Karpacz, May 16-25, 2024

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

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

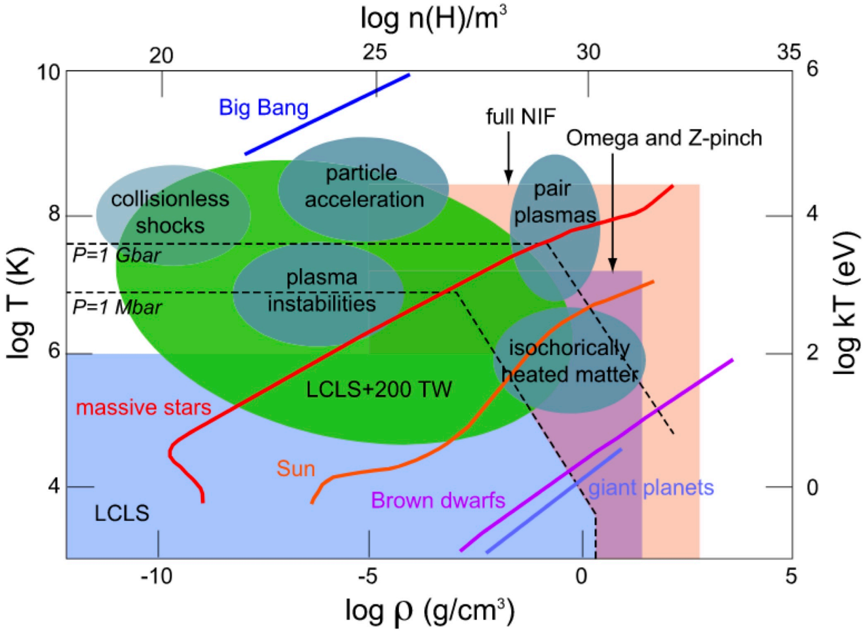
Fourier transform $V_{12,1'2'} = \frac{e_1 e_2}{\epsilon_0 \Omega |k_1 - k_1'|^2} \delta_{k_1+k_2,k_1'+k_2'} \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} \delta_{c_1c_1'} \delta_{c_2c_2'}$

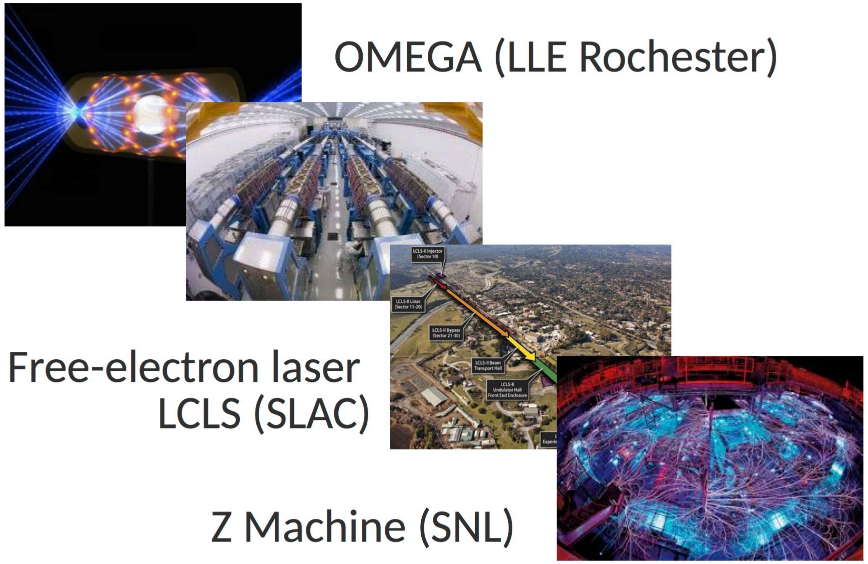
Ω: volume

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





National Ignition Facility (LLNL)

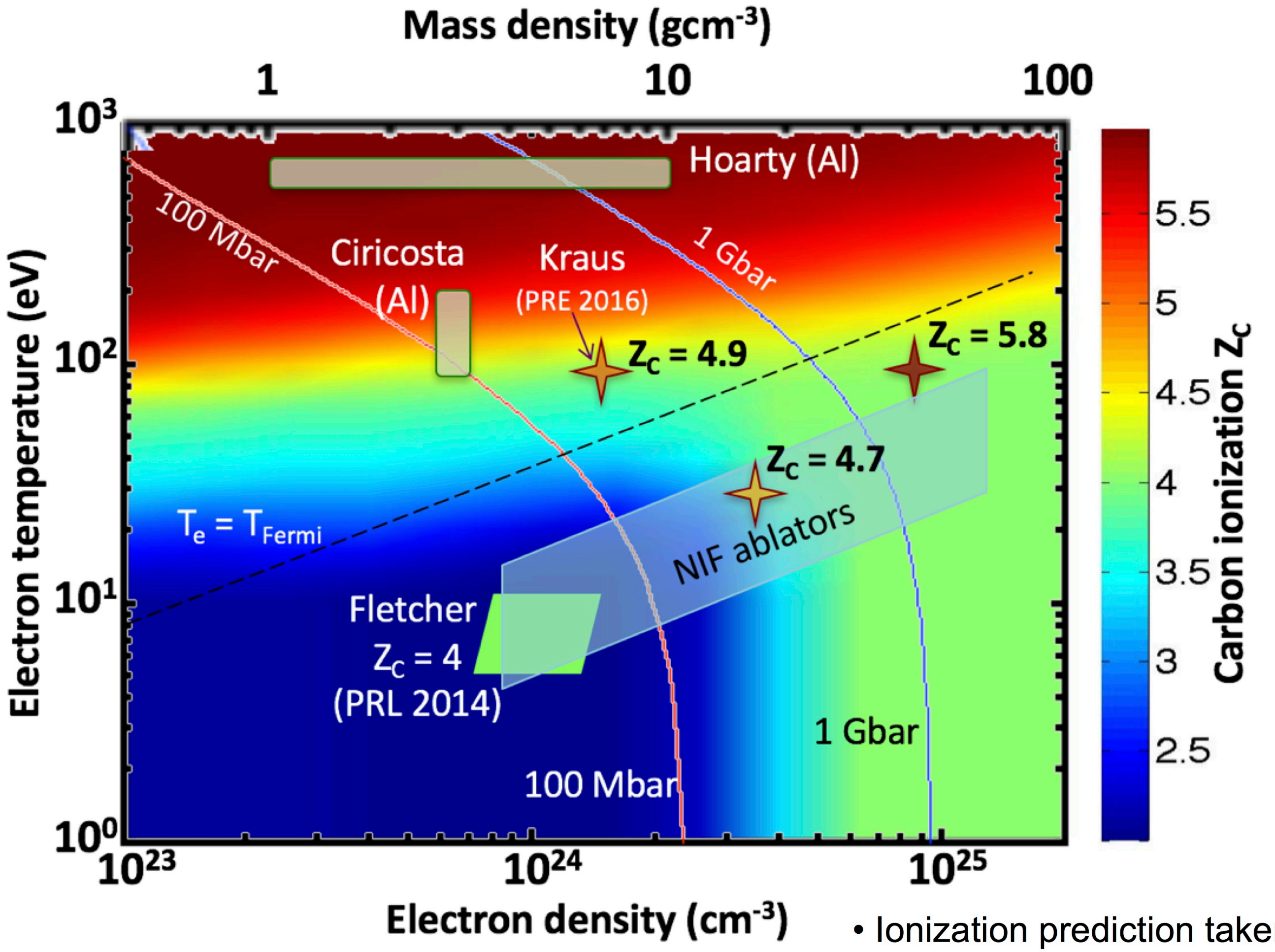
OMEGA (LLE Rochester)

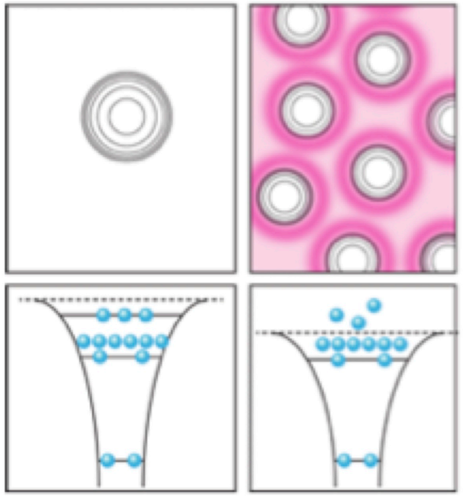
Free-electron laser
LCLS (SLAC)

Z Machine (SNL)

- 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)

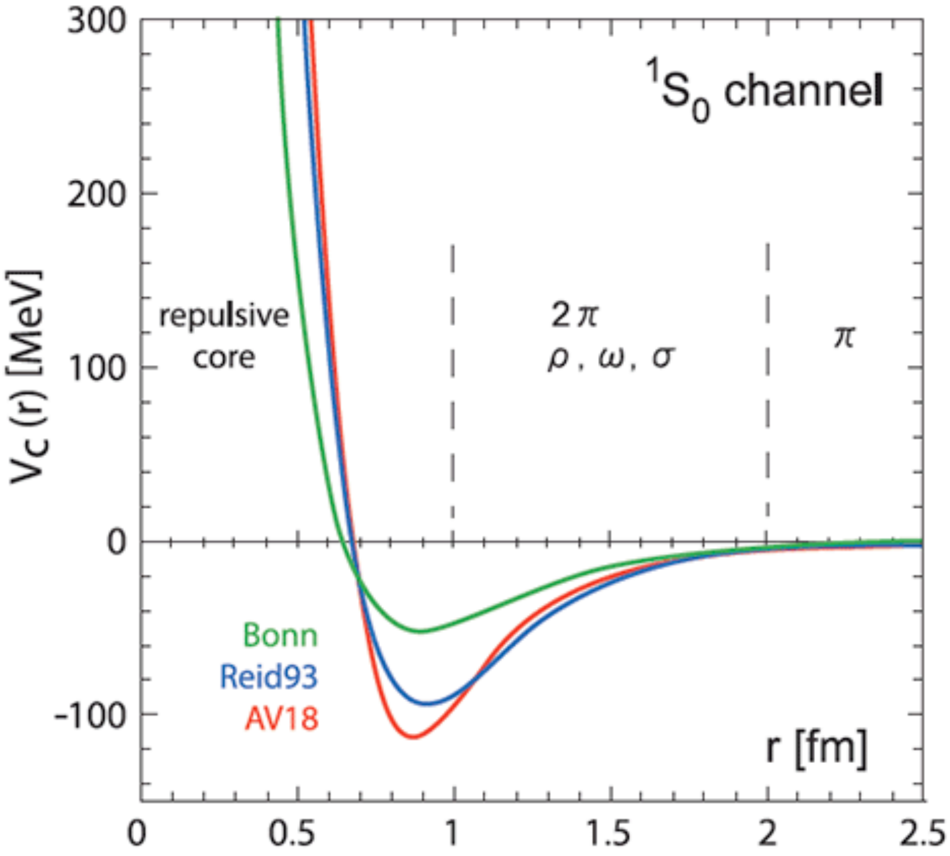
Preliminary, from Tilo Döppner et al., LLNL

Nuclear systems

- baryons: neutrons, protons,…(strange particles)
- Bound states: nuclei (deuteron ^{2}H, triton ^{3}H, helion ^{3}He, alpha ^{4}He,…)
- 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)

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

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 $\langle H \rangle = U$ $\quad \langle \hat{N}_c \rangle = N_c = n_c \Omega$

$$\delta[\langle S \rangle - \lambda_0 \langle 1 \rangle - \lambda_c \langle \hat{N}_c \rangle - \lambda_T \langle H \rangle] = 0$$

$$\hat{N}_c = \sum_{\bar{1}} a^+_{\bar{1}} a_{\bar{1}}$$

- 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

$$S = S^{(0)} + S^{(1)} + S^{(2)} + \dots$$
$$= \ln Z(T, \Omega, \mu) + \sum_k s^{(1)}_k c^+_k c_k + \sum_{k_1 k_2, k'_1 k'_2} s^{(2)}_{k_1 k_2, k'_1 k'_2} c^+_{k_1} c^+_{k_2} c_{k'_2} c_{k'_1} + \dots$$

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

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

- Coulomb systems: long-range Coulomb interaction

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

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

- Hydrogen bound states: internal partition function

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

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

Phase transitions

thermodynamic stability

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

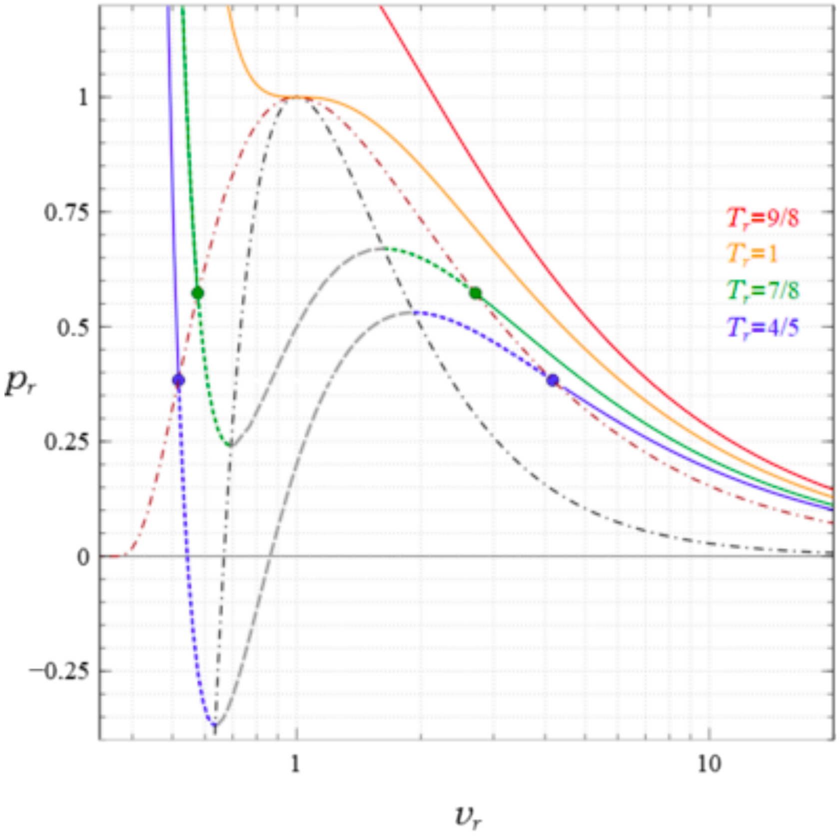
model:
Van der Waals equation of state

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

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

b: excluded volume

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



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)

transport coefficients: electrical, thermal,…

density

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

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

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

Dyson series

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

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

Sandwich expression

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

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

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

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

$\overbracket{A_1A_2}\overbracket{A_3A_4}$:	$(+1)\cdot\langle A_1A_2\rangle\cdot\langle A_3A_4\rangle$	[$\mathfrak{p}$ even]
$A_1A_2A_3A_4$:	$(-1)\cdot\langle A_1A_3\rangle\cdot\langle A_2A_4\rangle$	[$\mathfrak{p}$ odd]
$\overbracket{A_1\overbracket{A_2A_3}A_4}$:	$(+1)\cdot\langle A_1A_4\rangle\cdot\langle A_2A_3\rangle$	[$\mathfrak{p}$ even]

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

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

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 $(H-\mu N)\left|n\right\rangle = \epsilon_n \left|n\right\rangle$

define the single-particle spectral density

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

It is the Fourier transform of

$$\left\langle a_{1'}^{+} a_1(\tau)\right\rangle = G_1^{<}\left(11',\tau\right) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi} I_1\left(11',\omega'\right)\mathrm{e}^{-\omega'\tau}$$

$$\left\langle a_1(\tau) a_{1'}^{+}\right\rangle = -G_1^{>}\left(11',\tau\right) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}\mathrm{e}^{\beta\omega'} I_1\left(11',\omega'\right)\mathrm{e}^{-\omega'\tau}$$

and is connected with the Matsubara Green's function

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

Analytical continuation into the whole complex z-plane

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

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

Cauchy-type integral,
branch cut at the real axis

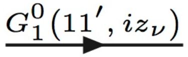
$$\begin{aligned} G_1\left(11',\omega-i\varepsilon\right) - G_1\left(11',\omega+i\varepsilon\right) &= 2i\mathrm{Im}\left\{G_1\left(11',\omega-i\varepsilon\right)\right\} \\ &= iA_1\left(11',\omega\right) \quad . \end{aligned}$$

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

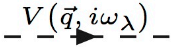
Diagrammatic representation of the perturbative series for the Green's functions

elements: free propagator



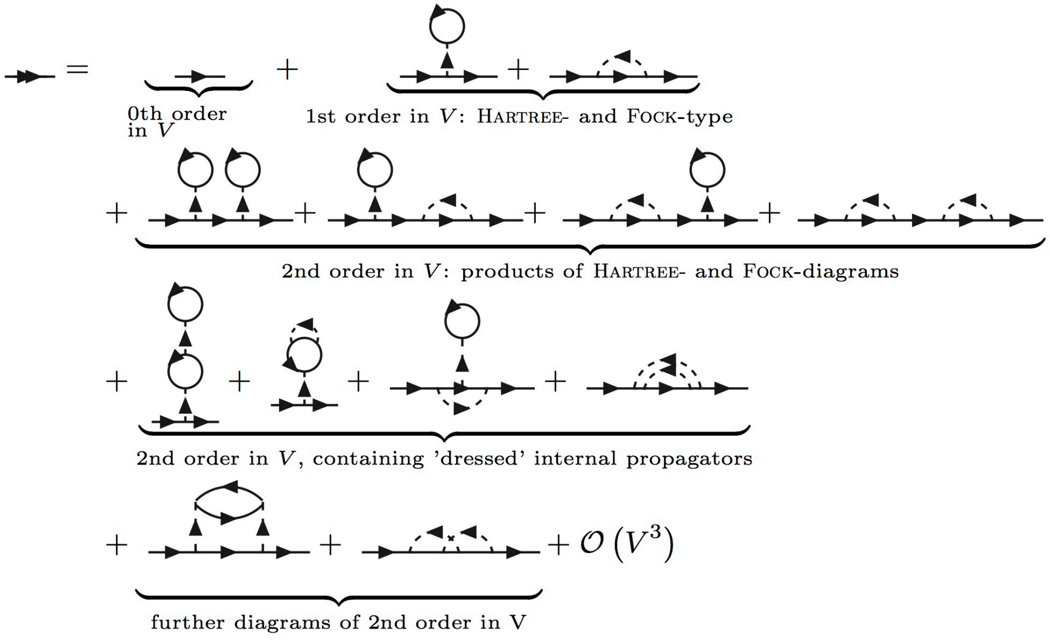
$$G_1^0\left(11', iz_\nu\right) = \frac{\delta_{11'}}{iz_\nu - \epsilon_1}$$

interaction



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

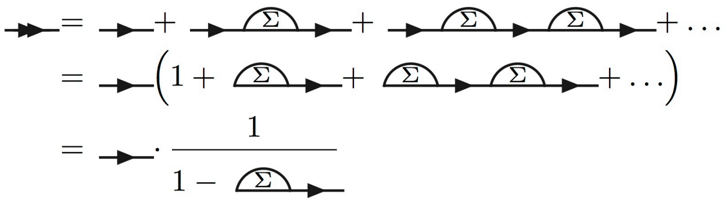
G_1:



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

Partial summations

- Dyson equation and self-energy

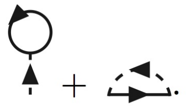


$$= G_1^0(1, iz_\nu) \frac{1}{1 - \Sigma_1(1, iz_\nu) G_1^0(1, iz_\nu)}$$

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

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

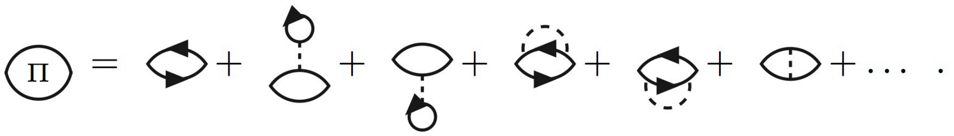
  - Hartree-Fock $\Sigma_1^{\mathrm{HF}}(1, iz_\nu) =$



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

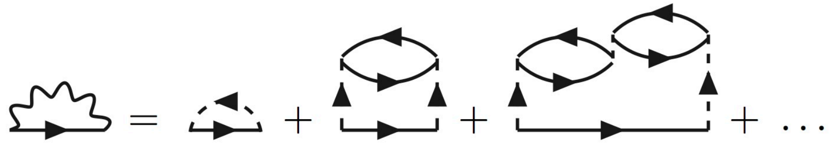
$$A_1(1, \omega) = \lim_{\varepsilon \searrow 0} 2 \frac{\mathrm{Im}\{\Sigma_1(1, \omega - i\varepsilon)\}}{[\omega - \epsilon_1 - \mathrm{Re}\{\Sigma_1(1, \omega - i\varepsilon)\}]^2 + [\mathrm{Im}\{\Sigma_1(1, \omega - i\varepsilon)\} - \varepsilon]^2}$$

- 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 $V^D(r) = \frac{e_1 e_2}{4\pi\varepsilon_0} \cdot \frac{\mathrm{e}^{-\kappa r}}{r}$ 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.

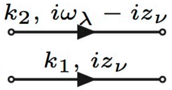
- Nonequilibrium statistics, fluctuations… (Flicker noise, Zips law,…)

- Convergence of perturbation expansions, analytical behavior

- Bound/free state contribution? Ionization degree?

Bethe-Salpeter equation

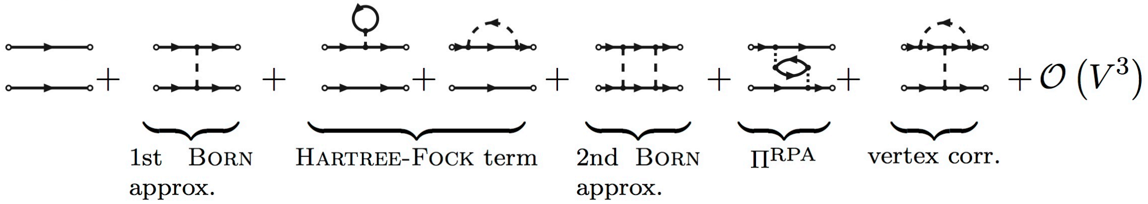
Free two-particle propagator $G_2^0\left(12,1'2',i\omega_\lambda\right) =$



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

Full two-particle propagator

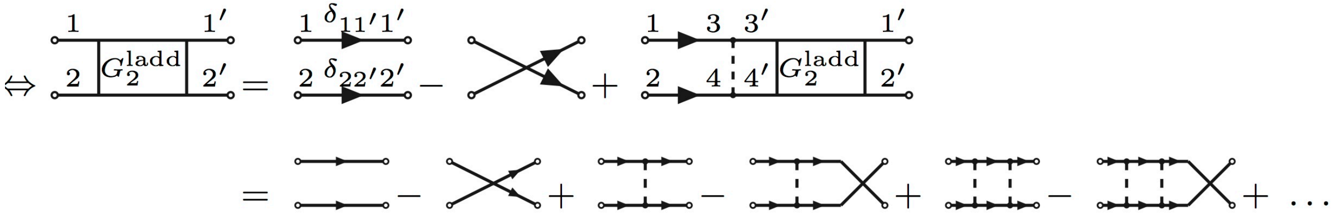
$G_2\left(12,1'2',i\omega_\lambda\right) =$



Bethe-Salpeter equation

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

Ladder summation

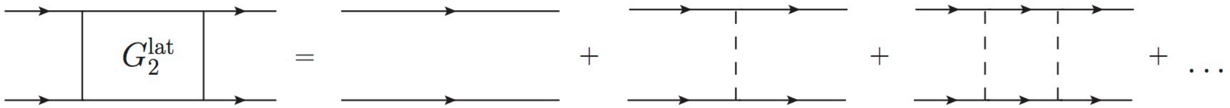


Solution low-density limit $\quad G_2^{\mathrm{ladd.}}\left(12,1'2',i\omega_\lambda\right) = \sum_{nP}\psi_{nP}(12)\frac{1}{i\omega_\lambda - E_{nP} + \mu_{12}}\psi_{nP}^*(1'2')$

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

Beth-Uhlenbeck formula

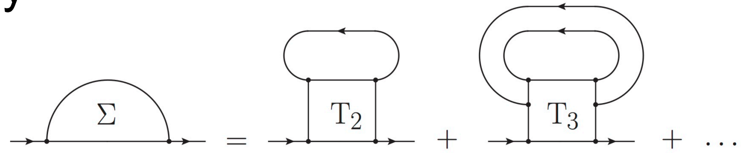
Two-particle correlations



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

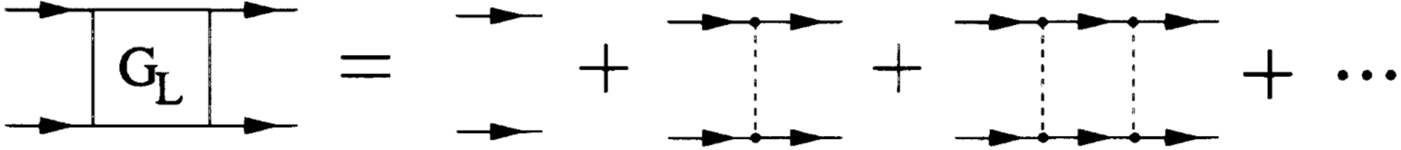
- Expansion for small Im $\Sigma(1, \omega + i\eta)$

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

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

- 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

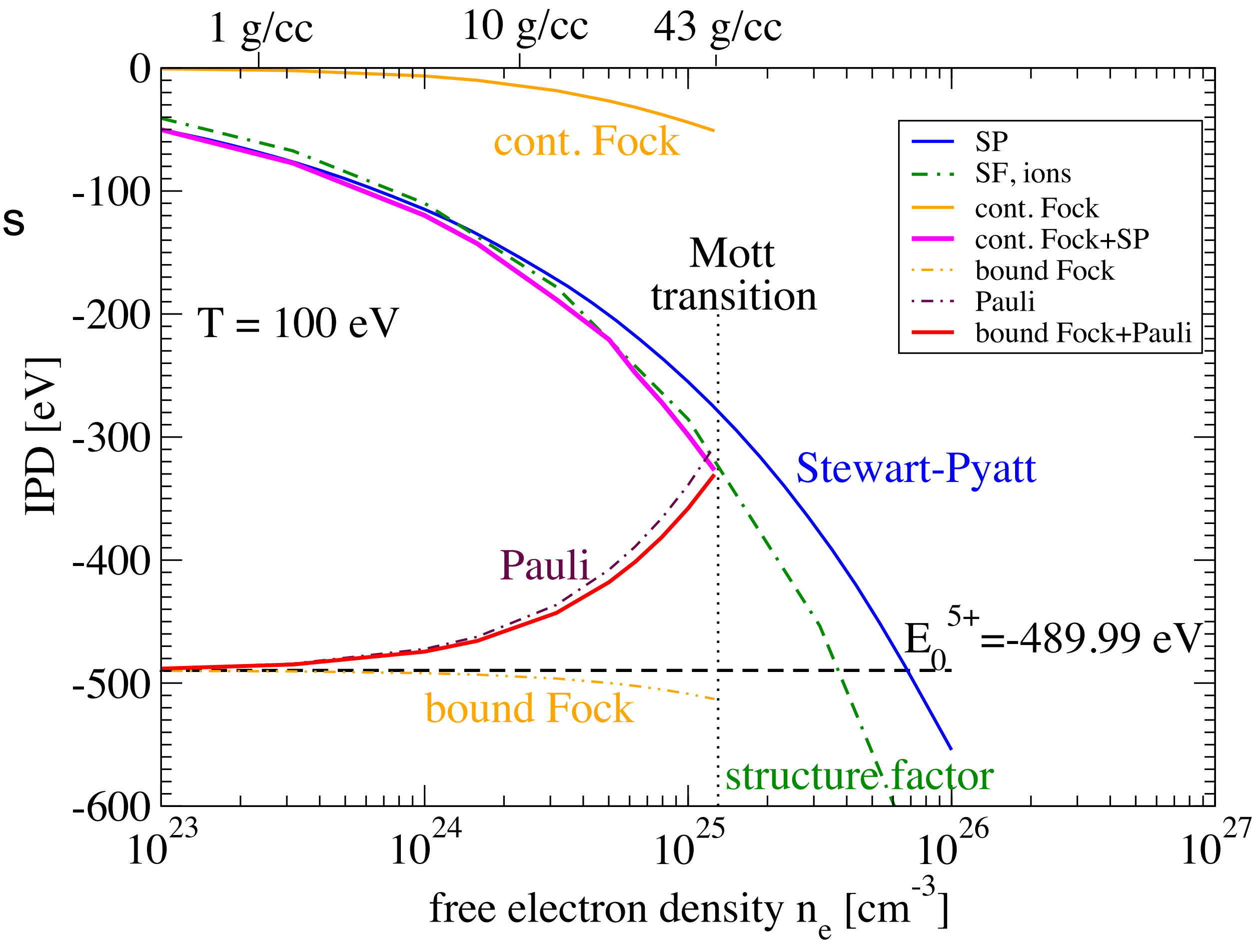
R. Zimmermann, K. Kilimann, W. D. Kraeft, D. Kremp and G. Röpke
Phys. Stat. sol. (b) **90**, 175 (1978)

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,

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

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

- quasiparticle concept

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

- generalized Beth-Uhlenbeck formula (quasiparticles)

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

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

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

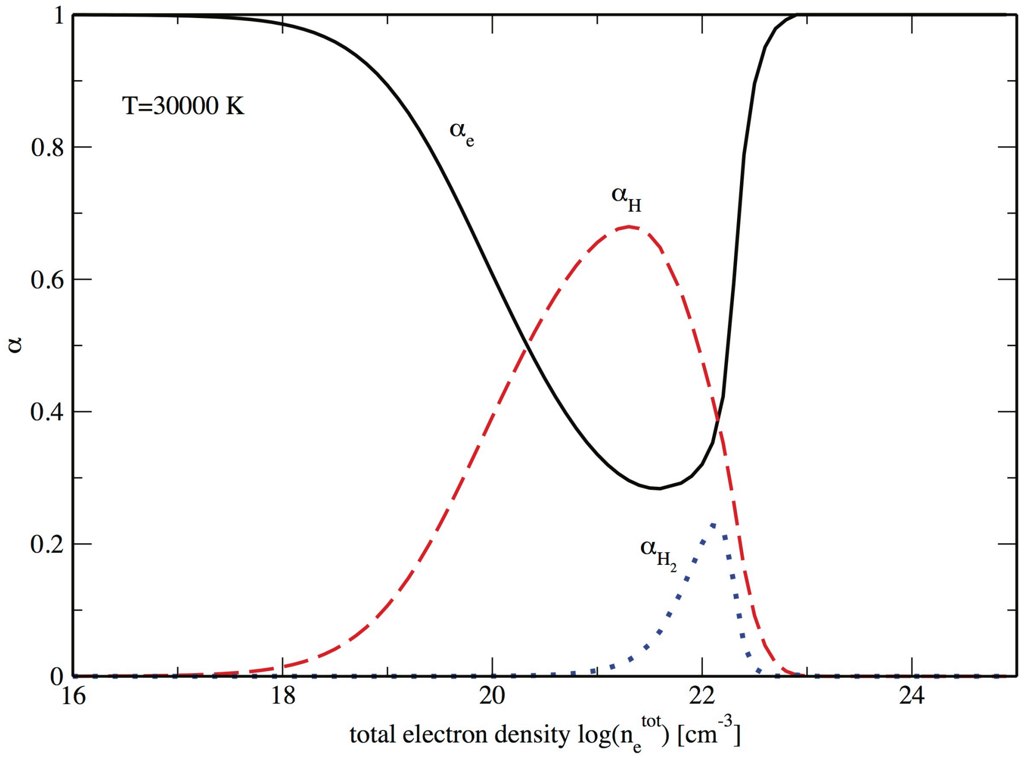
medium modifications

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

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

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

$$v_0(T) = -\frac{\sqrt{\pi}}{T^{1/2}}, \qquad v_1(T) = -\frac{\pi}{2T^2},$$

$$v_2(T) = -\frac{\pi}{T}\left[\frac{1}{2} - \frac{\sqrt{\pi}}{2}(1+\ln(2))\frac{1}{T^{1/2}} + \left(\frac{C}{2} + \ln(3) - \frac{1}{3} + \frac{\pi^2}{24}\right)\frac{1}{T} - \sqrt{\pi}\sum_{m=4}^{\infty}\frac{m}{2^m\Gamma(m/2+1)}\left(\frac{-1}{T^{1/2}}\right)^{m-1}[2\zeta(m-2) - (1-4/2^m)\zeta(m-1)]\right],$$

$$v_3(T) = -\frac{3\pi^{3/2}}{2T^{7/2}}.$$

(atomic units)

fourth virial coefficient? $v_4(T)$

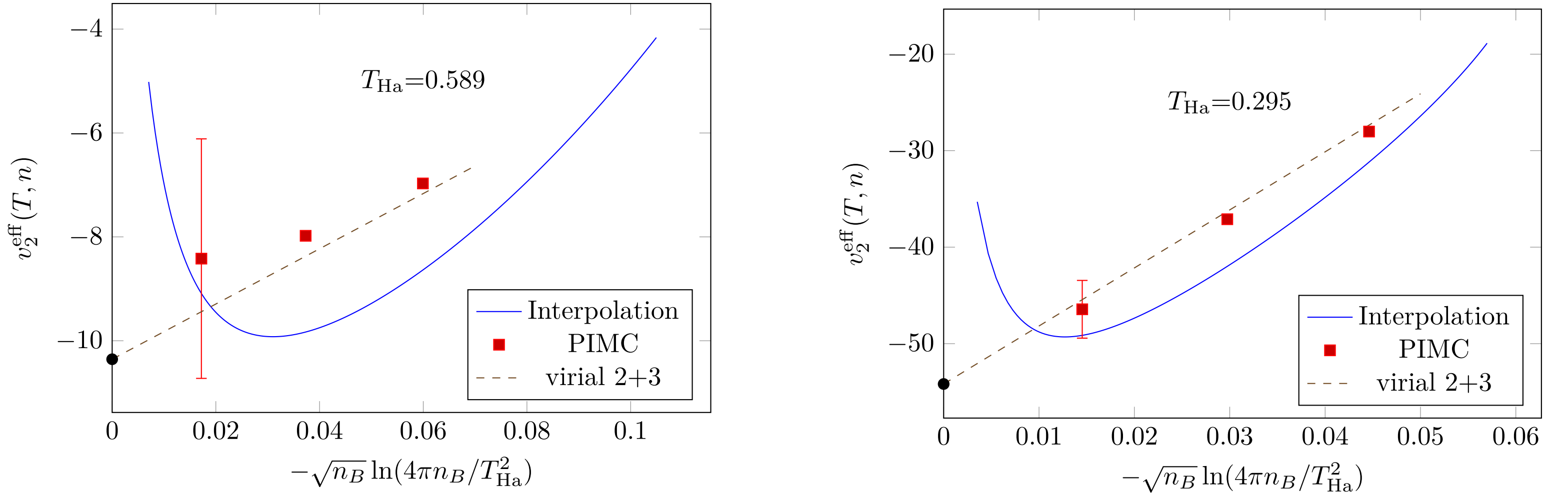
analytical expressions from perturbation theory

Virial plots for isotherms

reduced thermodynamic functions:
subtraction of known terms

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

- isotherms from PIMC simulations



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

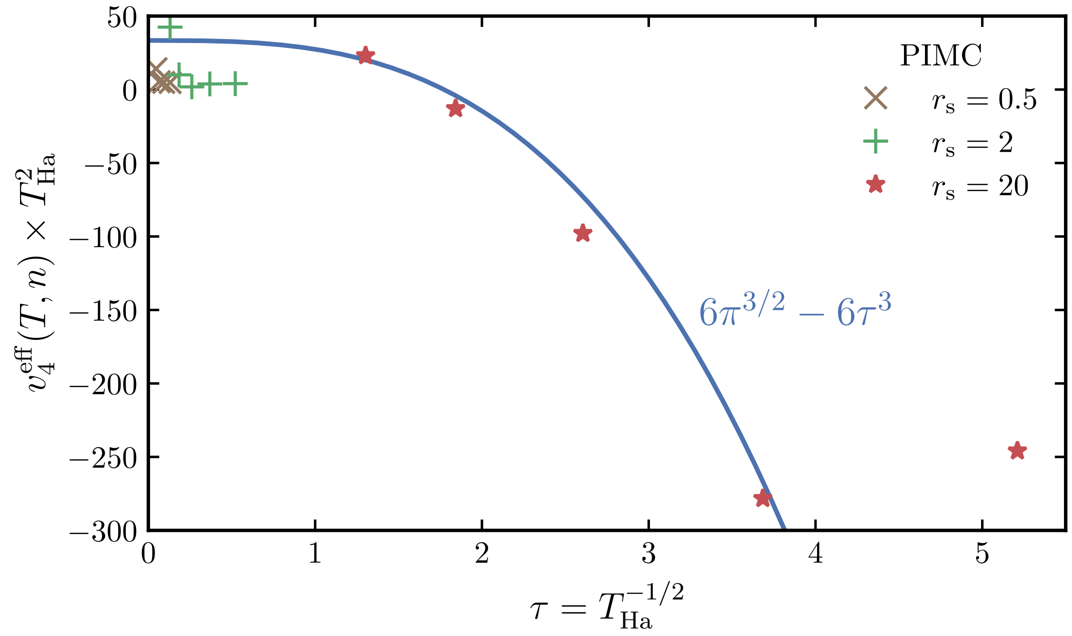
G.R., T.Dornheim, J Vorberger, D.Blaschke, B.Mahato, Phys. Rev. E **109**, 025202 (2024)

Fourth virial coefficient

extraction of the fourth virial coefficient

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

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



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

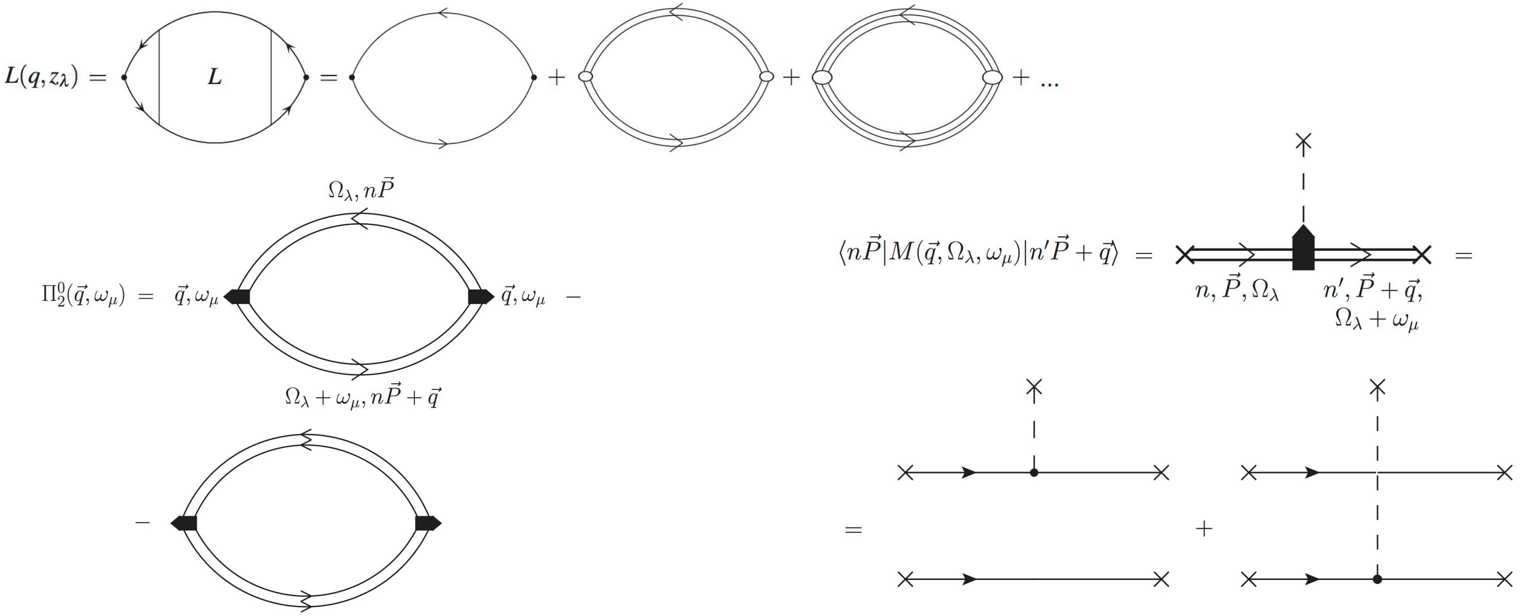
Optical (dynamic) conductivity, dynamical collision frequency

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

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

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

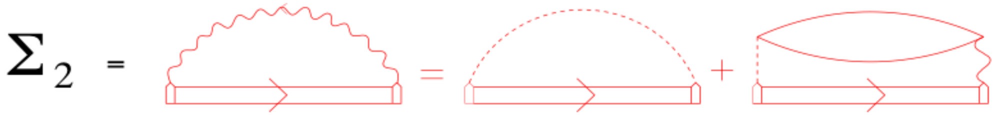
unperturbed energies $E^0_{n,P}$

Doppler broadening

Polarization function: bound state contribution

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

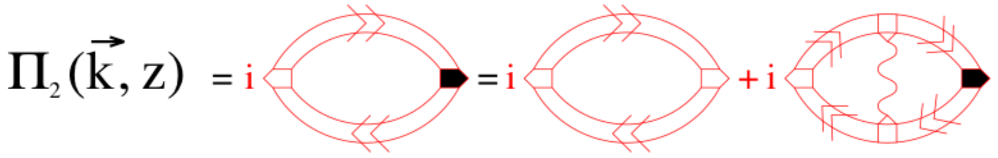
screened Born approximation



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