HNC calculations for the structure of dense multi-component plasmas

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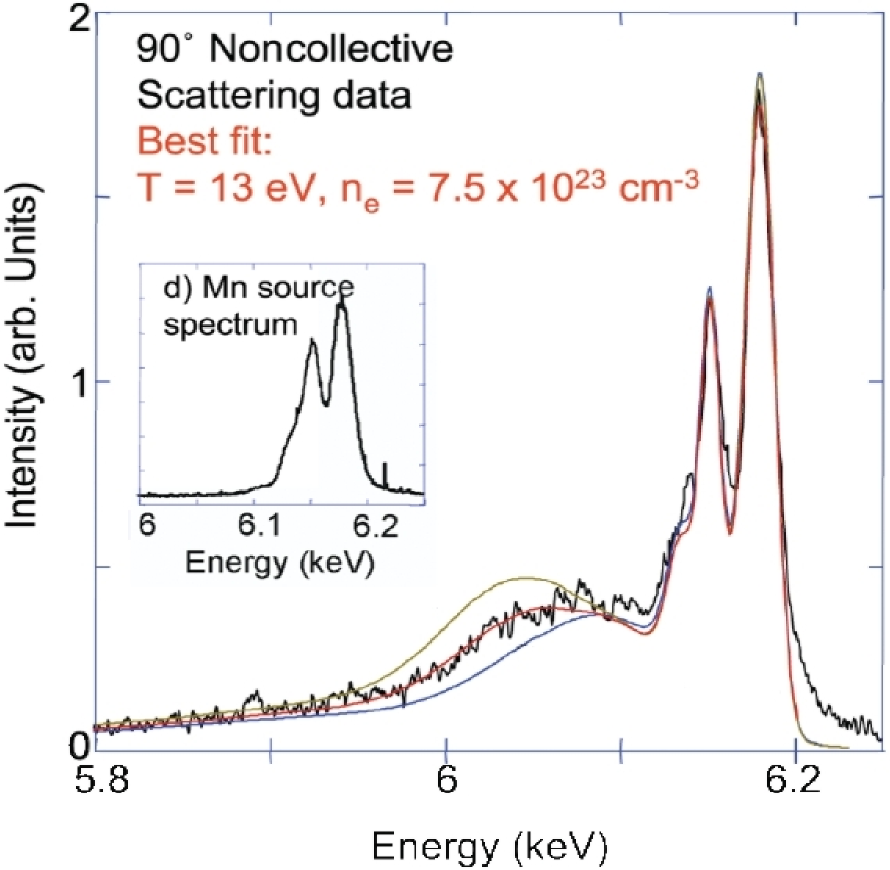
Outline

- Introduction
- Structure factor calculation
- Results
- Conclusion

Beryllium X-Ray Thomson Scattering Spectra



$$\frac{d^2\sigma}{d\omega d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} \frac{\omega_1}{\omega_0}\left[Z_f S_{ee}^0(k,\omega) + |f(k)+\rho(k)|^2 S_{ii}(k,\omega) + Z_b \int d\omega' \tilde{S}^{\mathrm{ce}}(k,\omega-\omega') S_s(k,\omega')\right]$$

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J. Chihara, J. Phys. F **17**, 295 (1987); J. Chihara, J. Phys.: Condens. Matter **12**, 231 (2000).

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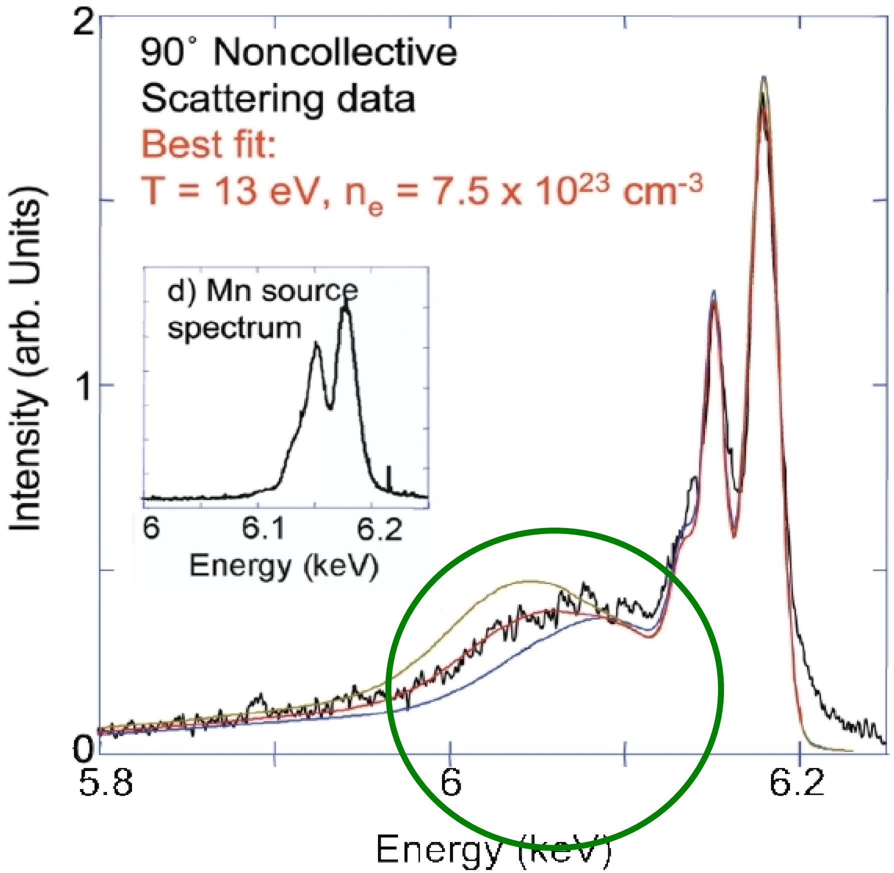

$$S_{ee}^{0}(k,\omega)=\left|1+\Pi_{ee}^{\mathrm{R}}(k,\omega)\frac{V_{ee}(k)}{\varepsilon^{\mathrm{R}}(k,\omega)}\right|^{2} S_{e}^{0}(k,\omega)$$

$$S_{e}^{0}(k,\omega)=\frac{n_e m_e}{k\sqrt{2\pi m_e k_B T}}\exp\left[\frac{m_e\left(\frac{\omega}{k}+\frac{\hbar k}{2m_e}\right)^{2}}{2k_B T}\right]$$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\omega\mathrm{d}\Omega}=\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{Th}}\frac{\omega_1}{\omega_0}\left[Z_f S_{ee}^{0}(k,\omega)+\left|f(k)+\rho(k)\right|^{2} S_{ii}(k,\omega)+Z_b\int \mathrm{d}\omega' \tilde{S}^{\mathrm{ce}}(k,\omega-\omega')S_{\mathrm{s}}(k,\omega')\right]$$

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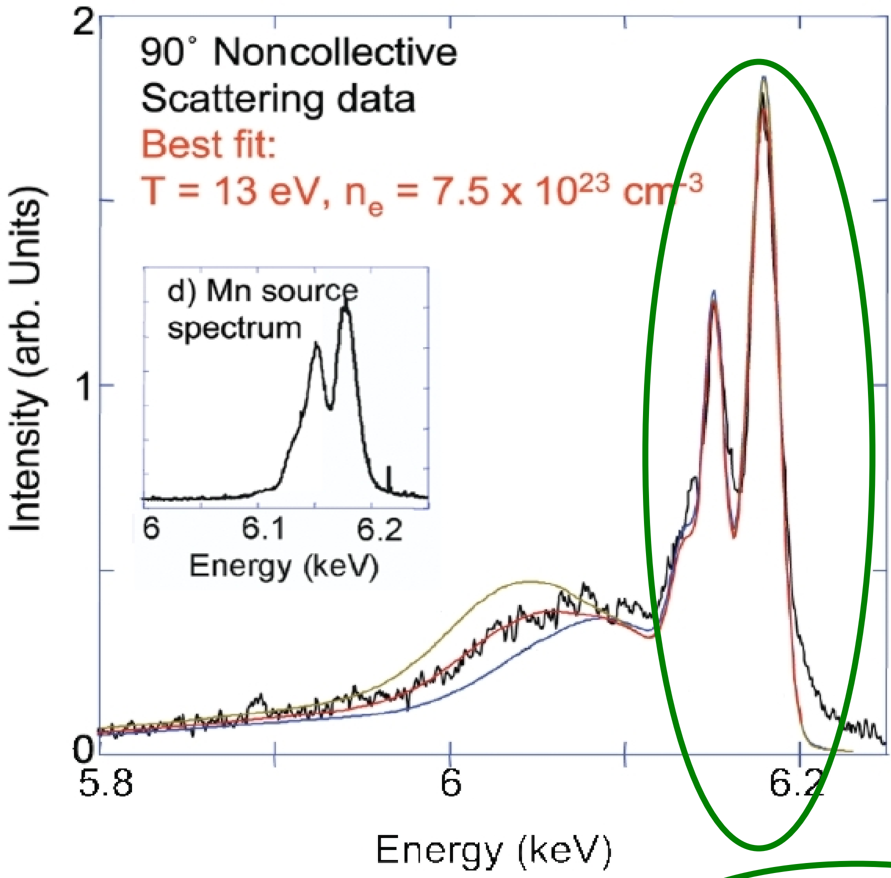

$$S_{ee}^{i}(k,\omega)=\left|f(k)+\rho(k)\right|^2 S_{ii}(k,\omega)$$

$$S_{ei}(k)=\frac{\rho(k)}{\sqrt{Z_f}}S_{ii}(k)$$

$$\frac{d^2\sigma}{d\omega d\Omega}=\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}}\frac{\omega_1}{\omega_0}\left[Z_f S_{ee}^{0}(k,\omega)+\left|f(k)+\rho(k)\right|^2 S_{ii}(k,\omega)+Z_b\int d\omega' \tilde{S}^{ce}(k,\omega-\omega')S_s(k,\omega')\right]$$

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Structure Factor Calculation

$$S_{ab}(k) = \delta_{ab} + \sqrt{n_a n_b} \int \mathrm{d}^3\mathrm{r}_{12} \exp(-i\mathbf{k}\mathbf{r}_{12})[g_{ab}(r_{12}) - 1]$$

ansatz for closed solution (BBGKY hierarchy) – Ornstein-Zernike equation:

$$g_{ab}(r_{12}) - 1 \equiv h_{ab}(r_{12}) = c_{ab}(r_{12}) + \sum_c n_c \int \mathrm{d}^3 r_3 c_{ac}(r_{13})\, h_{cb}(r_{23})$$

a closure relation (approximation) for the direct correlation function is needed, e.g. HNC

$$c_{ab}(r_{12}) = h_{ab}(r_{12}) - \ln g_{ab}(r_{12}) - \beta V_{ab}(r_{12})$$

applicable for multi-component plasmas, i.e. electrons, ions of multiple charge state

V. Schwarz, T. Bornath, W.-D. Kraeft, S. Glenzer, A. Höll, R. Redmer, Contrib. Plasma Phys. **47**, 324–330 (2007).
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Effective (quantum) Pair Potential

general ansatz: two-particle classical partition function equals quantum mechanical Slater sum:

$$\exp\left[-\beta V_{ab}^{\mathrm{eff}}(r_{12})\right] = \mathcal{S}_{ab}(r_{12})$$

typical representatives – Kelbg and Deutsch potential:

$$V_{ab}^{K}(r_{12}) = \frac{q_a q_b}{4\pi\varepsilon_0 r}\left[1 - \exp\left(-4\pi\frac{r^2}{\lambda_{ab}^2}\right) + 2\pi\frac{r}{\lambda_{ab}}\operatorname{erfc}\left(2\sqrt{\pi}\frac{r}{\lambda_{ab}}\right)\right]$$

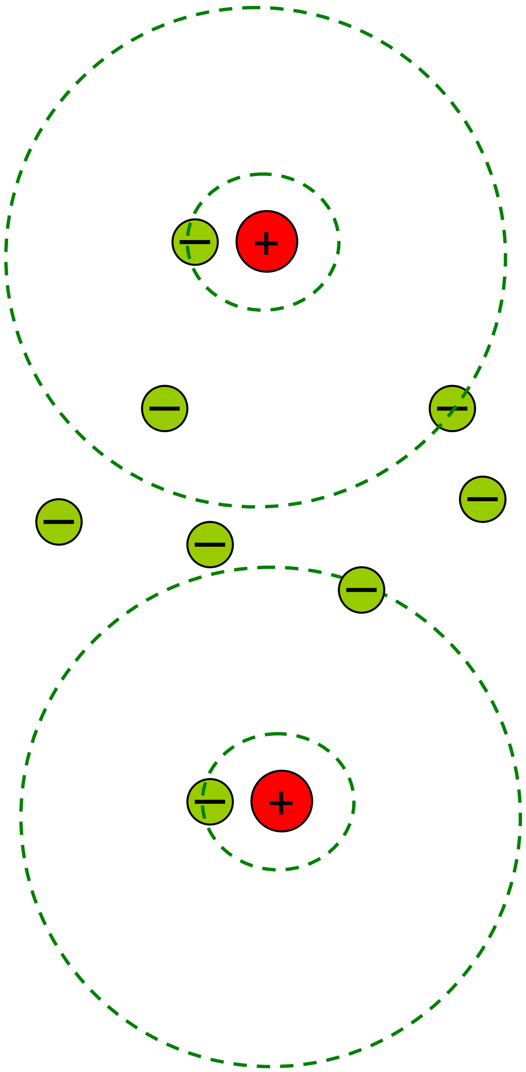
$$V_{ab}^{D}(r_{12}) = \frac{q_a q_b}{4\pi\varepsilon_0 r}\left[1 - \exp\left(-2\pi\frac{r}{\lambda_{ab}}\right)\right]$$

$$\lambda_{ab}^2 = \frac{2\pi\hbar^2}{m_{ab}k_B T} \qquad m_{ab}^{-1} = m_a^{-1} + m_b^{-1}$$

Kelbg potential is used for the repulsive interactions, $V_{ee}(r_{12})$ and $V_{ii}(r_{12})$

T. Morita, Prog. Theor. Phys. **22**, 757–774 (1959).
T. Morita, K. Hiroike, Prog. Theor. Phys. **23**, 1003–1027 (1960).
A. V. Filinov, V. O. Golubnychiy, M. Bonitz, W. Ebeling, J. W. Dufty, Phys. Rev. E **70**, 046411 (2004).

Effective (quantum) Pair Potential, $V_{ei}(r_{12})$



How to distinguish between free and weakly bound electrons far away from the core?

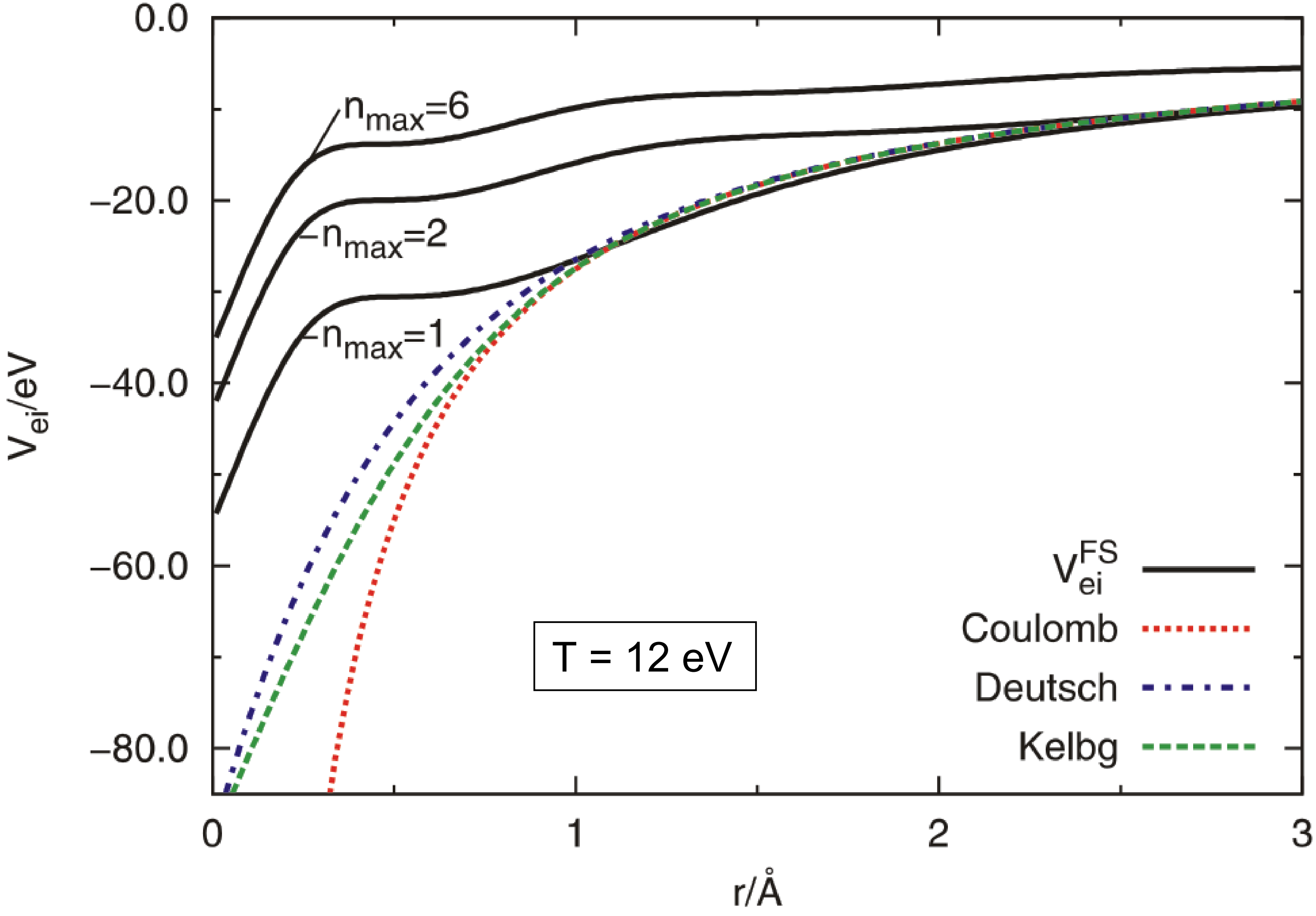
How to avoid Coulomb divergence for small distances?

ansatz: separate two-particle quantum mechanical Slater sum into scattering and bound part:

$$\exp\left[-\beta V_{ei}^{\mathrm{eff}}\left(r_{12}\right)\right]=\mathcal{S}_{ei}\left(r_{12}\right)-\mathcal{S}_{ei}^{b}\left(r_{12},n_{\max}\right)$$

F. J. Rogers, Phys. Rev. A 29, 868-879 (1984).

Effective (quantum) Pair Potential, $V_{ei}(r_{12})$

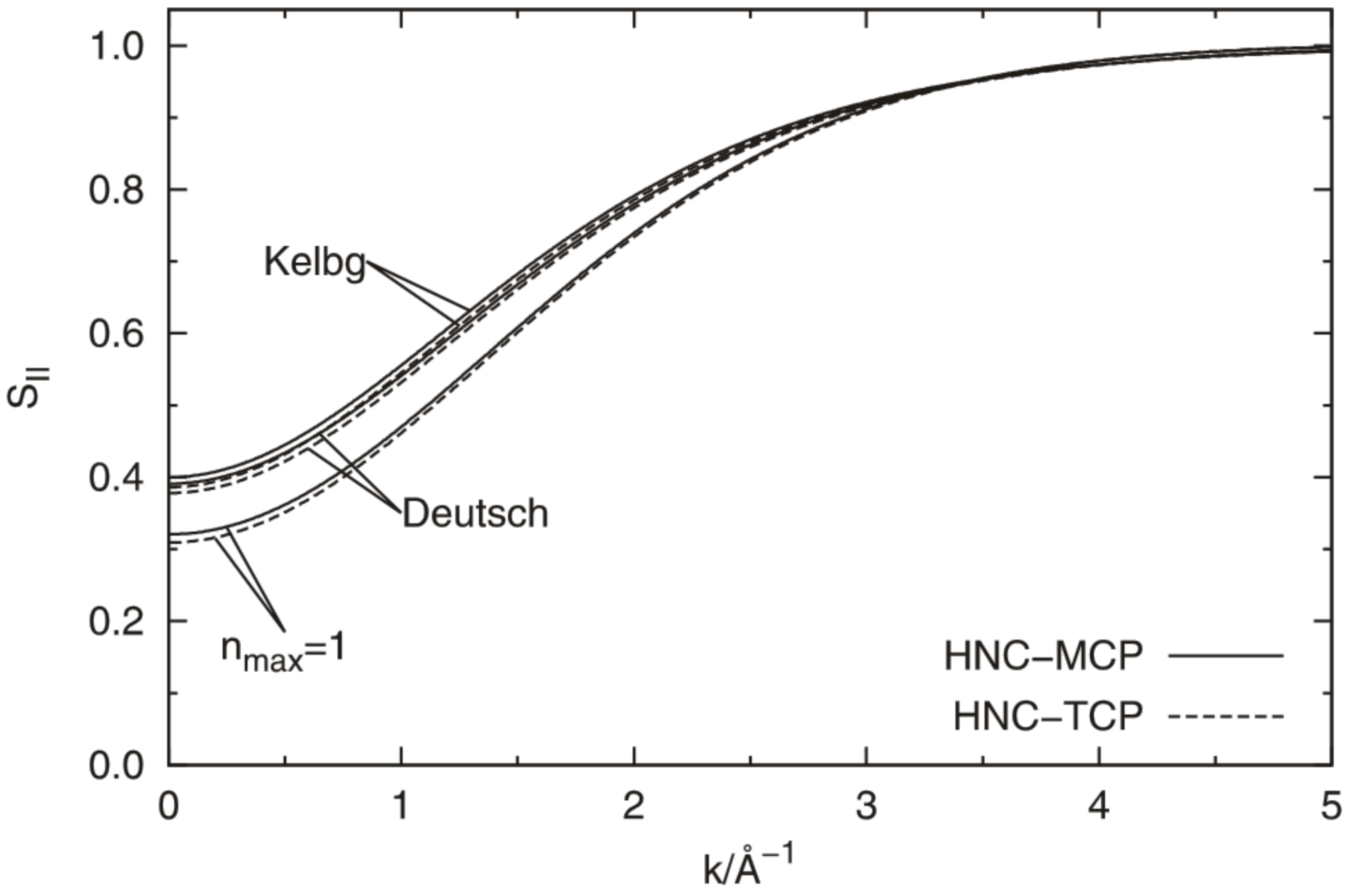


Results (MCP vs. TCP)

Multi-component Beryllium, solid density, T=40 eV:

MCP 3 components (Z=2@63%,Z=3@36%,Z=4@1%),

TCP Z_{eff}=2.38



Results (experimental conditions)

FT-DFT-MD simulations were performed using VASP, PAW potentials and GGA

ionic pair correlation function:

$$g_{ii}(r) = \frac{V}{4\pi r^2 N_i (N_i - 1)} \sum_{j=1}^{N_i} \sum_{\substack{k=1 \\ k \neq j}}^{N_i} \delta(r - r_j - r_k)$$

electron ion pair correlation function:

$$g_{ei}(\mathbf{r}) = \frac{V}{N_i N_e} \sum_{j=1}^{N_i} n_e(\mathbf{r_j} - \mathbf{r})$$

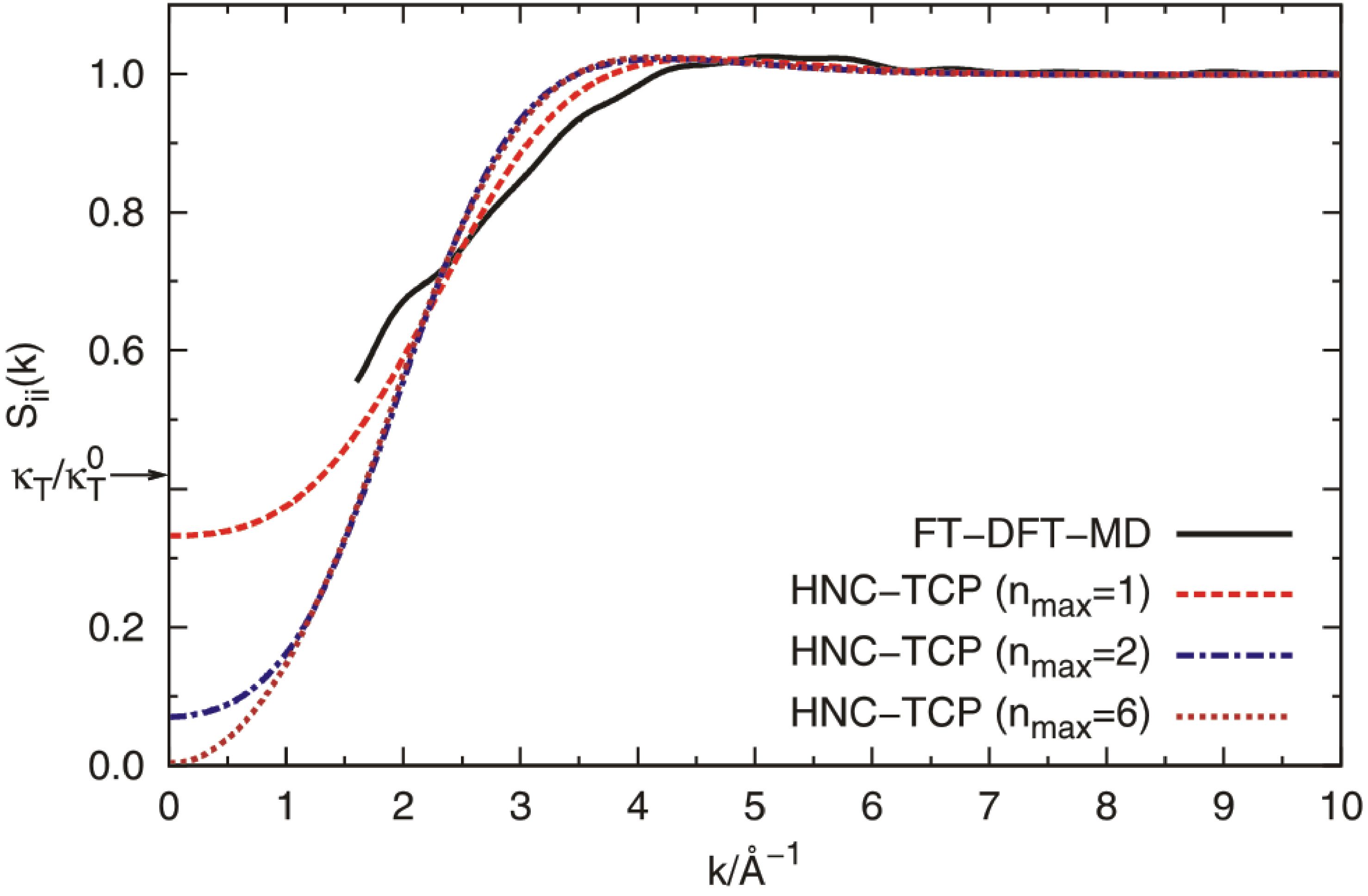
limiting cases:

$$S_{ii}(k=0) = \kappa_T \quad n_i k_B T \qquad\qquad \kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{T,n}$$

G. Kresse, J. Hafner, Phys. Rev. B **47**, 558 (1993). G. Kresse, J. Hafner, Phys. Rev. B **49**, 14251 (1994). G. Kresse, J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
G. Kresse, D. Joubert, Phys. Rev. B **59**, 1758 (1999).
J. P. Perdew, K. Burke, M. Enzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

Results (experimental conditions)

TCP Be, solid density, T=12 eV, Z_{eff}=2



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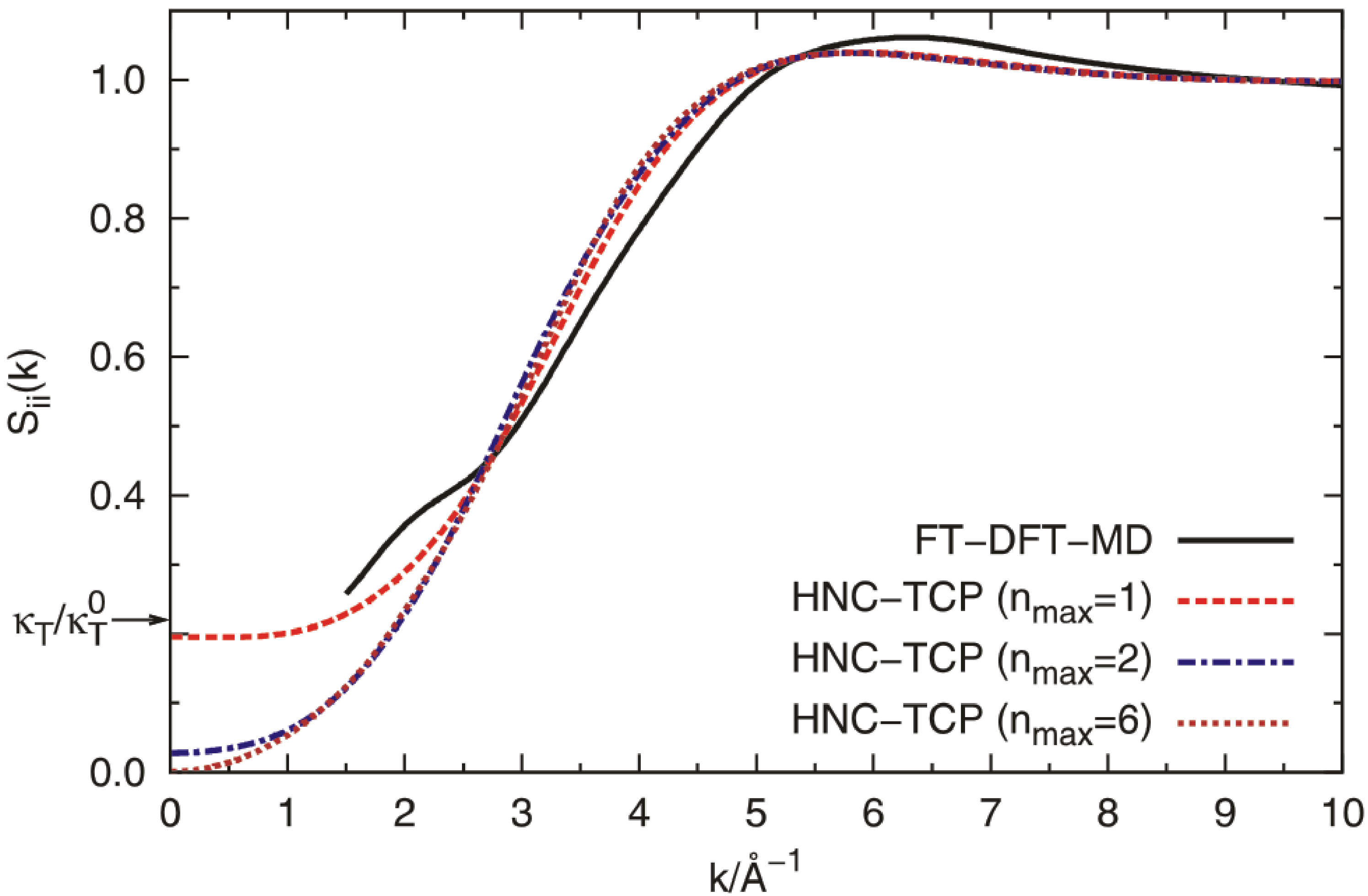
Results (experimental conditions)

TCP Be, three times solid density, T=13 eV, Z_{eff}=2



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Generalization to multi-temperature plasma

multi-temperature Ornstein-Zernike equation:

$$\frac{\partial h_{ab}(r_{12})}{\partial \mathbf{r}_{12}} - \frac{\partial c_{ab}(r_{12})}{\partial \mathbf{r}_{12}} = \beta_{ab} \frac{m_b}{m_a + m_b} \sum_c n_c \int \mathrm{d}^3 \mathrm{r}_3 \frac{1}{\beta_{ac}} \frac{\partial c_{ac}(r_{13})}{\partial \mathbf{r}_1} h_{cb}(r_{23})$$

$$- \beta_{ab} \frac{m_a}{m_a + m_b} \sum_c n_c \int \mathrm{d}^3 \mathrm{r}_3 \frac{1}{\beta_{bc}} \frac{\partial c_{bc}(r_{23})}{\partial \mathbf{r}_2} h_{ca}(r_{13})$$

corresponding multi-temperature closure relation, e.g. HNC:

$$c_{ab}(r_{12}) = h_{ab}(r_{12}) - \ln g_{ab}(r_{12}) - \beta_{ab} V_{ab}(r_{12})$$

mass-weighted temperature: $\beta_{ab}^{-1} = k_B T_{ab} = k_B \frac{m_a T_b + m_b T_a}{m_a + m_b}$

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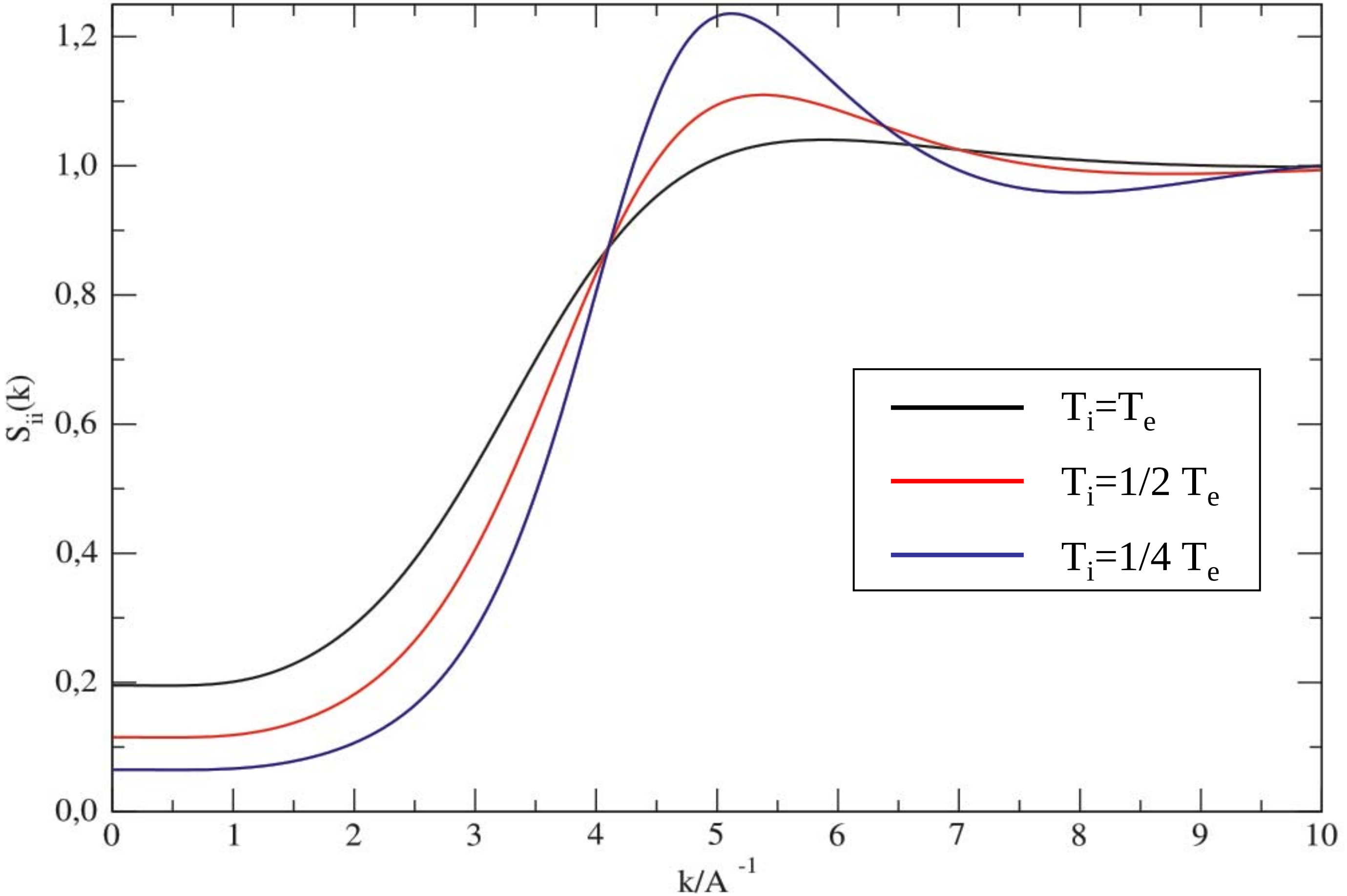
P. Seuferling, J. Vogel, C. Toepffer, Phys. Rev. A 40, 323 (1989).

Results (multi-temperature plasma)

Influence of $T_e \neq T_i$, i.e. two-temperature plasma

Beryllium, three times solid density T_e=13 eV, Z_{eff}=2



Conclusions

1. The approximation of a TCP with effective charge is reasonable.

2. Using an integral equation method in combination with effective (quantum) potentials it is possible to reproduce ab initio data for $S_{ii}(k)$.

3. We can treat also two-temperature plasmas.

Integral equation method is an efficient and reliable tool for structure calculations.

The results presented here can be applied to X-Ray Thomson Scattering Spectra [1].

[1] S. H. Glenzer, O. L. Landen, P. Neumayer, R. W. Lee, K. Widmann, S. W. Pollaine, R. J. Wallace, G. Gregori, A. Höll, T. Bornath, R. Thiele, V. Schwarz, W.-D. Kraeft, R. Redmer, Phys. Rev. Lett. **98**, 065002 (2007).

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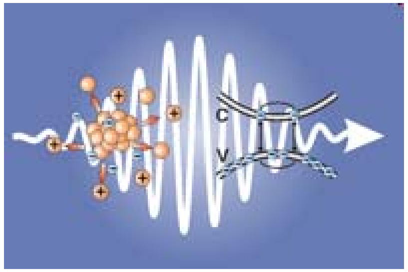

SFB 652

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grant FSP 301-FLASH, project No. KS7HRA

Helmholtz Gesellschaft Virtual Institute VH-VI-104
„Plasma physics research using FEL radiation“

Thank you for your attention.

$$\mathcal{S}_{ei}^{b}\left(r_{12}, n_{\max}\right) = \frac{2\sqrt{\pi}}{T^{3/2}} \sum_{n=1}^{n_{\max}} \sum_{l=0}^{n-1} \exp\left(\frac{1}{n^2 T}\right) (2l+1) \left| R_{nl}\left(r_{12}\right) \right|^2$$

$$R_{nl}\left(r_{12}\right) = \frac{2^{l+1}}{n^{2+l}} \sqrt{\frac{(n-1-l)!}{(n+l)!}} \exp\left(-\frac{r_{12}}{n}\right) \; r_{12}^{l} \, \mathrm{La}_{n-1-l}^{2l+1}\left(\frac{2r_{12}}{n}\right)$$