Goerlitz, 04. 12. 2023

Polish-German WE-Heraeus Seminar & Max Born Symposium Many-particle systems under extreme conditions

## Cluster-virial expansions for correlated matter G. Röpke, Rostock



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



## Nuclear matter phase diagram



## Outline

- 1. Equation of state and virial expansions in plasmas Virial coefficients for the uniform electron gas, interpolation formulas
- 2. Electrical conductivity: virial expansion for hydrogen plasmas Inclusion of electron-electron collisions
- 3. Beth-Uhlenbeck formula for the second virial coefficient In-medium Schroedinger equation for nuclear matter
- 4. Cross-over Bose Einstein condensate BCS pairing Quartetting in low-density nuclear matter, Hoyle state and  $\alpha$  decay
- 5. Cluster Beth-Uhlenbeck formula, few-body problem, continuum Cluster-mean field, composition, freeze-out concept

#### 1. Equations of state

many-particle system, temperature *T*, volume  $\Omega$ , 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

1

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

quantum statistical approach: grand canonical ensemble

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

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

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

 $\begin{aligned} & \text{Fermi function} \\ & \text{Tr}\{\rho\,\psi^{\dagger}(1',t')\,\psi(1,t)\} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\frac{i}{\hbar}\omega(t'-t)} f(\omega) A(1,1';\omega) \\ & \text{spectral function} \end{aligned}$ 

Correlation function Green's function method

path integral Monte Carlo (PIMC) simulations

## Virial expansions

short-range interaction

1

$$p^{\rm sr}(T,n) = b_1^{\rm sr}(T)n + b_2^{\rm sr}(T)n^2 + b_3^{\rm sr}(T)n^3 + \dots$$
  
second virial coefficient: classical limit  $b_2^{\rm sr}(T) = k_B T \int d^3r \left(e^{-V(r)/k_B T} - 1\right)$ 

Coulomb systems: long-range Coulomb interaction

$$\begin{split} F(T,\Omega,N) &= \Omega k_B T \left\{ n \ln n + [\ln(\Lambda^3) - 1] n \\ &-A_0(T) n^{3/2} - A_1(T) n^2 \ln n - A_2(T) n^2 \\ &-A_3(T) n^{5/2} \ln n - A_4(T) n^{5/2} + \mathcal{O}(n^3 \ln n) \right\} \\ \text{Debye} \quad A_0(T) &= \kappa^3 / (12\pi n^{3/2}) \qquad \text{screening parameter} \quad \kappa^2 = n e^2 / (\epsilon_0 k_B T) \\ \text{second virial coefficient} \qquad A_2(T) &= 2\pi \lambda^3 K(\xi) + \frac{\pi}{3} \left( \frac{e^2}{4\pi \epsilon_0 k_B T} \right)^3 \ln(\kappa \lambda / n^{1/2}) \\ \text{thermal wave length } \lambda^2 &= \hbar^2 / (m k_B T) \qquad \xi = -e^2 / (4\pi \epsilon_0 k_B T \lambda) = (\text{Hartree}/k_B T)^{1/2} \end{split}$$

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

#### Homogeneous (uniform) electron gas

specific mean potential energy 
$$v = V/N$$
  
 $\kappa^2 = \frac{ne^2}{\epsilon_0 k_B T}, \quad \lambda^2 = \frac{\hbar^2}{mk_B T}, \quad \tau = \frac{e^2 \sqrt{m}}{4\pi \epsilon_0 \sqrt{k_B T} \hbar}.$ 

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

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

fourth virial coefficient?  $v_4(T)$ 

analytical expressions from perturbation theory

## Mean potential energy

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

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

1.02 r<sub>s</sub>=20 Exact results, not debated: Debye, logarithmic  $\xi^3$ -term -0.01 1.01 V/V<sub>GDSMFB</sub> -0.02 V/N [Ha] -0.03  $\frac{V_1}{N k_B T} = -\frac{\kappa^3}{8\pi n} + \pi n \lambda^3 \xi^3 \ln(\kappa \lambda)$ 0.99 -0.04 -0.05 0.98  $v^{\rm red} = \frac{\Delta v}{\pi n \lambda^3 \xi \, k_B T} = \left[ \frac{V}{N \, k_B T} - \frac{V_1}{N \, k_B T} \right] \frac{1}{\pi n \lambda^3 \xi}$ 1 10 100 1000 1 10 100 1000 θ θ

r<sub>s</sub>=0.5

10

10

θ

θ

-0.1 -0.2

-0.3

-0.5

-0.6

-0.7

-0.8

-0.9

-0.1

-0.2

1

1

r<sub>s</sub>=2

V/N [Ha] -0.4

V/N [Ha]

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

1.02

1.01

1

0.99

0.98

1.02

1.01

0.99

0.98

1

V/VGDSMFB

1

0

10

10

θ

θ

100

100

1000

1000

10000

V/V<sub>GDSMFB</sub>

1000

1000

GDSMFB PIMC ..... PRL 2016

full virial

with E/6

100

100

DH ----no ξ/6 ·····

## Equation of state of the uniform electron gas



Figure 10. Dependence of the reduced interaction energy per particle  $v^{\text{red}}$  (56) on the Born parameter  $\xi$  for the density of  $r_s = 0.5$ . Red squares: PIMC data from this work, solid black line labelled v: virial expansion Eq. (45), dashed blue line: including the debated  $\xi/6$  term (denoted by w).

## Virial plot

extraction of the second virial coefficient

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

$$v_2^{\text{red}}(T,n) = \left[v^{\text{PIMC}} - v^{(1)}(T,n)\right] \frac{-T}{\pi n} = \frac{-T}{\pi} v_2(T) + \mathcal{O}(n^{1/2}\ln(n))$$
$$= \frac{1}{2} - \frac{\sqrt{\pi}}{2} (1 + \ln(2))\tau + \left(\frac{C}{2} + \ln(3) - \frac{1}{3} + \frac{\pi^2}{24}\right)\tau^2 + \mathcal{O}(\tau^3) + \mathcal{O}(n^{1/2}\ln(n))$$



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

#### Fourth virial coefficient

extraction of the fourth virial coefficient

$$\Delta v_3^{\text{red}}(T,n) = \left[ v^{\text{PIMC}} - v^{(1)}(T,n) - v_2(T)n - v_3(T)n^{3/2} \ln\left(\frac{4\pi n}{T^2}\right) \right] \frac{T}{\pi n}$$
$$v_4^{\text{eff}}(T,n) = \Delta v_3^{\text{red}}(T,n) \frac{\pi}{Tn^{1/2}} = v_4(T) + \mathcal{O}(n^{1/2}\ln(n))$$



#### Interpolation formulas:

G.R., T. Dornheim, J. Vorberger, D. Blaschke, B. Mahato, submitted, arXiv: 2310.17583

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)

#### Virial plots for isotherms



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

$$f_{\rm XC}^{\rm GDSMFB}(r_S,\Theta) = -\frac{1}{r_s} \frac{a(\Theta) + b(\Theta)\sqrt{r_s} + c(\Theta)r_s}{1 + d(\Theta)\sqrt{r_s} + e(\Theta)r_s} \qquad \qquad v(r_s,\Theta) = 2f_{\rm XC}(r_s,\Theta) + r_s \frac{\partial f_{\rm XC}(r_s,\Theta)}{\partial r_s}\Big|_{\Theta}$$

G.R., T.Dornheim, J Vorberger, D.Blaschke, B.Mahato, submitted, arXiv: 2310.17583

## 2. Electrical conductivity of plasmas

- Kinetic theory (Boltzmann equation): Spitzer (low-density limit)
- Linear response theory: Kubo formula (warm dense matter)

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

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

- Generalized linear response theory (unified)
- Fluctuation-dissipation theorem: equilibrium correlation functions
- Green functions: perturbation theory, diagram techniques

Kubo-Greenwood formula, DFT-MD simulations: electron-electron collisions included?

(M. P. Desjarlais et al. 2017, N.R. Shaffer and C.E. Starrett 2020)

$$\operatorname{Re}\left[\sigma(\omega)\right] = \frac{2\pi e^2}{3m_e^2\omega\Omega} \sum_k w_k \sum_{j=1}^N \sum_{i=1}^N \sum_{\alpha=1}^3 \left[f(\epsilon_{j,k}) - f(\epsilon_{i,k})\right] |\langle \Psi_{j,k}| \hat{p}_{\alpha} |\Psi_{i,k}\rangle|^2 \delta(\epsilon_{i,k} - \epsilon_{j,k} - \hbar\omega)$$

Conductivity of warm dense matter including electron-electron collisions: H. Reinholz, G. R., S. Rosmej, R. Redmer, Phys. Rev. E **91**, 043105 (2015). DFT-MD contains e-e interaction only in mean-field approximation, wrong low-density limit of electrical conductivity (Lorentz-model)

#### Virial Expansion of the Electrical Conductivity of Hydrogen Plasmas

dc conductivity  $\sigma(n,T) = \frac{(k_B T)^{3/2} (4\pi\epsilon_0)^2}{m_e^{1/2} e^2} \sigma^*(n,T)$ 

dimensionless resistivity: virial expansion

$$\rho^{*}(n,T) = 1/\sigma^{*}(n,T) = \rho_{1}(T) \ln \frac{1}{n} + \rho_{2}(T) + \rho_{3}(T) n^{1/2} \ln \frac{1}{n} + \dots$$
  
dimensionless parameters  $\Gamma = \frac{e^{2}}{4\pi\epsilon_{0}k_{B}T} \left(\frac{4\pi}{3}\hat{n}_{e}\right)^{1/3} \qquad \Theta = \frac{2m_{e}k_{B}T}{\hbar^{2}} (3\pi^{2}\hat{n}_{e})^{-2/3}$   
 $\rho^{*}(n,T) = \tilde{\rho}_{1}(T) \ln \left(\frac{\Theta}{\Gamma}\right) + \tilde{\rho}_{2}(T) + \dots$ 

 $\tilde{\rho}(x,T) = \frac{\rho^*}{\ln(\Theta/\Gamma)} = \tilde{\rho}_1(T) + \tilde{\rho}_2(T)x + \dots \qquad x = 1/\ln(\Theta/\Gamma) \qquad \text{virial plot}$ 

exact results $\rho_1^{\text{Spitzer}} = 0.846$  $\lim_{T \to \infty} \tilde{\rho}_2(T) = \tilde{\rho}_2^{\text{QLB}} = 0.4917$ (benchmarks)V. S. Karakhtanov, Contrib. Plasma Phys. 56, 343 (2016)

#### Virial Expansion of the Electrical Conductivity of Hydrogen Plasmas



Clerouin, Copeland: P. E. Grabowski et al. High Energy Dens. Phys. **37**, 100905 (2020), Review of the first charged-particle transport coefficient comparison Workshop

#### Ichimaru, Hubbard, Lee/More:

F. Lambert, V. Recoules, A. Decoster, J. Clerouin, M. Desjarlais, Phys. Plasmas 18, 056306 (2011)

### Free electron density

Kubo-Greenwood formula: conductivity, DFT-MD

Carbon, T = 100 eV, n = 50 g cm<sup>-3</sup>



M. Bethkenhagen et al., Phys. Rev. Research 2, 023260 (2020)

## Virial Expansion of the Electrical Conductivity of Hydrogen Plasmas

DFT-MD simulations: are electron-electron collisions rigorously included?



F. Lambert, V. Recoules, A. Decoster, J. Clerouin, M. Desjarlais, Phys. Plasmas 18, 056306 (2011)
M. Desjarlais, C.Scullard, L. Benedict, H. Whitley, R. Redmer, Phys. Rev. E 95, 033203 (2017)
G. R., M. Schoerner, M. Bethkenhagen, R. Redmer, Phys. Rev. E 104, 045204 (2021)

PIMC simulations can solve the problem of the contribution of e – e collisions

#### 3. 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

$$A(1,\omega) = 2 \operatorname{Im} G(1,\omega-i0) = 2 \operatorname{Im} \frac{1}{\omega - E(1) - \Sigma(1,\omega-i0)} \qquad E(1) = p_1^2/(2m)$$

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

$$A_e(1,\omega) \approx \frac{2\pi \,\delta(\omega - E_e^{\text{quasi}}(1))}{1 - \frac{d}{dz} \text{Re} \,\Sigma_e(1,z)|_{z=E_e^{\text{quasi}}-\mu_e}} - 2\text{Im} \,\Sigma_e(1,\omega+i0) \frac{d}{d\omega} \frac{\mathcal{P}}{\omega + \mu_e - E_e^{\text{quasi}}(1)}$$
$$E^{\text{quasi}}(1) = p_1^2/(2m) + \text{Re}\Sigma(1,\omega)|_{\omega = E^{\text{quasi}}(1)}$$

## Quantum statistical approach

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

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

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

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

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

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...)  $\gamma$ 

## 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)

# Effective wave equation for the deuteron in matter

Green functions, spectral function, quasiparticles, self energy, Bethe-Salpeter equation

In-medium two-particle wave equation in mean-field approximation

$$\frac{p_1^2}{2m_1} + \Delta_1 + \frac{p_2^2}{2m_2} + \Delta_2 \Psi_{d,P}(p_1, p_2) + \sum_{p_1', p_2'} (1 - f_{p_1} - f_{p_2}) V(p_1, p_2; p_1', p_2') \Psi_{d,P}(p_1', p_2')$$
self-energy
Pauli-blocking
$$= E_{d,P} \Psi_{d,P}(p_1, p_2)$$

phase space occupation: Fermi distribution function

$$f_p = \left[ e^{(p^2/2m - \mu)/k_B T} + 1 \right]^{-1}$$

medium:

uncorrelated mean field (-> shell model) correlated mean field (->  $\alpha$  matter)

Thouless criterion  $E_d(T,\mu) = 2\mu$ 

**BEC-BCS crossover:** 

#### Pauli blocking – phase space occupation



cluster wave function (atoms, ions, ...deuteron, alpha,...) in momentum space

P - center of mass momentum

The Fermi sphere is forbidden, deformation of the cluster wave function in dependence on the c.o.m. momentum *P* 

#### momentum space

The deformation is maximal at P = 0. It leads to the weakening of the interaction (disintegration of the bound state).

#### Shift of the deuteron bound state energy

Dependence on nucleon density, various temperatures, zero center of mass momentum



G.R., Nucl. Phys. A 867, 66 (2011)

#### Scattering phase shifts in matter



#### **Two-particle correlations**



M. Schmidt, G.R., H. Schulz Ann. Phys. **202**, 57 (1990)

FIG. 7. The composition of nuclear matter as a function of the density n for given temperature T = 10 MeV. The solid and dashed lines show the results of the generalized and classical Beth-Uhlenbeck approach, respectively. Note the distinct behavior of  $n_{\text{free}}$  and  $n_{\text{corr}}$  predicted by the two approaches in the low and high density limit!

#### Composition of dense nuclear matter

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

mass number A  
charge 
$$Z_A$$
  
energy  $E_{A,v,K}$   
 $f_{A(z)} = \frac{1}{\exp(z/T) - (-1)^A}$ 

v: internal quantum number excited states, continuum correlations

 Medium effects: correct behavior near saturation self-energy and Pauli blocking shifts of binding energies, Coulomb corrections due to screening (Wigner-Seitz, Debye)

#### Shift of Binding Energies of Light Clusters







#### **EOS: continuum contributions**

Partial density of channel A,c at P (for instance,  ${}^{3}S_{1} = d$ ):

$$z_{A,c}^{\text{part}}(\mathbf{P}; T, \mu_n, \mu_p) = e^{(N\mu_n + Z\mu_p)/T} \left\{ \sum_{\nu_c}^{\text{bound}} g_{A,\nu_c} \ e^{-E_{A,\nu_c}(\mathbf{P})/T} \ \Theta \left[ -E_{A,\nu_c}(\mathbf{P}) + E_{A,c}^{\text{cont}}(\mathbf{P}) \right] + z_{A,c}^{\text{cont}}(\mathbf{P}) \right\}$$

separation: bound state part – continuum part ?

$$z_{c}^{\text{part}}(\mathbf{P};T,n_{B},Y_{p}) = e^{[N\mu_{n}+Z\mu_{p}-NE_{n}(\mathbf{P}/A;T,n_{B},Y_{p})-ZE_{p}(\mathbf{P}/A;T,n_{B},Y_{p})]/T} \times g_{c} \left\{ \left[ e^{-E_{c}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p})/T} - 1 \right] \Theta \left[ -E_{c}^{\text{intr}}(\mathbf{P};T,n_{B},Y_{p}) \right] + v_{c}(\mathbf{P};T,n_{B},Y_{p}) \right\}$$

parametrization (d – like):  

$$v_c(\mathbf{P} = 0; T, n_B, Y_p) \approx \left[ 1.24 + \left( \frac{1}{v_{T_I=0}(T)} - 1.24 \right) e^{\gamma_c n_B/T} \right]^{-1}.$$

 $v^0_d(T) = v^0_{T_I=0}(T) \approx 0.30857 + 0.65327 \ e^{-0.102424 \ T/\text{MeV}}$  G. R., PRC 92,054001 (2015)

Few-body problem and continuum contributions ?

# 4. Effective wave equation for the deuteron in matter

Green functions, spectral function, quasiparticles, self energy, Bethe-Salpeter equation

In-medium two-particle wave equation in mean-field approximation

$$\frac{\left[\frac{p_1^2}{2m_1} + \Delta_1 + \frac{p_2^2}{2m_2} + \Delta_2\right]}{\left[\frac{p_1}{2m_1} + \Delta_2\right]} \Psi_{d,P}(p_1, p_2) + \sum_{p_1', p_2'} (1 - f_{p_1} - f_{p_2}) V(p_1, p_2; p_1', p_2') \Psi_{d,P}(p_1', p_2')$$

$$= E_{d,P} \Psi_{d,P}(p_1, p_2)$$

$$= E_{d,P} \Psi_{d,P}(p_1, p_2)$$

phase space occupation: Fermi distribution function

$$f_p = \left[ e^{(p^2/2m - \mu)/k_B T} + 1 \right]^{-1}$$

medium:

uncorrelated mean field (-> shell model) correlated mean field (->  $\alpha$  matter)

Thouless criterion  $E_d(T,\mu) = 2\mu$ 

**BEC-BCS crossover:** 

#### 2. Quantum condensate



Meng Jin, M. Urban, and P. Schuck, Phys. Rev. C 82, 024911 (2010)

#### Few-particle Schrödinger equation in a dense medium

 $\alpha$  particles are strongly bound (7.07 MeV/A) compared to deuterons (1.1MeV/A)

4-particle Schrödinger equation with medium effects

$$\begin{pmatrix} \left[ E^{HF}(p_{1}) + E^{HF}(p_{2}) + E^{HF}(p_{3}) + E^{HF}(p_{4}) \right] \end{pmatrix} \Psi_{n,P}(p_{1},p_{2},p_{3},p_{4}) \\ + \sum_{p_{1}^{'},p_{2}^{'}} (1 - f_{p_{1}} - f_{p_{2}}) V(p_{1},p_{2};p_{1}^{'},p_{2}^{'}) \Psi_{n,P}(p_{1}^{'},p_{2}^{'},p_{3},p_{4}) \\ + \left\{ permutations \right\} \\ = E_{n,P} \Psi_{n,P}(p_{1},p_{2},p_{3},p_{4})$$
Thouless criterion for quantum condensate:

 $E_{n,P=0}(T,\mu) = 4\mu$ 

## α-cluster-condensation (quartetting)



G.R., A.Schnell, P.Schuck, and P.Nozieres, PRL 80, 3177 (1998)

Is there a sharp transition from quartetting to pairing ?

#### Quantum condensate: quartetting

Ideal Bose condensate :  $|0\rangle = b_0^{\dagger} b_0^{\dagger} \cdots b_0^{\dagger} |vac\rangle$ 

 $\alpha$ -particle condensate :  $|\Phi_{\alpha C}\rangle = C^{\dagger}_{\alpha}C^{\dagger}_{\alpha}\cdots C^{\dagger}_{\alpha}|vac\rangle$ 

In *r*-space :  $\langle \vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{4n} | \Phi_{\alpha C} \rangle = \mathcal{A} \{ \Phi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \Phi(\vec{r}_5, \vec{r}_6, \vec{r}_7, \vec{r}_8) \cdots \Phi(\vec{r}_{4n-3}, \vec{r}_{4n-2}, \vec{r}_{4n-1}, \vec{r}_{4n}) \}$ 

In comparison with pairing :

$$\langle \vec{r}_1, \vec{r}_2, \cdots | BCS \rangle = \mathcal{A} \left\{ \Phi \left( \vec{r}_1, \vec{r}_2 \right) \Phi \left( \vec{r}_3, \vec{r}_4 \right) \cdots \right\}$$

A. Tohsaki et al., PRL 87, 192501 (2001)

### The $\alpha$ condensate state in 4n nuclei

The Hoyle state as Bose-like gas of 3  $\alpha$  clusters, shell model not applicable  $\alpha$  condensation is a general phenomenon: <sup>12</sup>C, <sup>16</sup>O, <sup>20</sup>Ne, ...

Container picture: B. Zhou et al., Phys. Rev. Lett. 110, 262501 (2013)



B. Zhou, Y. Funki, H. Horiuchi, Y. Ma, G. R., P. Schuck, A. Tohsaki, T. Yamada, to be published

Is there a sharp transition from quartetting to pairing ?

# 5. Cluster virial expansion for nuclear matter within a quasiparticle statistical approach

Generalized Beth-Uhlenbeck approach

$$n_1^{\rm qu}(T,\mu_p,\mu_n) = \sum_{A,Z,\nu} \frac{A}{\Omega} \sum_{\substack{\vec{P} \\ P > P_{\rm Mott}}} f_A(E_{A,Z,\nu}(\vec{P};T,\mu_p,\mu_n),\mu_{A,Z,\nu})$$

$$n_{2}^{qu}(T,\mu_{p},\mu_{n}) = \sum_{A,Z,\nu} \sum_{A',Z',\nu'} \frac{A+A'}{\Omega} \sum_{\vec{p}} \sum_{c} g_{c} \frac{1+\delta_{A,Z,\nu;A',Z',\nu'}}{2\pi} \times \int_{0}^{\infty} dE f_{A+A'} \left( E_{c}(\vec{P};T,\mu_{p},\mu_{n}) + E,\mu_{A,Z} + \mu_{A',Z'} \right) 2 \sin^{2}(\delta_{c}) \frac{d\delta_{c}}{dE}$$

avoid double counting



$$\underline{A}_{qu} = \underline{A} + \underline{$$

 $\Sigma^{\text{CMF}} = A \xrightarrow{qu} A \xrightarrow{qu} qu$ 

generating functional

G.R., N. Bastian, D. Blaschke, T. Klaehn, S. Typel, H. Wolter, NPA 897, 70 (2013)

### **Cluster - mean field approximation**

Cluster (A) interacting with a distribution of clusters (B) in the medium, fully antisymmetrized (correlated medium)

$$\sum_{1'\dots A'} \{H_A^0(1\dots A, 1'\dots A') + \sum_i \Delta_i^{A,mf} \delta_{k,k'} + \frac{1}{2} \sum_{i,j} \Delta V_{ij}^{A,mf} \delta_{l,l'} - E_{A\nu P} \delta_{k,k'} \} \psi_{A\nu P}(1'\dots A') = 0$$

self-energy

$$\Delta_1^{A,mf}(1) = \sum_2 V(12,12)_{ex} f^*(2) + \sum_{BvP} \sum_{2\dots B'} f_B(E_{BvP}) \sum_i V_{1i}(1i,1'i') \psi_{BvP}^*(1\dots B) \psi_{BvP}(1'\dots B')$$

effective interaction

$$\Delta V_{12}^{A,mf} = -\frac{1}{2} [f^*(1) + f^*(2)] V(12,1'2') - \sum_{B\nu P} \sum_{2^* \dots B^*} f_B(E_{B\nu P}) \sum_i V_{1i} \psi_{B\nu P}^*(22^* \dots B^*) \psi_{B\nu P}(2'2" \dots B")$$

phase space occupation 
$$f^*(1) = f_1(1) + \sum_{B \lor P} \sum_{2...B} f_B(E_{B \lor P}) |\psi_{B \lor P}(1...B)|^2$$

self-consistent solutions for clusters in a clustered medium ?

#### Light Cluster Abundances



Composition of symmetric matter in dependence on the baryon density  $n_B$ , T = 5 MeV. Quantum statistical calculation (full) compared with NSE (dotted).

G. R., PRC 92, 054001 (2015)

#### Core-collapse supernovae



snapshot

density

proton fraction, and

temperature profile

of a 15 solar mass supernova at 150 ms after core bounce as function of the radius.

Influence of cluster formation on neutrino emission in the cooling region and on neutrino absorption in the heating region ?

K.Sumiyoshi, G. R., Astrophys.J. **629**, 922 (2005)

#### Composition of supernova core



X

#### EoS at low densities from HIC



#### Nonequilibrium statistical operator (NSO)

principle of weakening of initial correlations (Bogoliubov, Zubarev)

$$\rho_{\epsilon}(t) = \epsilon \int_{-\infty}^{t} e^{\epsilon(t_1 - t)} U(t, t_1) \rho_{\mathrm{rel}}(t_1) U^{\dagger}(t, t_1) dt_1$$

time evolution operator  $U(t,t_0)$  relevant statistical operator  $ho_{
m rel}(t)$ 

selection of the set of relevant observables  $\{B_n\}$ 

 $\begin{array}{ll} \text{self-consistency relations} & \operatorname{Tr}\{\rho_{\mathrm{rel}}(t)B_n\} \equiv \langle B_n \rangle_{\mathrm{rel}}^t = \langle B_n \rangle^t \\ \text{maximum of information entropy} & S_{\mathrm{rel}}(t) = -k_{\mathrm{B}}\operatorname{Tr}\{\rho_{\mathrm{rel}}(t)\log\rho_{\mathrm{rel}}(t)\} \\ \text{generalized Gibbs distribution} & \rho_{\mathrm{rel}}(t) = \exp\left\{-\Phi(t) - \sum_n \lambda_n(t)B_n\right\} \\ \text{von Neumann equation} & \frac{\partial}{\partial t}\varrho_{\varepsilon}(t) + \frac{\imath}{\hbar}\left[H,\varrho_{\varepsilon}(t)\right] = -\varepsilon\left(\varrho_{\varepsilon}(t) - \varrho_{\mathrm{rel}}(t)\right) \\ \varrho(t) = \lim_{\varepsilon \to 0} \varrho_{\varepsilon}(t) \end{array}$ 

Expanding nuclear matter: freeze-out and reaction processes (feed-down)

#### Freeze-out at heavy ion collisions



**Fig. 1.** Chemical freezeout lines in the temperature density plane (phase diagram) together with Mott lines for light clusters. The coexistence regions for the nuclear gasliquid transition and for two examples of the hadron-quark matter transition are shown as grey shaded regions together with their critical endpoints. For details, see text.

D. Blaschke, G. Ropke, Yu. Ivanov, M. Kozhevnikova, and S. Liebing, The XVIII International Conference on Strangeness in Quark Matter (SQM 2019)

#### **Cluster formation at LHC/CERN**



Beth-Uhlenbeck formula for interaction with further particles:

B. Doenigus, G.R., D. Blaschke, Phys. Rev. C 106, 044908 (2022)

## **Outline/Conclusions**

- 1. Equation of state and virial expansions in plasmas Virial coefficients for the uniform electron gas, interpolation formulas: PIMC
- 2. Electrical conductivity: virial expansion for hydrogen plasmas Inclusion of electron-electron collisions: DFT-MD, PIMC
- 3. Beth-Uhlenbeck formula for the second virial coefficient In-medium Schroedinger equation for nuclear matter: Few-body problem
- 4. Cross-over Bose Einstein condensate BCS pairing Quartetting in low-density nuclear matter, Hoyle state and  $\alpha$  decay: AMD
- 5. Cluster Beth-Uhlenbeck formula, continuum correlations Cluster-mean field, composition, freeze-out concept: self-consistent cluster

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## Electron-electron collisions and transport coefficients

Lorentz limit: electron-electron collisions not included in DFT-MD simulations.

slope from quantum Lenard-Balescu: dynamical screening by electrons

 $\lim_{T\to\infty}\tilde{\rho}_2(T)=\tilde{\rho}_2^{\rm QLB}=0.4917$ 

slope: fit gives 0.9886, static screening by electrons and ions:

$$\lim_{T \to \infty} \tilde{\rho}_2(T) = \frac{\pi^{3/2}}{24\sqrt{2}} \left[ \frac{11}{2} - 3C + \ln\left(\frac{3}{2}\pi^2\right) \right] = 1.06036$$

PIMC simulations can solve the problem of the contribution of e – e collisions Higher order correlation functions?

Electronic transport coefficients from density functional theory across the plasma plane M. French, G. R., M. Schörner, M. Bethkenhagen, M. P. Desjarlais, R. Redmer Phys. Rev. E **105**, 065204 (2022)



Interpolation formulas, ERR: A Esser, R. Redmer, G. R., Contrib. Plasma Phys. 43, 33 (2003).

WKB: 
$$\tilde{\rho}_2(T_{\rm eV}) \approx 0.4917 + 0.846 \ln \left[ \frac{1 + 8.492/T_{\rm eV}}{1 + 25.83/T_{\rm eV} + 167.2/T_{\rm eV}^2} \right]$$

G. R., M. Schoerner, M. Bethkenhagen, R. Redmer, , Phys. Rev. E 104, 045204 (2021) Supplemental material

## 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



## 5. Nuclear structure and reactions

 $\alpha$  cluster structure of  ${\rm ^8Be}$ 



R.B. Wiringa et al., PRC **63**, 034605 (01)

Contours of constant density, plotted in cylindrical coordinates, for <sup>8</sup>Be(0+). The left side is in the laboratory frame while the right side is in the intrinsic frame.

#### Ionization degree for carbon

T = 100 eV



Ionization degree of carbon Z<sup>free</sup> derived from DFT- MD simulations (orange line) compared to predictions of OPAL (green line) and Beth-Uhlenbeck (BU) calculations (black lines).

BU results incorporate the EK and SP models, respectively.

Solid line takes into account Pauli blocking effects in addition.

M. Bethkenhagen et al., Phys. Rev. Research 2, 023260 (2020)

#### 3. Clusters in an external potential

c. o. m. coordinate R, relative coordinates s<sub>i</sub>

$$\Psi(\mathbf{R},\mathbf{s}_j) = \varphi^{\mathrm{intr}}(\mathbf{s}_j,\mathbf{R}) \Phi(\mathbf{R})$$

normalization  $\int dR |\Phi(\mathbf{R})|^2 = 1$   $\int ds_j |\varphi^{\text{intr}}(\mathbf{s}_j, \mathbf{R})|^2 = 1$ 

N. Gidopoulos, E. Gross (2014)

Wave equation for the c.o.m. motion

$$-\frac{\hbar^2}{2Am}\nabla_R^2\Phi(\mathbf{R}) - \frac{\hbar^2}{Am}\int ds_j\varphi^{\text{intr},*}(\mathbf{s}_j,\mathbf{R})[\nabla_R\varphi^{\text{intr}}(\mathbf{s}_j,\mathbf{R})][\nabla_R\Phi(\mathbf{R})] \\ -\frac{\hbar^2}{2Am}\int ds_j\varphi^{\text{intr},*}(\mathbf{s}_j,\mathbf{R})[\nabla_R^2\varphi^{\text{intr}}(\mathbf{s}_j,\mathbf{R})]\Phi(\mathbf{R}) + \int dR' W(\mathbf{R},\mathbf{R}')\Phi(\mathbf{R}') = E\,\Phi(\mathbf{R})$$

c.o.m. effective potential

$$W(\mathbf{R},\mathbf{R}') = \int ds_j \, ds'_j \, \varphi^{\text{intr},*}(\mathbf{s}_j,\mathbf{R}) \left[ T[\nabla_{s_j}] \delta(\mathbf{R}-\mathbf{R}') \delta(\mathbf{s}_j-\mathbf{s}'_j) + V(\mathbf{R},\mathbf{s}_j;\mathbf{R}',\mathbf{s}'_j) \right] \varphi^{\text{intr}}(\mathbf{s}'_j,\mathbf{R}')$$

Wave equation for the intrinsic motion

$$-\frac{\hbar^2}{Am} \Phi^*(\mathbf{R}) [\nabla_R \Phi(\mathbf{R})] [\nabla_R \varphi^{\text{intr}}(\mathbf{s}_j, \mathbf{R})] - \frac{\hbar^2}{2Am} |\Phi(\mathbf{R})|^2 \nabla_R^2 \varphi^{\text{intr}}(\mathbf{s}_j, \mathbf{R}) + \int dR' \, ds'_j \, \Phi^*(\mathbf{R}) \left[ T[\nabla_{s_j}] \delta(\mathbf{R} - \mathbf{R}') \delta(\mathbf{s}_j - \mathbf{s}'_j) + V(\mathbf{R}, \mathbf{s}_j; \mathbf{R}', \mathbf{s}'_j) \right] \Phi(\mathbf{R}') \varphi^{\text{intr}}(\mathbf{s}'_j, \mathbf{R}') = F(\mathbf{R}) \varphi^{\text{intr}}(\mathbf{s}_j, \mathbf{R}) G. R. et al., PRC 90, 034304 (2014)$$

#### **Quartet wave function**

Four-particle wave equation in position space representation

$$\begin{split} & [E_4 - \hat{h}_1 - \hat{h}_2 - \hat{h}_3 - \hat{h}_4] \Psi_4(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3 \mathbf{r}_4) = \int d^3 \mathbf{r}'_1 \, d^3 \mathbf{r}'_2 \langle \mathbf{r}_1 \mathbf{r}_2 | B \ V_{N-N} | \mathbf{r}'_1 \mathbf{r}'_2 \rangle \Psi_4(\mathbf{r}'_1 \mathbf{r}'_2 \mathbf{r}_3 \mathbf{r}_4) \\ & + \int d^3 \mathbf{r}'_1 \, d^3 \mathbf{r}'_3 \langle \mathbf{r}_1 \mathbf{r}_3 | B \ V_{N-N} | \mathbf{r}'_1 \mathbf{r}'_3 \rangle \Psi_4(\mathbf{r}'_1 \mathbf{r}_2 \mathbf{r}'_3 \mathbf{r}_4) + \text{four further permutations.} \\ & \text{Single-nucleon Hamiltonian} \qquad \hat{h} = \frac{\hbar^2 p^2}{2m} + [1 - \sum_i^{\text{occ.}} |n\rangle \langle n|] V^{\text{mf}}(r) \\ & \text{Pauli blocking B} \qquad B(1,2) = [1 - f_1(\hat{h}_1) - f_2(\hat{h}_2)] \end{split}$$

Local density approximation: momentum representation, no coupled gradient terms, Thomas-Fermi Intrinsic motion: in-medium interaction

c.o.m. effective potential  $W(\mathbf{R}) = W^{\text{ext}}(\mathbf{R}) + W^{\text{intr}}(\mathbf{R})$   $W^{\text{ext}}(\mathbf{R}) = W^{\text{mf}}(\mathbf{R}) = V^{\text{Coul}}_{\alpha = \Omega}(R) + V^{\text{N-N}}_{\alpha = \Omega}(R)$ 

$$W^{\text{intr}}(\mathbf{R}) = 4E_F[n_B(\mathbf{R})], \qquad E_F(n_B) = (\hbar^2/2m)(3\pi^2 n_B/2)^{2/3}.$$

 $W^{\text{intr}}(\mathbf{R}) = -B_{\alpha} + W^{\text{Pauli}}[n_B(\mathbf{R})], \qquad n_B \le n_{\text{crit}}$ 

 $W^{\text{Pauli}}(n_B) \approx 4515.9 \text{ MeV fm}^3 n_B - 100935 \text{ MeV fm}^6 n_B^2 + 1202538 \text{ MeV fm}^9 n_B^3$ 

# Nuclear statistical equilibrium (NSE)

#### Chemical picture:

Ideal mixture of reacting components Mass action law



Interaction between the components internal structure: Pauli principle

#### Physical picture:

"elementary" constituents and their interaction



Quantum statistical (QS) approach, quasiparticle concept, virial expansion



deuteron bound state -2.2 MeV

G. Roepke, J. Phys.: Conf. Series 569, 012031 (2014) Phys. Part. Nucl. 46, 772 (2015) [arXiv:1408.2654]

## **Different approximations**

#### Ideal Fermi gas:

protons, neutrons, (electrons, neutrinos,...)

#### bound state formation

Nuclear statistical equilibrium: ideal mixture of all bound states (clusters:) chemical equilibrium

#### medium effects

Quasiparticle quantum liquid: mean-field approximation BHF, Skyrme, Gogny, RMF

Chemical equilibrium with quasiparticle clusters: self-energy and Pauli blocking

### Single nucleon distribution function

Dependence on temperature



saturation density

Alm et al., PRC 53, 2181 (1996)

## **Different approximations**

#### Ideal Fermi gas: protons, neutrons, (electrons, neutrinos,...)

#### bound state formation

Nuclear statistical equilibrium: ideal mixture of all bound states (clusters:) chemical equilibrium

#### continuum contribution

Second virial coefficient: account of continuum contribution, scattering phase shifts, Beth-Uhl.Eq.

#### chemical & physical picture

Cluster virial approach: all bound states (clusters) scattering phase shifts of all pairs

#### medium effects

Quasiparticle quantum liquid: mean-field approximation BHF, Skyrme, Gogny, RMF

Chemical equilibrium of quasiparticle clusters: self-energy and Pauli blocking

#### Generalized Beth-Uhlenbeck formula:

medium modified binding energies, medium modified scattering phase shifts

#### Correlated medium:

phase space occupation by all bound states in-medium correlations, quantum condensates

## **Crossover from BEC to BCS pairing**



#### α-cluster-condensation (quartetting)



G.R., A.Schnell, P.Schuck, and P.Nozieres, PRL 80, 3177 (1998)

#### Suppresion of condensate fraction



# Clustering phenomena in nuclear matter below the saturation density



Overhauser: density-fluctuated states (DFSs) instead of plane-wave states.

Energy curves of DFSs due to  $\alpha$  and <sup>16</sup>O clustering in the symmetric nuclear matter. The density of matter is normalized by the saturation density of the uniform matter.

Hiroki Takemoto et al., PR C **69**, 035802 (2004)

#### Equation of state: chemical potential



Chemical potential for symmetric matter. T=1, 5, 10, 15, 20 MeV. QS calculation compared with RMF (thin) and NSE (dashed). Insert: QS calculation without continuum correlations (thin lines).

#### Symmetric matter: free energy per nucleon



Dashed lines: no continuum correlations

G. R., PRC 92, 054001 (2015)