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WIGNER PATH INTEGRAL REPRESENTATION OF DENSITY OF STATES AND RESPONSE FUNCTIONS. MONTE CARLO SIMULATION OF THE ONE- AND TWO-COMPONENT PLASMA MEDIA

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OUTLINE

The dynamic structure and response function characterize the excitation spectrum of the system and the amount of energy absorbed by the system when perturbed by an external field, for example, x-ray Thomson scattering and others. These functions contain information about inter-particle correlations and time evolution.

- Dynamic Structure Factor and Response Function in Heisenberg representation
- Wigner Representation of the Dynamic Structure Factor and Response Function
- Path integral representation of the time propagator matrix elements
- Path integral representation of the Wigner function
- Wiener–Khinchin theorem applied to the stochastic trajectories in path integrals
- Quantum density of state
- Radial distributions, dynamic structure factor and response function for ideal system of scatterers, strongly coupled soft-spheres and plasma media

Dynamic Structure Factor and Response Function

The Hamiltonian of the system of N particles $\hat{H} = \hat{K} + \hat{U}$ contains the kinetic $\hat{K}$ and the interaction $\hat{U} = \sum_{i<j}^{N} \phi(r_{ij})$ energy operators. We assume the presence of a perturbation field:

$$\hat{H}_A = \hat{H} + a(t)\hat{A} \tag{1}$$

where $a(t)$ is some kind of field (c-number) and $\hat{A}$ is the dynamical system variable (operator) coupled to the field. The $a(t)\hat{A})$ perturbs the equilibrium state of the system, the response will be measured as an expectation value of a dynamical variable $\hat{B}$.

$$\mathrm{Tr}(e^{-\beta \hat{H}_A}\hat{B}) - \mathrm{Tr}(e^{-\beta \hat{H}}\hat{B}) = \int_{-\infty}^{t} \mathrm{d}t' \tilde{\chi}_{BA}(t-t')a(t'), \tag{4}$$

where $\tilde{\chi}_{BA}(t)$ is real, independent of $a(t)$ function and $\tilde{\chi}_{BA}(t) = 0$ for $t < 0$. The response function can be presented as

$$\begin{aligned} &\tilde{\chi}_{BA}(t-t') = \mathrm{i}\theta(t-t')\mathrm{Tr}\rho_0[\hat{B}(t), \hat{A}(t')] = \\ &\mathrm{i}\theta(t-t')\langle[\hat{B}(t), \hat{A}(t')]\rangle_0 = \mathrm{i}\theta(\Delta t)\langle[\hat{B}(\Delta t), \hat{A}(0)]\rangle_0, \end{aligned} \tag{5}$$

where $\Delta t = t - t'$, $\langle[\hat{B}(t), \hat{A}(t')]\rangle_0 = \langle\hat{B}(t)\hat{A}(t')\rangle_0 - \langle\hat{B}(t')\hat{A}(t)\rangle_0$ and operators $\hat{B}(t)$ and $\hat{A}(t)$ are in the Heisenberg representation for $\hat{H}$. The Θ-function guarantees causality, i.e., contributions to the induced fluctuations at time t can only arise from perturbations for $t' \leq t$.

a(t)	A
magnetic field	magnetization
electric field	electric polarization
sound wave	mass density

Dynamic Structure Factor and Response Function

$$S(\omega) = Z^{-1} \int \mathrm{d}\Delta t \, \mathrm{Tr}\left(e^{\mathrm{i}\hat{H}t_c} \hat{B} e^{-\mathrm{i}\hat{H}t_c^*} \hat{A} \right) e^{-\mathrm{i}\omega\Delta t} = \exp\left(-\frac{\omega}{2}\right) S_{BA}(\omega)$$

$$= \exp\left(-\frac{\omega}{2}\right) Z^{-1} \int \mathrm{d}\Delta t \, \mathrm{Tr}\left(e^{-\beta\hat{H}} e^{\mathrm{i}\hat{H}\Delta t} \hat{B} e^{-\mathrm{i}\hat{H}\Delta t} \hat{A} \right) e^{-\mathrm{i}\omega\Delta t}, \qquad (2)$$

where $\beta = 1/T$ is the reciprocal temperature, $t_c = \Delta t - \mathrm{i}\beta/2$ is a complex-valued quantity, i is the imaginary unit and $Z(N, V, T) = \mathrm{Tr}(\hat{\rho}_0) = \mathrm{Tr}(e^{-\beta\hat{H}})$ is the canonical partition function of the system of N particle in volume V. So $S(\omega)$ is

$$S(\omega) = Z^{-1} \int \mathrm{d}\Delta t \, e^{-\mathrm{i}\omega\Delta t} \int \mathrm{d}\bar{q} \, \mathrm{d}\bar{\bar{q}} \, \mathrm{d}\tilde{q} \, \mathrm{d}\tilde{\tilde{q}}$$

$$\left\langle \bar{q} \left| \hat{B} \right| \bar{\bar{q}} \right\rangle \left\langle \bar{\bar{q}} \left| e^{\mathrm{i}\hat{H}t_c^*} \right| \tilde{q} \right\rangle \left\langle \tilde{q} \left| \hat{A} \right| \tilde{\tilde{q}} \right\rangle \left\langle \tilde{\tilde{q}} \left| e^{-\mathrm{i}\hat{H}t_c} \right| \bar{q} \right\rangle . \qquad (3)$$

According to the fluctuation-dissipation theorem the imaginary part of the time and spacial Fourier transforms (IMRF) of the density-density response function (RF) can be presented through the dynamic structure factor $S_{BA}(k, \omega)$ [1, 2, 43]

$$\chi(k, \omega) \equiv \mathrm{Im}\tilde{\chi}_{BA}(k, k'|_{k'=k}, \omega) = \rho\pi S_{BA}(k, \omega) \left(e^{-\omega} - 1 \right), \qquad (6)$$

The name fluctuation-dissipation theorem arises from the fact that DSF determines the scattering intensity of particles by density fluctuations in the system. It determines the amount of energy absorbed by the system when perturbed by an external potential and determines also the imaginary part of the inverse dielectric function.

Wigner Representation of the Dynamic Structure Factor and Response Function

The Wigner representation of the density-density correlation function $S(k,\omega)$ can be identically rewritten in the form that includes the Weyl symbols of operators and the generalization of the the Wigner–Liouville function W:

$$
\begin{aligned}
S(k,\omega) &= \exp\left(-\frac{\omega}{2}\right) S_{BA}(k,\omega) \\
&= (2\pi)^{-12N} \int \mathrm{d}\overline{PQ}\,\mathrm{d}\widetilde{PQ}\, B(k,\overline{PQ}) A(k,\widetilde{PQ}) \int \mathrm{d}\Delta t e^{-\mathrm{i}\omega\Delta t} W\left(\overline{PQ};\widetilde{PQ};\Delta t\right) \\
&= (2\pi)^{-12N} \int \mathrm{d}\overline{PQ}\,\mathrm{d}\widetilde{PQ}\, B(k,\overline{PQ}) A(k,\widetilde{PQ})\, W\left(\overline{PQ};\widetilde{PQ};\omega\right), \qquad (7)
\end{aligned}
$$

where we have introduced a short-hand notation for $6N$-dimensional phase space points, viz., $\overline{PQ}$ and $\widetilde{PQ}$, with the momenta and coordinates, respectively, of all the particles in the system. Here $B(k,\overline{PQ}))$ and $A(k,\widetilde{PQ})$ denotes the Weyl symbol [28] of the density operators, which describe system perturbations by different external fields

the system. Here $B(k,PQ))$ and $A(k,PQ)$ denotes the Weyl symbol [28] of the density operators, which describe system perturbations by different external fields

$$
\begin{aligned}
B(k,\overline{PQ}) &= \int \mathrm{d}\bar{\xi} \exp(-\mathrm{i}\langle\overline{P}|\bar{\xi}\rangle) \left\langle \overline{Q} - \frac{\bar{\xi}}{2} \middle| \hat{B} \middle| \overline{Q} + \frac{\bar{\xi}}{2} \right\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\langle k|\overline{Q}_j\rangle} = \rho(\overline{Q},k)\ ,
\end{aligned}
$$

Wigner Representation of the time propagator matrix elements

$$W\left(\overline{PQ};\widetilde{PQ};\Delta t\right)=Z^{-1}\int\int \mathrm{d}\overline{\xi}\,\mathrm{d}\widetilde{\xi}\,e^{\mathrm{i}\langle\overline{P}|\overline{\xi}\rangle}e^{\mathrm{i}\langle\widetilde{P}|\widetilde{\xi}\rangle}G\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right),$$

$$G\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)\equiv G^{+}\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)G^{-}\left(\widetilde{Q\xi};\overline{Q\xi};\Delta t\right)$$

$$=\left\langle\overline{Q}+\frac{\overline{\xi}}{2}\left|e^{\mathrm{i}\hat{H}t_{\mathrm{c}}^{*}}\right|\tilde{Q}-\frac{\widetilde{\xi}}{2}\right\rangle\left\langle\tilde{Q}+\frac{\widetilde{\xi}}{2}\left|e^{\mathrm{i}\hat{H}(t_{\mathrm{c}}^{*})}\right|\overline{Q}-\frac{\overline{\xi}}{2}\right\rangle^{*}. \tag{9}$$

$W\left(\overline{PQ};\widetilde{PQ};\Delta t\right)$ is presented by the Fourier transforms of the product of the "symmetric in time directions" propagators $G^{+}=\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)$ and $G^{-}\left(\widetilde{Q\xi};\overline{Q\xi};\Delta t\right)$ with related Fourier transforms

$$G^{+}\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)\equiv\left\langle\overline{Q}+\frac{\overline{\xi}}{2}\left|e^{\mathrm{i}\hat{H}t_{\mathrm{c}}^{*}}\right|\tilde{Q}-\frac{\widetilde{\xi}}{2}\right\rangle,$$

$$F^{+}\left(\overline{Q\xi};\widetilde{Q\xi};\omega\right)\equiv\int \mathrm{d}\Delta t\,G^{+}\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)e^{-\mathrm{i}\omega\Delta t}$$

$$=2\pi\left\langle\overline{Q}+\frac{\overline{\xi}}{2}\left|\delta\left(\omega\hat{\mathrm{I}}-\hat{H}\right)e^{-\beta\hat{H}/2}\right|\tilde{Q}-\frac{\widetilde{\xi}}{2}\right\rangle, \tag{10}$$

$$G^{-}\left(\widetilde{Q\xi};\overline{Q\xi};\Delta t\right)\equiv\left\langle\tilde{Q}+\frac{\widetilde{\xi}}{2}\left|e^{\mathrm{i}\hat{H}t_{\mathrm{c}}^{*}}\right|\overline{Q}-\frac{\overline{\xi}}{2}\right\rangle^{*}$$

Path integral representation of the time propagator matrix elements

$$F^{+}\left(\overline{Q\xi};\widetilde{Q\xi};\omega\right) \equiv \int \mathrm{d}\Delta t \left\langle \overline{Q}+\frac{\overline{\xi}}{2} \left| e^{\mathrm{i}\hat{H}t_c^*} \right| \tilde{Q}-\frac{\tilde{\xi}}{2} \right\rangle e^{-\mathrm{i}\omega\Delta t} = \int \mathrm{d}\Delta t \int \prod_{j=1}^{M} \mathrm{d}q_j \mathrm{d}\underline{q}_j$$

$$\times \left\langle \overline{Q}+\frac{\overline{\xi}}{2} \left| e^{-\mathrm{i}\Delta t(\omega\hat{\mathrm{I}}-\hat{H})/M} \right| \underline{q}_1 \right\rangle \left\langle \underline{q}_1 \left| e^{-\beta\hat{H}/2M} \right| \underline{q}_2 \right\rangle$$

$$\times \left\langle \underline{q}_2 \left| e^{-\mathrm{i}\Delta t(\omega\hat{\mathrm{I}}-\hat{H})/M} \right| q_2 \right\rangle \left\langle q_2 \left| e^{-\beta\hat{H}/2M} \right| q_3 \right\rangle$$

$$\times \left\langle q_3 \left| e^{-\mathrm{i}\Delta t(\omega\hat{\mathrm{I}}-\hat{H})/M} \right| \underline{q}_3 \right\rangle \left\langle \underline{q}_3 \left| e^{-\beta\hat{H}/2M} \right| \underline{q}_4 \right\rangle \ldots$$

$$\times \left\langle \underline{q}_M \left| e^{-\mathrm{i}\Delta t(\omega\hat{\mathrm{I}}-\hat{H})/M} \right| q_M \right\rangle \left\langle q_M \left| e^{-\beta\hat{H}/2M} \right| \tilde{Q}-\frac{\tilde{\xi}}{2} \right\rangle. \quad (14)$$

The Weyl symbol of the operator $\hat{H}$ can be presented as the Hamiltonian function $H(p,q) = \sum_{i=1}^{N} p_i^2/m_i + \sum_{i<j}^{N} \phi(r_{ij})$ [27, 28]

$$H(p,q) = \int \mathrm{d}\xi \exp(\mathrm{i}\langle p|\xi\rangle) \left\langle q+\xi/2 \left| \hat{H} \right| q-\xi/2 \right\rangle, \quad (15)$$

The final expression for the product at $\overline{\xi}=0$ and $\tilde{\xi}=0$ is equal to

$$\left\langle \overline{Q} \left| \exp\frac{-\mathrm{i}\Delta \mathrm{t}}{M}(\omega\hat{\mathrm{I}}-\hat{H}) \right| \underline{q}_1 \right\rangle \prod_{j=2}^{M} \left\langle q_j \left| \exp\frac{-\mathrm{i}\Delta \mathrm{t}}{M}(\omega\hat{\mathrm{I}}-\hat{H}) \right| \underline{q}_j \right\rangle$$

$$\approx \left(\frac{1}{2\pi}\right)^{3NM} \times \prod_{j=1}^{M} \int \mathrm{d}P_j \exp(-\mathrm{i}\langle P_j|\xi_j\rangle) \exp\frac{-\mathrm{i}\Delta \mathrm{t}}{M}(\omega - H(P_j,Q_j)),$$

Canonical ensemble

In (3) we tacitly assumed that the operators H, A and B do not depend on the spin variables. Therefore, the summation over spins can be safely moved here and below, so we do not explicitly mention the spin variables, as if they are not essential. However, the spin variables σ and the Fermi statistics can be taken into account by the following redefinition of $W^+(P,Q)$ in the canonical ensemble with temperature T

$$W^+(P,Q) = \frac{1}{Z(\beta)N!}\sum_{\sigma}\sum_{\mathcal{P}}(-1)^{\kappa_{\mathcal{P}}}\mathcal{S}(\sigma,\mathcal{P}\sigma')\big|_{\sigma'=\sigma}\int d\xi e^{-i\langle P|\xi\rangle}\left\langle \underline{q}_1\middle|e^{-\beta\hat{H}/2M}\middle|\underline{q}_2\right\rangle$$
$$\times\left\langle q_2\middle|e^{-\beta\hat{H}/2M}\middle|q_3\right\rangle\times\left\langle \underline{q}_3\middle|e^{e^{-\beta\hat{H}/2M}}\middle|\underline{q}_4\right\rangle\cdots\left\langle q_M\middle|e^{e^{-\beta\hat{H}/2M}}\middle|\mathcal{P}\tilde{Q}\right\rangle$$
$$=\frac{1}{Z(\beta)N!}\int d\xi\exp(-i\langle P|\xi\rangle)\rho^{(1)}\ldots\rho^{(M-1)}\sum_{\sigma}\sum_{\mathcal{P}}(-1)^{\kappa_{\mathcal{P}}}\mathcal{S}(\sigma,\mathcal{P}\sigma')\big|_{\sigma'=\sigma},\mathcal{P}\rho^{(M)}\big|_{\mathcal{P}\tilde{Q}},\qquad(24)$$

where the sum is taken over all permutations $\mathcal{P}$ with the parity $\kappa_{\mathcal{P}}$, index j labels the

Path integral representation of the Wigner function

$$W(P,Q) \approx \frac{\tilde{C}(M)}{Z(\beta)N!} \exp\Big[-\sum_{j=1}^{M}\Big(\pi|\eta_j|^2 + \frac{1}{M}U\Big(Q_1+\zeta_j\Big)\Big)\Big]$$

$$\times \exp\left\{\frac{M}{4\pi}\sum_{j=1}^{M}\left\langle \mathrm{i}P_j + (-1)^{(j-1)}\frac{1}{2M}\frac{\partial U(Q_1+\zeta_j)}{\partial Q_1}\right| \mathrm{i}P_j + (-1)^{(j-1)}\frac{1}{2M}\frac{\partial U(Q_1+\zeta_j)}{\partial Q_1}\right\rangle\right\}$$

$$\times \det\|\tilde{\phi}_{kt}\|_1^{N/2} \det\|\tilde{\phi}_{kt}\|_{(N/2+1)}^{N_e}, \quad (14)$$

where

$$\tilde{\phi}_{kt} = \exp\{-\pi\,|r_{kt}|^2/M\} \exp\left\{-\frac{1}{2M}\sum_{j=1}^{M}\left(\phi\left(\left|r_{tk}\frac{2j}{M} + r_{kt} + (\zeta_j^k - \zeta_j^t)\right|\right) - \phi\left(\left|r_{kt} + (\zeta_j^k - \zeta_j^t)\right|\right)\right)\right\}$$

$\eta_j \equiv \zeta_j - \zeta_{(j+1)}$, $r_{kt} \equiv (Q_1^k - Q_1^t)$, $(k,t = 1,\ldots,N)$. The constant $\tilde{C}(M)$ is canceled in Monte Carlo calculations.

Let us stress that approximation (14) have the correct limits to the cases of weakly and strongly degenerate fermionic systems. Indeed, in the classical limit the main contribution comes from the diagonal matrix elements due to the factor $\exp\{-\pi\,|r_{kt}|^2/M\}$ and the differences of potential energies in the exponents are equal to zero (identical permutation). At the same time, when the thermal wavelength is of the order of the average interparticle distance and the trajectories are highly entangled the

$$Q_j = (\tilde{P}Q_{(M+1)} - Q_1)\frac{j-1}{M} + Q_1 + \zeta_j$$

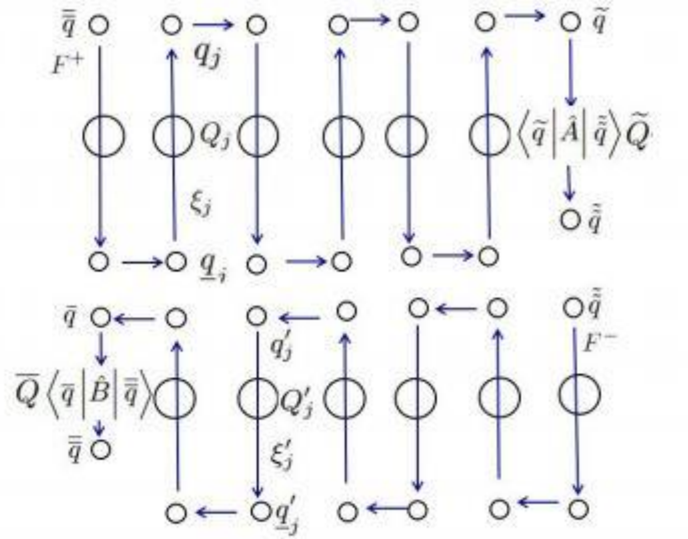


Figure 1. (Color online) The symbolic representation of the DSF and the propagator $G\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)$ by Eq. (9). The "vertical" $\left\langle q_j \left| \exp \frac{\mathrm{i}\Delta t}{M}(\omega \hat{\mathrm{I}} - \hat{H}) \right| \underline{q}_j \right\rangle$ and "horisontal" $\left\langle q_j \left| \exp -\beta \hat{H}/2M \right| q_{(j+1)} \right\rangle$ ($\left\langle \underline{q}_j \left| \exp -\beta \hat{H}/2M \right| \underline{q}_{(j+1)} \right\rangle$) matrix elements are shown by the related arrows. Matrix elements $G^+\left(\overline{Q\xi};\widetilde{Q\xi};\Delta t\right)$ and $G^-\left(\widetilde{Q\xi};\overline{Q\xi};\Delta t\right)$ correspond to the upper and bottom trajectories with "the oppisite time directions" and linking matrix elements $\left\langle \widetilde{Q} - \frac{\tilde{\xi}}{2} \left| \hat{A} \right| \widetilde{Q} + \frac{\tilde{\xi}}{2} \right\rangle$ and $\left\langle \overline{Q} - \frac{\bar{\xi}}{2} \left| \hat{B} \right| \overline{Q} + \frac{\bar{\xi}}{2} \right\rangle$ respectively (here, for example, $M = 6$). For the DSF the variables $\bar{\xi}$ and $\tilde{\xi}$ have to be equal to zero due to arising $\delta(\xi)$ in matrix elements of the operators $\hat{B}$ and $\hat{A}$ not depending on momentum.

Wiener–Khinchin theorem

a distribution $W = W^+W^-$. Then making use of the Wiener–Khinchin theorem [49, 50, 51, 52] we present the product of the expected values of the spectral densities of these trajectories $F^+\left(\overline{Q\xi};\widetilde{Q\xi};\omega\right)F^-\left(\widetilde{Q\xi};\overline{Q\xi};\omega\right)$ as the Fourier transform of the expected value of their correlation function, which defines the DSF

$$
\begin{aligned}
&(2\pi)^{-12N}\int \mathrm{d}\overline{PQ}\,\mathrm{d}\widetilde{PQ}\mathrm{d}\overline{\xi}\,\mathrm{d}\widetilde{\xi}\,e^{\mathrm{i}\langle\overline{P}|\overline{\xi}\rangle}e^{\mathrm{i}\langle\widetilde{P}|\widetilde{\xi}\rangle}\\
&\times\rho(\widetilde{Q},k)\rho(\overline{Q},k)F^+\left(\overline{Q\xi};\widetilde{Q\xi};\omega\right)F^-\left(\widetilde{Q\xi};\overline{Q\xi};\omega\right)\\
&=(2\pi)^{-12N}\int \mathrm{d}\overline{PQ}\,\mathrm{d}\widetilde{PQ}\mathrm{d}\overline{\xi}\,\mathrm{d}\widetilde{\xi}\,e^{\mathrm{i}\langle\overline{P}|\overline{\xi}\rangle}e^{\mathrm{i}\langle\widetilde{P}|\widetilde{\xi}\rangle}\rho(\widetilde{Q},k)\rho(\overline{Q},k)\\
&\times\int \mathrm{d}t e^{-\mathrm{i}\omega t}G^+\left(\overline{Q\xi};\widetilde{Q\xi};t\right)G^-\left(\widetilde{Q\xi};\overline{Q\xi};t\right)=S(k,\omega).
\end{aligned}
\tag{29}
$$

For an isotropic system we can average over angles so the DSF becomes

$$
\begin{aligned}
S(|k|,\omega)&=\frac{8\pi^3}{(2\pi)^{6N}N}\int \mathrm{d}\overline{Q}\,\mathrm{d}\widetilde{Q}\\
&\times F^+\left(\overline{Q0};\widetilde{Q0};\omega\right)F^-\left(\widetilde{Q0};\overline{Q0};\omega\right)\sum_{i,j}\frac{\sin(|k||\widetilde{Q}_j-\overline{Q}_i|)}{|k||\widetilde{Q}_j-\overline{Q}_i|}\\
&=\frac{8\pi^3}{(2\pi)^{6N}N}\int \mathrm{d}\overline{Q}\,\mathrm{d}\widetilde{Q}\left|\left\langle\overline{Q}\right|\delta\left(\omega\hat{\mathrm{I}}-\hat{H}\right)e^{-\beta\hat{H}/2}\left|\widetilde{Q}\right\rangle\right|^2\sum_{i,j}\frac{\sin(|k||\widetilde{Q}_j-\overline{Q}_i|)}{|k||\widetilde{Q}_j-\overline{Q}_i|}.
\end{aligned}
\tag{30}
$$

Thus, the DSF calculation is reduced to a WPIMC simulation of random trajectories in the phase space with a distribution $W = W^+W^-$ (see Figure 1). According to Eqs. (2, 6 and 30) the IMRF and DSF are defined by the WPIMC averaged **histogram** of the value $\frac{1}{N}\sum_{i,j}\frac{\sin(|k||\widetilde{Q}_j-\overline{Q}_i|)}{|k||\widetilde{Q}_j-\overline{Q}_i|}$ versus the full energy ω of the trajectories connecting $\widetilde{Q}_j$ and $\overline{Q}_i$. The WPIMC can be also used for the WPIMC simulation of thermodynamic properties. In the classical limit the W is reduced to the Boltzmann distribution.

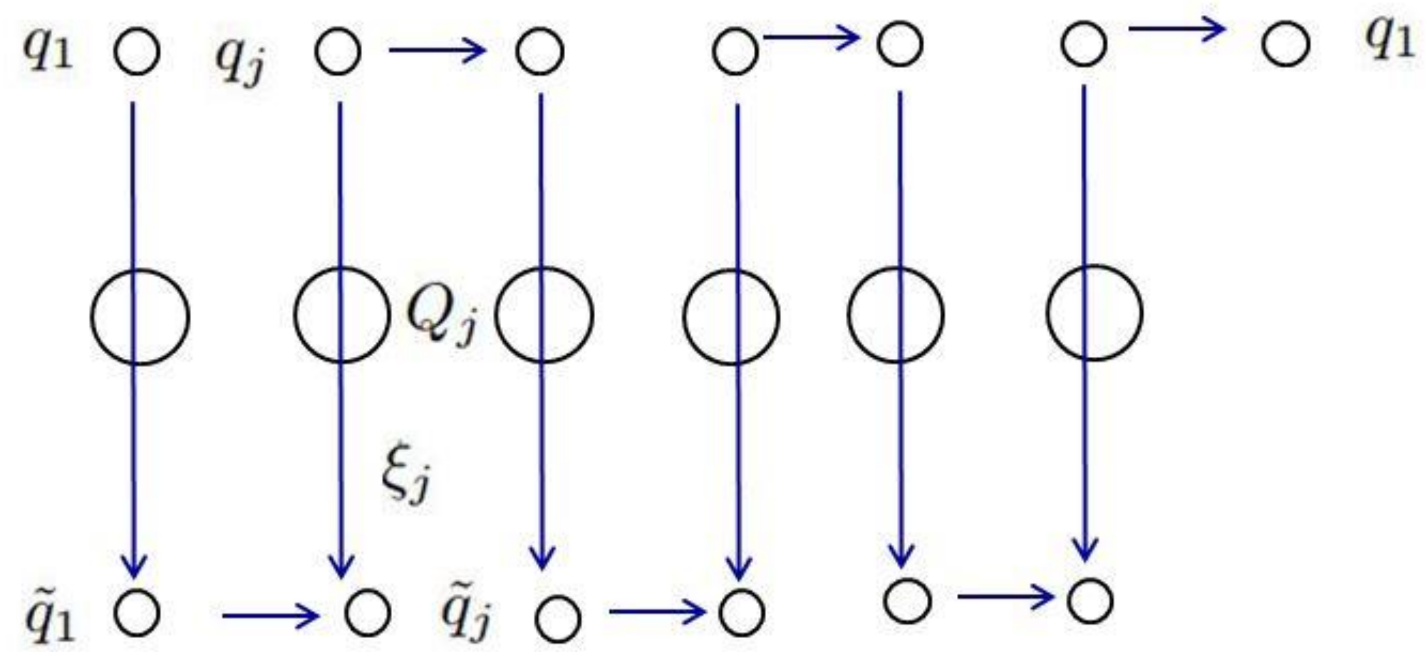
Quantum density of state

In our approach we are going to rewrite $\Omega(E)$ in an identical form using the property of the delta function

$$\Omega(E) = \mathrm{Tr}\{\delta(E\hat{\mathrm{I}} - \hat{H})\hat{\mathrm{I}}\} = \mathrm{Tr}\{\delta(E\hat{\mathrm{I}} - \hat{H})\exp(E\hat{\mathrm{I}} - \hat{H})\}$$
$$= \frac{1}{2\pi}\int \mathrm{d}\omega \mathrm{Tr}\{\exp \mathrm{i}\omega(\mathrm{E}\hat{\mathrm{I}} - \hat{\mathrm{H}})\exp(\mathrm{E}\hat{\mathrm{I}} - \hat{\mathrm{H}})\} = \frac{1}{2\pi}\int \mathrm{d}\omega \mathrm{Tr}\{\exp \kappa(\omega)(\mathrm{E}\hat{\mathrm{I}} - \hat{\mathrm{H}})\}$$
$$= \frac{1}{2\pi}\int \mathrm{d}\omega \int \mathrm{d}q_1 \left\langle q_1 \left| \exp \kappa(\omega)(E\hat{\mathrm{I}} - \hat{H}) \right| q_1 \right\rangle, \quad (1)$$

where $\kappa(\omega) = 1+\mathrm{i}\omega$, angular brackets $\langle q|\tilde{q}\rangle$ mean the scalar products of the eigenvectors $|q\rangle$ and $|\tilde{q}\rangle$ of the coordinate operator $\hat{q}$ ($\langle\hat{q}|q\rangle = q|q\rangle$, $\langle q|\tilde{q}\rangle = \delta(q-\tilde{q})$), $\hat{\mathrm{I}} = \int |q\rangle \mathrm{d}q\langle q|$ is the unit operator, $\psi(q) = \langle q|\psi\rangle$ is the wave function [35]), the angular brackets in expression $\langle q_1|A|q\rangle$ mean the scalar products of vectors $|q_1\rangle$ and $|\hat{A}|q\rangle$ arising after the action of operator $\hat{A}$ on vector $|q\rangle$, i is the imaginary unit. Further in the text, it

The symbolic representation of the DOS by the path integrals.
The ``vertical'' and ``horizontal " arrows are the matrix elements.



Energy distribution functions and density of state at rs~2 and T=60 K (2D)

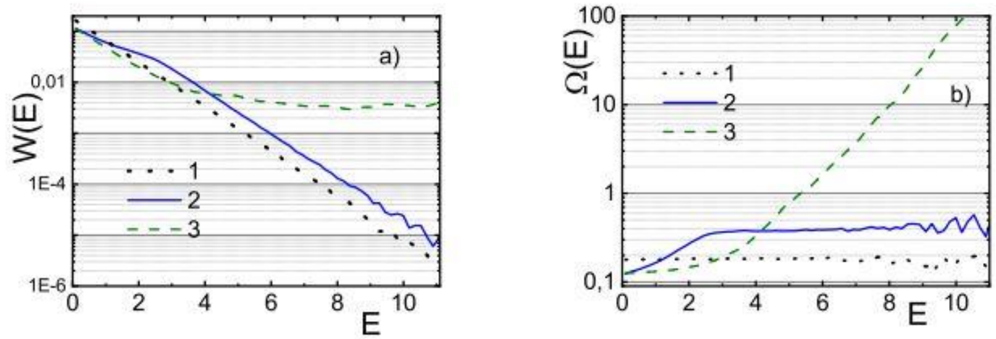


Figure 3. (Color online) The energy distribution $W(E)$ (panel a) and DOS (panel b) for the system of soft-sphere fermions at a fixed density $r_s = 2.2$ and temperature $T = 60$ K ($\int W(E)\mathrm{d}E = 1$, $\Omega(E)$ in conditional units). Lines: 1—ideal system; 2—$n = 0.6$; 3—$n = 1$. Small oscillations indicate the Monte-Carlo statistical error.

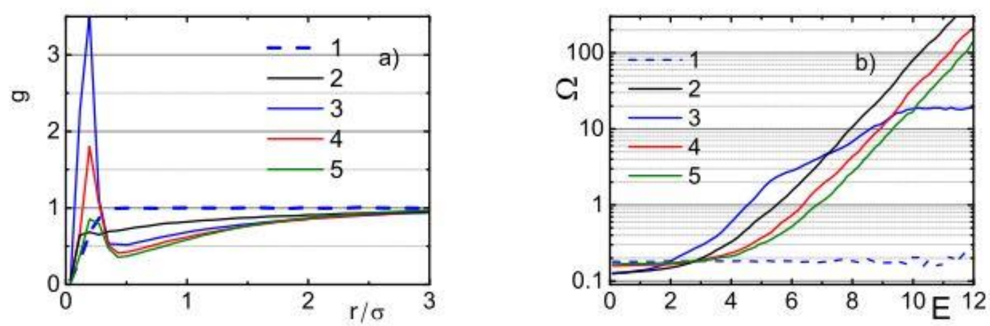


Figure 4. (Color online) The RDFs for the same spin projections (panel a) and DOS (panel b) for a system of soft-sphere fermions at a fixed density $r_s = 2.1$ and temperature $T = 60$ K.
Lines: 1—ideal system; 2 —$n = 0.2$; 3—$n = 0.6$; 4—$n = 1.0$; 5—$n = 1.4$.
Small oscillations indicate the Monte-Carlo statistical error.

He-3: radial and energy distribution functions, density of state (3D)

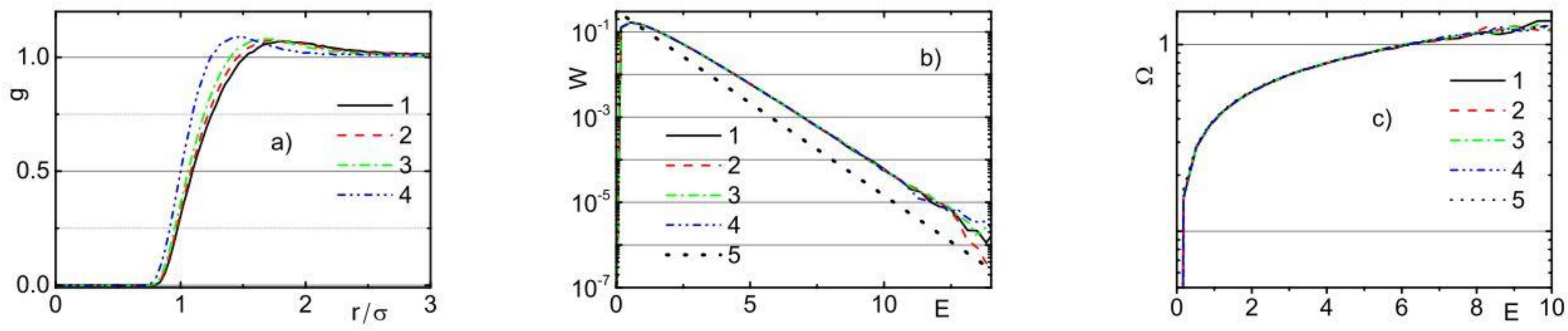


Figure 1: (Color online) The RDF $g(r)$, IED $W(E)$ and DOS $\Omega(E)$) at $r_s = 9$.
Lines: $1 - T = 3.5$ K, $2 - T = 4.2$ K, $3 - T = 5.4$ K, $4 - T = 13$ K, $5 - e^{-E}$ (panel b) and $\Omega \sim \sqrt{E}$ (panel c).
Results are in conditional units. Small oscillations indicate the Monte-Carlo statistical error.

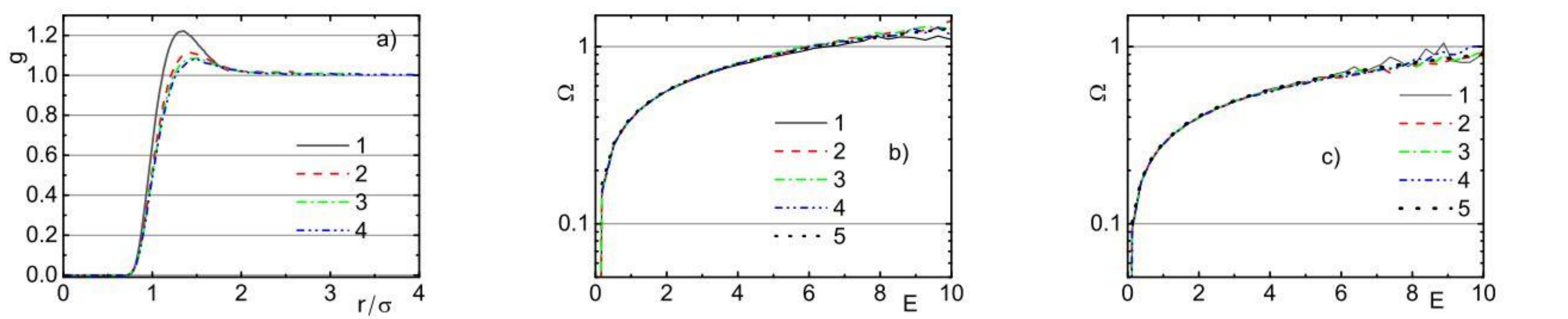


Figure 2: (Color online) The RDF $g(r)$ and DOSs $\Omega(E)$ at $T = 13$ K (panel a) and b)) and $\Omega(E)$ at $T = 2$ K K (panel c)).
Lines: $1 - r_s = 5$, $2 - r_s = 7$, $3 - r_s = 9$, $4 - r_s = 12$, $5 - \Omega \sim \sqrt{E}$ (panel c) . Results are in conditional units. Small oscillations indicate the Monte-Carlo statistical error.

Monte Carlo simulation of the two-component plasma media. Energy distribution functions and density of state for plasma and non correlated uniformly distributed in space protons (OCP).

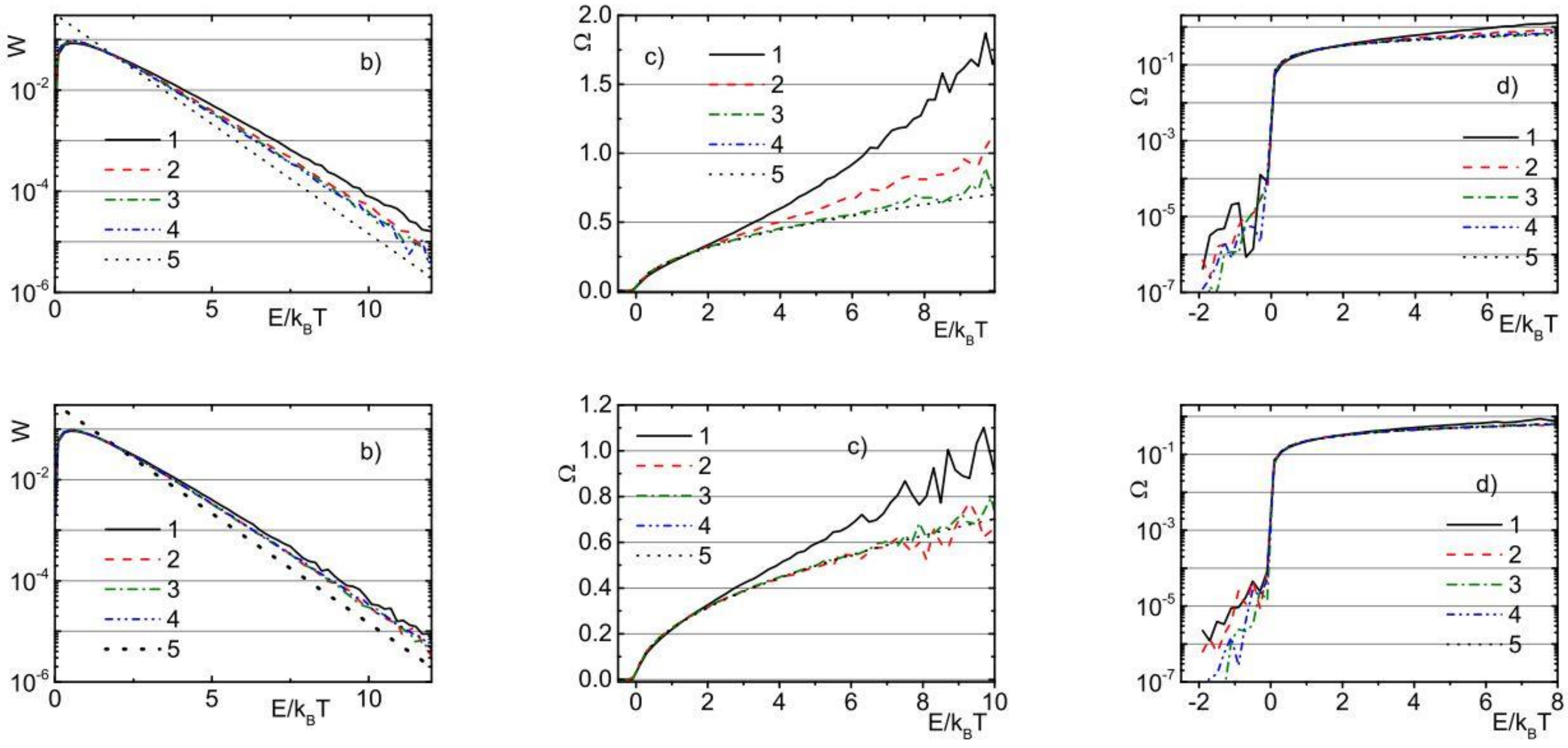


Figure 2: (Color online) The typical IEDs (panels a)) and DOSs (panels b and c) for TCP (upper row) and OCP (bottom row) at $r_s = 4$. Lines: $1 - T = 0.5\,\mathrm{Ha}$, $2 - T = 1\,\mathrm{Ha}$, $3 - T = 1.5\,\mathrm{Ha}$, $4 - T = 2\,\mathrm{Ha}$, 5 – 'ideal plasma" (panel a)) and DOS Ω (panel b) and c)) respectively. Small oscillations at large and negative energies indicate the Monte-Carlo statistical error. The $W(E)$ is normalized to unity.

Radial distributions, dynamic structure factor and response function for ideal Fermi Systems.

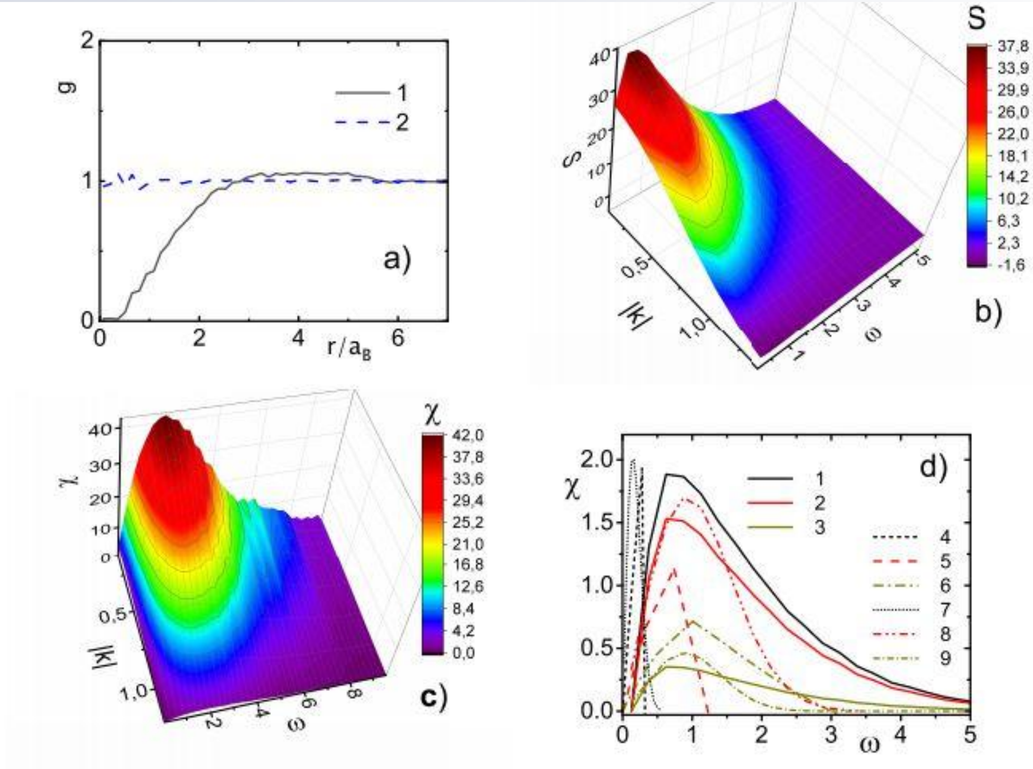


Figure 2. (Color online) The ideal fermions for $r_s = 6.8$. The WPIMC RDFs at $T = 20$ K (panel a), lines: 1 - the same spin projections, 2 - the opposite spin projections. The opposite spin WPIMC DSF (panel b)) and WPIMC IMRF (panels c) and d)). The WPIMC IMRF at $T = 20$ K , lines: 1 - $|k| = 0.1$, 2 - $|k| = 0.4$, 3 - $|k| = 1$. The analytical estimations of the IMRF. The Lindhard's IMRF for the ground state at $T = 0$ [55], lines: 4 - $|k| = 0.1$, 5 - $|k| = 0.4$, 6 - $|k| = 1$. The IMRF for the point-like uncorrelated classical scatterers at $T = 20$ K (Eq. (32)), lines: 7 - $|k| = 0.1$, 8 - $|k| = 0.4$, 9 - $|k| = 1$. The DSF and IMRF are scaled in conditional units.

Radial distributions and response functions for strongly coupled soft sphere systems.

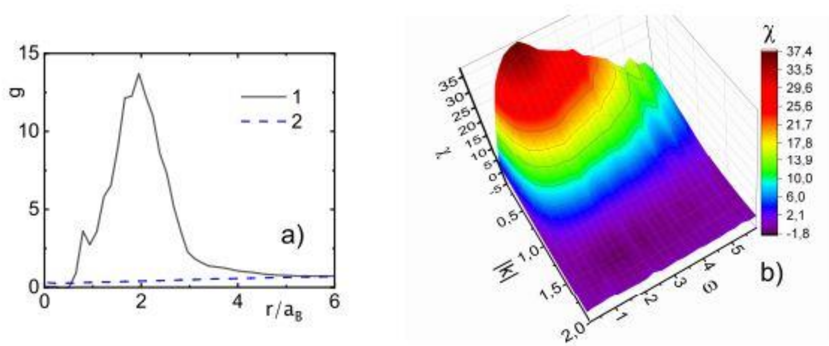


Figure 3. (Color online) The WPIMC simulations for $T = 20$ K and $r_s = 6.8$. Panel a). Lines: 1 - the same spin projections RDFs, 2 - the opposite spin projections RDFs. Panel b) - IMRF for opposite spin fermions. Panel c) - IMRF for the same spin fermions . IMRFs are in conditional units. Irregular oscillations indicate the Monte-Carlo statistical error. The ω is normalized by temperature equal to $T = 20$ K.

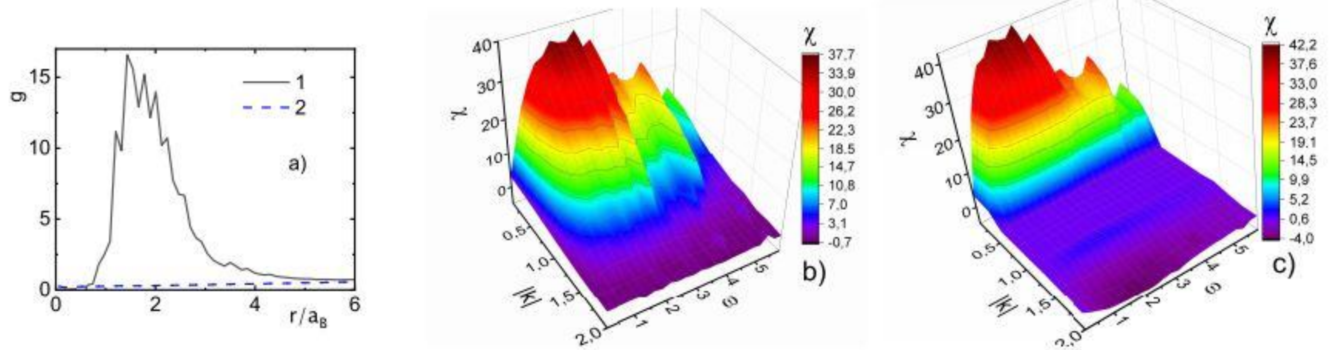


Figure 4. (Color online) The WPIMC simulations for $T = 20$ K and $r_s = 5.4$. Panel a): 1—the same spin projections RDFs, 2—the opposite spin projections RDFs. Panel b): IMRF for opposite spin fermions. Panel c): IMRF for the same spin fermions. IMRFs are in conditional units.

Basic results

The Wigner formulation of quantum mechanics is used to derive a new path integral representation of quantum density of states, dynamic structure factor and response function .

A path integral Monte Carlo approach is developed for the numerical investigation of the density of states, internal energy and spin--resolved radial distribution functions for a strongly correlated soft--sphere fermions.

The peculiarities of the quantum density of states, dynamic structure factors and response functions of the soft—spheres plasma media are investigated and explained.

Thank you for attention.

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