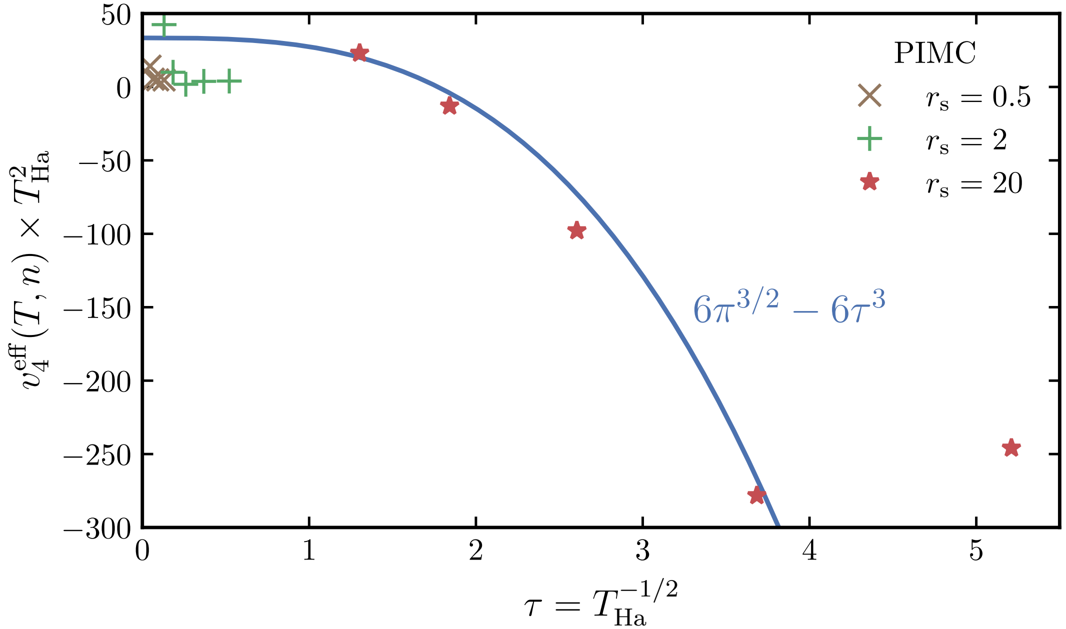
G.R., T.Dornheim, J Vorberger, D.Blaschke, B.Mahato, Phys. Rev. E **109**, 025202 (2024)

Fourth virial coefficient

extraction of the fourth virial coefficient

$$\Delta v_3^{\rm red}(T,n) = \left[v^{\rm PIMC} - v^{(1)}(T,n) - v_2(T)n - v_3(T)n^{3/2}\ln\left(\frac{4\pi n}{T^2}\right)\right]\frac{T}{\pi n}.$$

$$v_4^{\rm eff}(T,n) = \Delta v_3^{\rm red}(T,n)\,\frac{\pi}{T n^{1/2}} = v_4(T) + \mathcal{O}(n^{1/2}\ln(n))$$



Interpolation formulas:

G.R., T. Dornheim, J. Vorberger, D. Blaschke, B. Mahato, Phys. Rev. E **109**, 025202 (2024)

Two-component plasmas: Thermodynamics of atomic and ionized hydrogen: Analytical results versus equation-of-state tables and Monte Carlo data

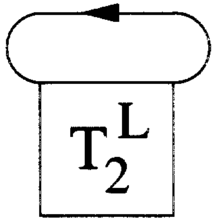
A. Alastuey and V. Ballenegger, Phys. Rev. E **86**, 066402 (2012)

Inclusion of bound states

low density limit:

$$G_2^L(12,1'2',i\lambda) = \sum_{n\mathbf{P}} \Psi_{n\mathbf{P}}(12) \frac{1}{i\omega_\lambda - E_{n\mathbf{P}}} \Psi^*_{n\mathbf{P}}(12)$$

$\Sigma =$



$$n(\beta,\mu) = \sum_1 f_1(E^{\text{quasi}}(1)) + \sum_{2,n\mathbf{P}}^{\text{bound}} g_{12}(E_{n\mathbf{P}})$$

$$+ \sum_{2,n\mathbf{P}} \int_0^\infty \mathrm{d}k\, \delta_{\mathbf{k},\mathbf{p}_1-\mathbf{p}_2} g_{12}(E^{\text{quasi}}(1) + E^{\text{quasi}}(2)) 2\sin^2\delta_n(k) \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}k}\delta_n(k)$$

- generalized Beth-Uhlenbeck formula
  correct low density/low temperature limit:
  mixture of free particles and bound clusters

Beth-Uhlenbeck formula

rigorous results at low density: virial expansion

Beth-Uhlenbeck formula

$$
\begin{aligned}
n(T,\mu) &= \frac{1}{V}\sum_p e^{-(E(p)-\mu)/k_BT} \\
&+ \frac{1}{V}\sum_{nP} e^{-(E_{nP}-2\mu)/k_BT} \\
&+ \frac{1}{V}\sum_{\alpha P}\int_0^\infty \frac{dE}{2\pi} e^{-(E+P^2/4m-2\mu)/k_BT}\frac{d}{dE}\delta_\alpha(E) \\
&+ \ldots
\end{aligned}
$$

$\delta_\alpha(E)$: scattering phase shifts, channel α

Ideal mixture of reacting nuclides

$$n_p(T,\mu_p,\mu_n) = \frac{1}{V}\sum_{A,\nu,K} Z_A f_A\{E_{A,\nu K} - Z_A\mu_p - (A-Z_A)\mu_n\}$$

$$n_n(T,\mu_p,\mu_n) = \frac{1}{V}\sum_{A,\nu,K} (A-Z_A) f_A\{E_{A,\nu K} - Z_A\mu_p - (A-Z_A)\mu_n\}$$

$$f_{A(z)} = \frac{1}{\exp(z/T) - (-1)^A}$$

mass number *A*,
charge Z_A,
energy $E_{A,\nu,K}$,
ν internal quantum number,
~*K* center of mass momentum

Chemical equilibrium, mass action law,
Nuclear Statistical Equilibrium (NSE)

Quantum statistical approach

1. Perturbation expansion:
   diagram representation, partial summations

   - pressure and two-particle Green function

$$p(\beta,\mu_e,\mu_i) = p_{\rm id} - \frac{1}{2V}\int_0^1 \frac{d\lambda}{\lambda}\int d1 d\tilde{1} V(1\tilde{1}) G_2(1,\tilde{1},1^{++},1^{+} : \tilde{t}_1 = t_1^{+})$$

   - density and single-particle Green function

$$n_c(\beta,\mu_{c'}) = \frac{g_c}{\Omega}\sum_p \frac{1}{2\pi}\int_{-\infty}^{\infty} f_1(\omega;\beta,\mu_c) A(1,\omega;\beta,\mu_{c'}) d\omega$$

$$f_1(\omega;\beta,\mu_c) = [\exp(\beta(\omega-\mu_c))+1]^{-1}$$

$$A(1,\omega) = \frac{2{\rm Im}\Sigma(1,\omega-i0)}{[\omega - E(1) - {\rm Re}\Sigma(1,\omega)]^2 + [{\rm Im}\Sigma(1,\omega-i0)]^2}$$

2. Numerical methods:
   simulations, together with Local density approximations (LDA)

Virial expansion of the pressure

Chemical potentials - fugacities

$$z_a = \frac{2s_a + 1}{\Lambda_a^3} \exp(\beta\mu_a) = n_a \exp(\beta\mu_a^{\mathrm{ex}})$$

(excess part of the chemical potentials)

$$\beta p = z_e + z_i + \frac{\kappa_g^3}{12\pi} f(\kappa_g \lambda) + 8\pi z_e z_i \lambda^3 \exp[1 + \beta e^2 \kappa_g] \sigma_{\mathrm{BPL}}(T) + \cdots ,$$

$$\kappa_g^2 = 4\pi\beta(z_e + z_i)e^2$$

$$f(x) = \left[1 - \frac{3\sqrt{\pi}}{16} x + \frac{1}{10} x^2 + \cdots \right]$$

Brillouin-Planck-Larkin internal partition function

W. Ebeling, W.D. Kraeft, G.R.,
On the quantum statistics of bound states within the Rutherford model of matter,
Ann. Phys. (Berlin) **525**, 311 (2012)

Quantum statistical approach

The total density as well as the DoS are given by the spectral function A,

$$n_e^{\text{total}}(T, \mu_e, \mu_a) = \frac{1}{\Omega} \sum_1 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hat{f}_e(\omega) A_e(1, \omega) = \int_{-\infty}^{\infty} d\omega \hat{f}_e(\omega) D_e(\omega)$$

$$|1\rangle = |\mathbf{p}_1, \sigma_1\rangle$$

which is related to the Green function and the self-energy as

$$A(1, \omega) = 2\,\mathrm{Im}\, G(1, \omega - i0) = 2\,\mathrm{Im} \frac{1}{\omega - E(1) - \Sigma(1, \omega - i0)}$$

$$E(1) = p_1^2/(2m)$$

A cluster decomposition for the self-energy is possible so that a quasiparticle (free) contribution can be separated,

$$A_e(1, \omega) \approx \frac{2\pi\, \delta(\omega - E_e^{\text{quasi}}(1))}{1 - \frac{d}{dz} \mathrm{Re}\, \Sigma_e(1, z)|_{z = E_e^{\text{quasi}} - \mu_e}} - 2\mathrm{Im}\, \Sigma_e(1, \omega + i0) \frac{d}{d\omega} \frac{\mathcal{P}}{\omega + \mu_e - E_e^{\text{quasi}}(1)}$$

$$E^{\text{quasi}}(1) = p_1^2/(2m) + \mathrm{Re}\Sigma(1, \omega)|_{\omega = E^{\text{quasi}}(1)}$$

We obtain the generalized Beth-Uhlenbeck formula (quasiparticles) after calculating the self-energy in ladder approximation.
Bound states appear as solution of an in-medium Schrödinger equation.

Quantum statistical approach

The total density as well as the DoS are given by the spectral function A,

$$n_e^{\text{total}}(T,\mu_e,\mu_a) = \frac{1}{\Omega}\sum_1 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hat{f}_e(\omega) A_e(1,\omega) = \int_{-\infty}^{\infty} d\omega \hat{f}_e(\omega) D_e(\omega)$$

$$A(1,\omega) = 2\,\mathrm{Im}\,G(1,\omega - i0) = 2\,\mathrm{Im}[\omega - E(1) - \Sigma(1,\omega - i0)]^{-1}$$

A cluster decomposition for the self-energy is possible so that a quasiparticle (free) contribution can be separated,

$$A_e(1,\omega) \approx \frac{2\pi\,\delta(\omega - E_e^{\text{quasi}}(1))}{1 - \frac{d}{dz}\mathrm{Re}\,\Sigma_e(1,z)|_{z=E_e^{\text{quasi}}-\mu_e}} - 2\mathrm{Im}\,\Sigma_e(1,\omega + i0)\frac{d}{d\omega}\frac{\mathcal{P}}{\omega + \mu_e - E_e^{\text{quasi}}(1)}$$

We obtain the generalized Beth-Uhlenbeck formula (quasiparticles)

$$n_e^{\text{total}}(T,\mu_e,\mu_a) = \frac{1}{\Omega}\sum_1 f_e(E^{\text{quasi}}(1))$$

$$+\frac{1}{\Lambda^3}\sum_{i,\gamma} Z_i e^{\beta\mu_i}\left[\sum_{\nu}^{\text{bound}}(e^{-\beta E_{i,\gamma,\nu}} - 1) + \frac{\beta}{\pi}\int_0^{\infty} dE e^{-\beta E}\left\{\delta_{i,\gamma}(E) - \frac{1}{2}\sin[2\delta_{i,\gamma}(E)]\right\}\right]$$

In-medium Schrödinger equation for $E_{i,\gamma,\nu}(T,\mu)$, $\delta_{i,\gamma}(T,\mu)$, channel (spin…) γ

nucleon-nucleon interaction potential

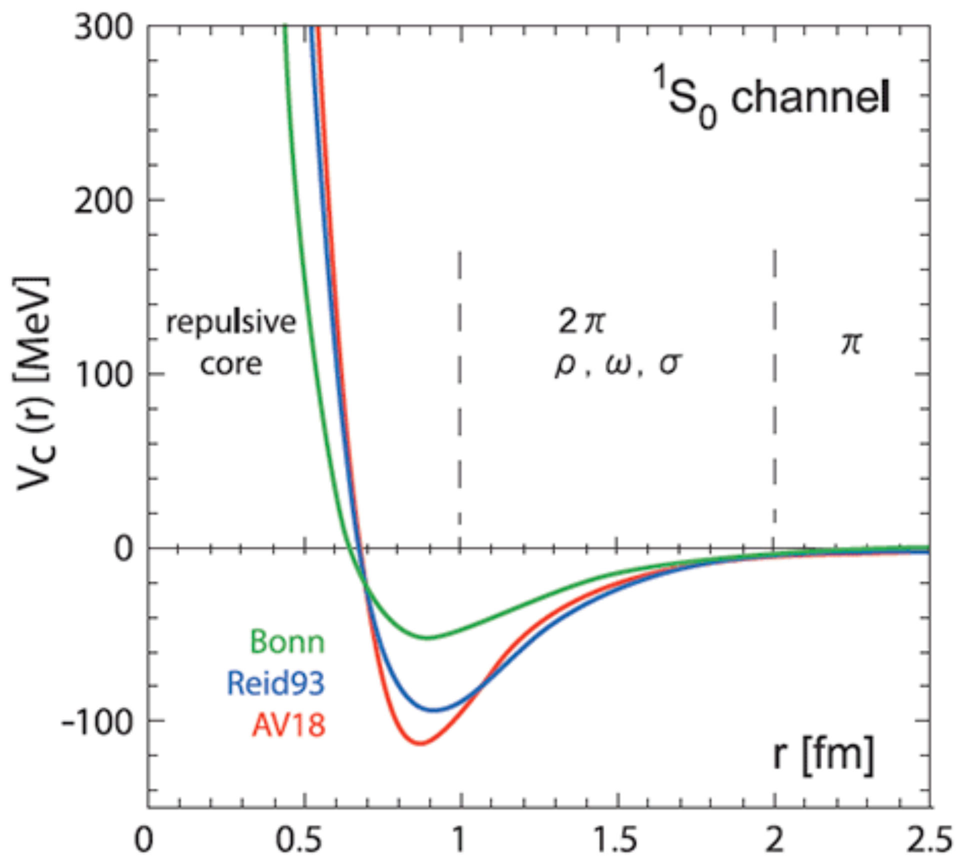
- Effective potentials
  (like atom-atom potential)
  binding energies, scattering

- non-local, energy-dependent?
  QCD?

- microscopic calculations
  (AMD, FMD)

- single-particle descriptions:
  Thomas-Fermi approximation
  shell model
  density functional theory (DFT)

- correlations, clustering
  low-density nα nuclei, Volkov



Virial expansions

short-range interaction

$$p^{\rm sr}(T,n) = b_1^{\rm sr}(T)n + b_2^{\rm sr}(T)n^2 + b_3^{\rm sr}(T)n^3 + \ldots .$$

second virial coefficient: classical limit $b_2^{\rm sr}(T) = k_BT \int d^3r \left(e^{-V(r)/k_BT} - 1\right)$

Coulomb systems: long-range Coulomb interaction

$$\begin{aligned} F(T,\Omega,N) = \Omega k_BT \{ & n\ln n + [\ln(\Lambda^3) - 1]n \\ & -A_0(T)n^{3/2} - A_1(T)n^2\ln n - A_2(T)n^2 \\ & -A_3(T)n^{5/2}\ln n - A_4(T)n^{5/2} + \mathcal{O}(n^3\ln n)\} \end{aligned}$$

Debye $A_0(T) = \kappa^3/(12\pi n^{3/2})$ screening parameter $\kappa^2 = ne^2/(\epsilon_0 k_BT)$

second virial coefficient $A_2(T) = 2\pi\lambda^3 K(\xi) + \frac{\pi}{3}\left(\frac{e^2}{4\pi\epsilon_0 k_BT}\right)^3 \ln(\kappa\lambda/n^{1/2})$

thermal wave length $\lambda^2 = \hbar^2/(mk_BT)$ $\xi = -e^2/(4\pi\epsilon_0 k_BT\lambda) = ({\rm Hartree}/k_BT)^{1/2}$

W.-D. Kraeft, D. Kremp, W. Ebeling, G.R., *Quantum Statistics of Charged Particle Systems,* 1986