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

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## Outlook

- 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

## Structure of matter

energy scale	fermions	interaction	bound states	density effects	condensed phase
$1 \dots 10 \text{ meV}$	electrons, holes	Coulomb	$\operatorname{excitons}$	screening	electron-hole liquid
$1 \dots 10   \mathrm{eV}$	electrons, nuclei	Coulomb	ions, atoms	screening	liquid metal
$1 \dots 10 \text{ MeV}$	protons, neutrons	N-N int.	nuclei	Pauli blocking	nuclear matter
$0.1 \dots 1  { m GeV}$	quarks	QCD	hadrons	deconfinement	quark-gluon plasma

Fermion systems: ideal Fermi gases

Interaction - correlations

Low densities: bound states, quantum condensates High densities: condensed phase

- Plasma physics: Ionization potential depression (IPD)
- Nuclear physics: Weakly bound nuclei in nuclear systems
- QCD: Deconfinement, Quark Gluon phase transition in neutron-star mergers

## 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



## Binding energy per nucleon



#### Semi-empirical mass formula

Liquid drop model: Bethe-Weizsaecker mass formula

$$B(A,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + a_P \frac{1}{A^{1/2}}$$

bulk contribution:  $a_V = 15.75$  MeV surface contribution:  $a_S = 17.8$  MeV Coulomb repulsion:  $a_C = 0.711$  MeV asymmetry term:  $a_A = 23.7$  MeV pairing:  $a_P = 11.18$  MeV (even-even), = 0 (even-odd), = -11.18 MeV (odd-odd) shell structure and magic numbers

proton fraction 
$$Y_p = \frac{Z}{A} = \frac{Z}{N+Z}, \quad \frac{N}{Z} = 1 + \frac{a_C}{2a_A}A^{2/3}$$

## Models of nuclei

Constituents: protons, neutrons

Shell model of nucleus: potential well

Droplet model: Bethe-Weizsäcker-Formel

C. F. von Weizsäcker: *Zur Theorie der Kernmassen.* In: *Zeitschrift für Physik.* **96** (1935), S. 431–458.





magic numbers: 2; 8; 20; 28; 50; 82; 126

Hans Jensen, Maria Goeppert-Mayer

O. Haxel, J.H.D. Jensen, H. E. Suess *Zur Interpretation der ausgezeichneten Nukleonenzahlen im Bau der Atomkerns*, Die Naturwissenschaften, Band **35**, (1949) S.376

## Nuclear radii

ms<sup>2</sup> = 
$$\frac{\int_0^\infty dr \ r^4 \ \rho(r)}{\int_0^\infty dr \ r^2 \ \rho(r)}$$

root mean square radius (charge or point): rms

mass – radius relation: R = 1.18 A<sup>1/3</sup> [fm]  $\rightarrow$  n<sub>B</sub> = 0.15 fm<sup>-3</sup> =  $\rho_{sat}$ 



I. Angeli, Atomic Data and Nuclear Data Tables 87, (2004)

## **Correlations in nuclei**

- Liquid droplet (Bethe Weizsaecker)
- Shell model (Jensen)
- Pairing (odd-even staggering) quartetting
- Hoyle state in <sup>12</sup>C
- $\alpha$  formation and  $\alpha$  decay

#### $\alpha$ cluster structure of <sup>8</sup>Be



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.

#### Big-Bang nucleosynthesis: H, He, Li, \_\_\_\_



Take home textbook knowledge

- Three minutes after the Big Bang
- Three chemical elements: H, He, Li
- Three observed abundances: <sup>2</sup>H, <sup>4</sup>He, <sup>7</sup>Li

#### The Hoyle state in <sup>12</sup>C

<sup>12</sup>C: from astrophysics: excited state predicted near the 3  $\alpha$  threshold energy (F. Hoyle).

a 0<sup>+</sup> state at 0.39 MeV above the 3  $\alpha$  threshold energy has been found.

not described by shell structure calculations,  $3 \alpha$  cluster interact predominantly in relative S waves, gas-like structure, THSR state

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

 $\alpha$ -particle condensation in low-density nuclear matter,  $\rho$  below  $\rho_{sat}/5$ 

n $\alpha$  nuclei: <sup>8</sup>Be, <sup>12</sup>C, <sup>16</sup>O, <sup>20</sup>Ne, <sup>24</sup>Mg, ... cluster type structures near the n  $\alpha$  breakup threshold energy

## **Excited light nuclei**



#### Decay modes of nuclei





## Preformation: $\alpha$ decay of <sup>212</sup>Po



## Hot and dense matter

- Early universe
- Compact objects in astrophysics
- Heavy ion collisions
- Spontaneous fission

## Nuclear matter phase diagram



#### 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

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

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

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

## 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)

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

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

## **Different approximations**

Ideal Fermi gas:

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

#### **Partial summations**



## **Different approximations**

medium effects

Ideal Fermi gas:

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

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

## Medium effects: Quasiparticle approximation

- Skyrme / Gogny
- relativistic mean field (RMF)

Lagrangian: non-linear sigma, TM1 parameters, single particle modifications, energy shift, effective mass

- DD-RMF [S.Typel, Phys. Rev. C 71, 064301 (2007)]: expansion of the scalar field and the vector fields in powers of proton/neutron densities
- Dirac-Brueckner Hartree Fock (DBHF)
- Density functional theory

## Quasiparticle picture: RMF and DBHF



## Quasiparticle approximation for nuclear matter Equation of state for symmetric matter

10NLo NLoð DBHF DD $D^{2}C$ KVR KVOR DD-F  $E_0$  [MeV] But: cluster -10 formation Incorrect low-density -20<sup>L</sup> 0.3 0.2 limit 0.1n [fm<sup>-3</sup>] Klaehn et al., PRC 2006

#### **Bethe-Salpeter equation**



#### **Beth-Uhlenbeck formula**



## Cluster decomposition of the self-energy



T<sub>n</sub>-matrices: n-particle Schroedinger equation, n-particle bound states, (we neglect here scattering states).

Including clusters like new components chemical picture, mass action law, nuclear statistical equilibrium (NSE)

#### Ideal mixture of reacting nuclides

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

mass number A, charge  $Z_A$ , energy  $E_{A,v,K}$ , v internal quantum number,  $\sim K$  center of mass momentum

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

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

# Nuclear statistical equilibrium (NSE)

#### Chemical picture:

Ideal mixture of reacting components Mass action law



## **Different approximations**

#### medium effects

#### Ideal Fermi gas:

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

bound state formation

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

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

Inclusion of the light clusters (d,t,<sup>3</sup>He,<sup>4</sup>He)

## Composition of symmetric matter Ideal mixture of nuclides



## **Different approximations**

#### medium effects

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

#### bound state formation

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## **Different approximations**

#### Ideal Fermi gas:

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#### medium effects

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

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

# 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

#### **Bethe-Salpeter equation**



## Effective wave equation for the deuteron in matter

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

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

phase space occupation: Fermi distribution function

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

(screening and vertex correction neglected)

#### 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)

#### Shift of Binding Energies of Light Clusters







## **Full virial expansion**

- Excited states, resonances, scattering states
- Full expression for the second virial coefficient
- Scattering phase shifts
- Exact in second order of density
- Beth-Uhlenbeck equation, Dashen-Ma-Bernstein: S-matrix

## **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.E.

#### medium effects

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

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

#### **Beth-Uhlenbeck formula**



#### Alpha-particle fraction in the low-density limit

symmetric matter, T=2, 4, 8 MeV



C.J.Horowitz, A.Schwenk, Nucl. Phys. A 776, 55 (2006)

## Effective wave equation for the deuteron in matter

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

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

phase space occupation: Fermi distribution function

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

solution for bound and scattering states

## **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.

#### 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

## Levinson's theorem

- Bound states disappear at increasing density, merge with the continuum
- No discontinuity in the partition function, jump in the bound state contribution is compensated by a jump in the scattering phase contribution
- Levinson's theorem: scattering phase shift at zero energy is given by the number of bound states multiplied by pi

#### 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)



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

#### 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

## **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):  

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

 $v_d^0(T) = v_{T_I=0}^0(T) \approx 0.30857 + 0.65327 \ e^{-0.102424 \ T/\text{MeV}}$ 

G. Roepke, PRC 92,054001 (2015)

## Single nucleon distribution function

Dependence on temperature



saturation density

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

#### Pauli blocking, correlated medium

In-medium Schroedinger equation

$$[E_{\tau_1}(\mathbf{p}_1; T, \mu_n, \mu_p) + \dots + E_{\tau_A}(\mathbf{p}_A; T, \mu_n, \mu_p) - E_{A\nu}(\mathbf{P}; T, \mu_n, \mu_p)]\psi_{A\nu\mathbf{P}}(1 \dots A) + \sum_{1' \dots A'} \sum_{i < j} [1 - n(i; T, \mu_n, \mu_p) - n(j; T, \mu_n, \mu_p)]V(ij, i'j') \prod_{k \neq i, j} \delta_{kk'}\psi_{A\nu\mathbf{P}}(1' \dots i' \dots j' \dots A') = 0$$

effective occupation numbers

$$n(1) = f_{1,\tau_1}(1) + \sum_{B=2}^{\infty} \sum_{\bar{\nu},\bar{\mathbf{P}}} \sum_{2...B} B f_B \left( E_{B,\bar{\nu}}(\bar{\mathbf{P}};T,\mu_n,\mu_p) \right) |\psi_{B\bar{\nu}\bar{\mathbf{P}}}(1\ldots B)|^2$$

effective Fermi distribution

$$\begin{split} n(1;T,\mu_n,\mu_p) &\approx f_{1,\tau_1}(1;T_{\rm eff},\mu_n^{\rm eff},\mu_p^{\rm eff}) & \mbox{blocking by all nucleons} \\ n(1;T,\mu_n,\mu_p) &\approx \tilde{f}_{1,\tau_1}(1;T_{\rm eff},n_B,Y_p) \\ & \mbox{effective temperature} & T_{\rm eff} &\approx 5.5 \, {\rm MeV} + 0.5 \, T + 60 \, n_B \, \, {\rm MeV} \, {\rm fm}^3 \end{split}$$

G. Roepke, PRC 92,054001 (2015)

## **In-medium effects**

- Self energy, mean-field approximation
- Quasiparticle picture of elementary particles
- Full antisymmetrization: Pauli blocking
- Bound states as new quasiparticles
- Continuum correlations
- Correlated medium
- Quantum statistical approach.
- Excluded volume (Hempel, Schaffner-Bielich,...)
- Generalized relativistic mean field: clusters as quasiparticles (Typel, Pais,...)

## **EoS including correlations**

- Composition
- Chemical potential, nuclear matter and stellar matter ( $\beta$  equilibrium)
- Free energy and related quantities, symmetry energy,...
- Phase transition
- Quantum condensates: pairing, quartetting,...

#### 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)

## Pauli blocking in symmetric matter



Free proton fraction as function of density and temperature in symmetric matter. QS calculations (solid lines) are compared with the NSE results (dotted lines). Mott effect in the region  $n_{\text{saturation}}/5$ .

#### 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).