

Cluster expansion for ideal Fermi systems in the 'fixed-node approximation'

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2001 J. Phys. A: Math. Gen. 34 1665

(<http://iopscience.iop.org/0305-4470/34/8/312>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.106

The article was downloaded on 02/06/2010 at 09:56

Please note that [terms and conditions apply](#).

Cluster expansion for ideal Fermi systems in the ‘fixed-node approximation’

Vladimir Filinov

Russian Academy of Sciences, Institute for High Energy Density, Izhorskaya Street 13–19,
Moscow 127412, Russia

E-mail: Vladimir_Filinov@mail.ru, vs_filinov@hotmail.com and filinov@ok.ru

Received 18 October 2000

Abstract

Over the last ten years the ‘fixed-node approximation’, well known in the literature, has been widely used for a numerical treatment of thermodynamic properties of strongly correlated Fermi systems. Results of the direct path integral Monte Carlo simulation performed here show that the ‘fixed-node approximation’ describes the thermodynamic properties of the strongly coupling fermions rather well at ‘weak and moderate’ degeneracy. To analyse the reasons for the increasing difference between the ‘fixed-node approximation’ and the results of direct path integral Monte Carlo simulations for highly degenerate fermions, the correctness of the ‘fixed-node approximation’ for ideal Fermi systems has been analysed by analytical methods. A rigorous proof has been given of the fact that the exact Fermi function with index $\frac{5}{2}$ describing the logarithm of the grand partition function of ideal fermions cannot be reproduced in the ‘fixed-node approximation’, which means that the ‘fixed-node approximation’ does not give the correct ideal Fermi gas limit.

PACS numbers: 0510L, 0530, 5225K, 5265

1. Introduction

Theoretical studies of strongly interacting fermions are currently of great interest in many different fields of physics, including the physics of low temperatures, solid state and condensed matter physics, plasma theory, astrophysics and so on. The most interesting physical phenomena in such systems are the phase transitions in fermi liquids, metallic and superconducting states, particle bound states and so on [1–6].

Over the last few years significant progress has been observed in studies of the thermodynamic properties of strongly correlated degenerate systems at non-zero temperatures, which is mainly conditioned by the application of mathematical simulations [3, 4, 7–10]. The reason for this success is the possibility of an explicit representation of the low-temperature density matrix and partition function in the form of a finite-dimensional approximation of the

Wiener path integrals [11] without any preliminary physical approximations, which require the physical parameters to be small. Different Monte Carlo methods have been developed and used for calculations of the obtained path integral representations [7–9].

The main difficulty for path integral Monte Carlo studies (PIMC) of Fermi systems is the requirement of antisymmetrization of the density matrix in the partition function [11]. As a result of the antisymmetrization all thermodynamic quantities are presented as the sum of alternating sign terms related to all permutations of particles. So the thermodynamic quantities are equal to the small difference of two large numbers, which are the sums of positive and negative terms. The numerical calculation in this case is severely hampered. The given difficulty is known in the literature as the ‘sign problem’. To overcome the ‘sign problem’ some approaches have been developed, among which the ‘fixed-node approximation’ [12–15] is widely known.

The main idea of the ‘fixed-node approximation’ consists in introducing an additional functional called the ‘trial antisymmetric density matrix’, which is used to reduce the domain of integration in the integral representation of the partition function. The new domain of integration is bounded by the positive domain of the ‘trial density matrix’. This transformation results in the reduction of the sum over all permutations to the reduced sum of positive terms related to the even permutations. This transformation of the partition function is called the ‘fixed-node approximation’. The ‘trial density matrix’ is chosen in the form of a density matrix of the ideal fermions or to improve the accuracy of the approximation in the more complicated form [15]. The background for this transformation is the statement that with an appropriate choice of the ‘trial density matrix’ the properties of the Fermi system can be described exactly [12–14]. The Monte Carlo methods developed for calculations in the ‘fixed-node approximation’ are known as the ‘restricted path integral Monte Carlo simulation’ (RPIMC).

An alternative approach for studies of Fermi systems without preliminary approximations and transformations is known in the literature as the ‘direct path integral Monte Carlo simulation’ (DPIMC) [10, 16–20]. In this approach the sum over all permutations is represented identically as a determinant, which can be calculated by the direct methods of linear algebra. The accuracy of this approach depends only on the errors of the finite-dimensional approximations of the path integrals and can be improved systematically.

A comparison of the numerical results for thermodynamic properties of a dense hydrogen plasma obtained by these two approaches (this work and [21]) has demonstrated rather good agreement for weak and moderate degeneracy. However, the difference obtained increases systematically with the growth of the degeneracy for large density and lower temperature.

The purpose of this work is the consideration of the reasons for this systematic difference. The equation of state of ideal fermions has been considered using the analytical methods developed by Ruelle [22, 23]. It has been rigorously proved that any modification of the domain of integration in the partition function as well as a reduction of the sum over permutations results in replacing the exact Fermi function with index $\frac{5}{2}$ describing fermions in a grand canonical ensemble by another function. An analogous replacement is valid in a canonical ensemble. Let us note, nevertheless, that the performed calculations have shown that the difference between RPIMC and DPIMC in the equations of state for a dense hydrogen plasma is reasonably small at weak and moderate degeneracy. For other fermi systems further investigations are required.

2. Path integrals and the ‘fixed-node approximation’

Let us consider the main ideas of the path integral representation of thermodynamic quantities [11]. As is known the thermodynamic quantities are equal to the appropriate derivatives

of the logarithm of the partition function $Q_N = \text{Tr}[\rho_\beta]$. Here ρ_β is the low-temperature density matrix of a quantum system. The quantum statistical mechanics of the system may be incorporated via Feynman’s path integral formulation, which expresses the low-temperature density matrix of the system in terms of its high-temperature density matrix ρ_τ (Trotter formula),

$$\rho_\beta = e^{-\beta\hat{H}} = (e^{-\tau\hat{H}})^M \quad \tau = \beta/M.$$

Once the coordinate representation of the density matrix is known, the thermodynamic quantity or average value quantum operator are computed as

$$\begin{aligned} \langle \hat{O} \rangle &\equiv \frac{\text{Tr}[\hat{O}\rho_\beta]}{Q_N} \\ &= \frac{\int_{\Omega} dR dR^1 \dots dR^{M-1} \sum_P (-1)^{\kappa P} \langle R | \hat{O} \rho_\tau | R^1 \rangle \langle R^1 | \rho_\tau | R^2 \rangle \dots \langle R^{M-1} | \rho_\tau | P R \rangle}{\int_{\Omega} dR dR^1 \dots dR^{M-1} \sum_P (-1)^{\kappa P} \langle R | \rho_\tau | R^1 \rangle \langle R^1 | \rho_\tau | R^2 \rangle \dots \langle R^{M-1} | \rho_\tau | P R \rangle} \end{aligned}$$

where $R = \{R_1, R_2, \dots, R_N\}$ and $R^{(l)} = \{R_1^{(l)}, R_2^{(l)}, \dots, R_N^{(l)}\}$ are the coordinates of all particles ($l = 1, \dots, M - 1$). The sum is taken over all permutations with odd permutations yielding a negative contribution. The negative sign is problematic for Monte Carlo methods and is eliminated using the ‘fixed-node approximation’ [12–14]. In this approximate formulation, the domain of integration is limited to the positive domain of a ‘trial density matrix’, and permutations are restricted to even exchange cycles. The observable expression then becomes

$$\langle \hat{O} \rangle_{FNA} = \frac{\sum_{P^+} \int_{\Omega_{P^+}} dR dR^1 \dots dR^{M-1} \langle R | \hat{O} \rho_\tau | R^1 \rangle \langle R^1 | \rho_\tau | R^2 \rangle \dots \langle R^{M-1} | \rho_\tau | P^+ R \rangle}{\sum_{P^+} \int_{\Omega_{P^+}} dR dR^1 \dots dR^{M-1} \langle R | \rho_\tau | R^1 \rangle \langle R^1 | \rho_\tau | R^2 \rangle \dots \langle R^{M-1} | \rho_\tau | P^+ R \rangle}$$

where P^+ corresponds to positive permutations and Ω_{P^+} is the modified domain of integration. The ‘trial density matrix’ in [12–15] was chosen as the density matrix of ideal fermions or the variational density matrix taking interactions into account.

It is of interest to derive the cluster and virial expansions for ideal fermions in the ‘fixed-node approximation’ and to compare them with similar exact expansions. Most convenient for this purpose, apparently, is the algebraic approach developed by Ruelle [22, 23].

3. Basic expressions

As was mentioned above the exact partition function of ideal fermions has the form:

$$\text{Tr}(\rho_\beta) = N!^{-1} Q_N = N!^{-1} \int \dots \int_{\Omega} \sum_P (-1)^{\kappa P} \rho((q)_N, (Pq)_N) d(q)_N dR^{(1)} \dots dR^{(M-1)}$$

$$(-1)^{\kappa P} \equiv \pm 1$$

where $\rho((q)_N, (Pq)_N) \equiv \prod_{k=1}^N \rho_{k, Pk}$ and $\rho_{k, Pk} = \rho_0(q_k, R_k^{(1)}) \rho_0(R_k^{(1)}, R_k^{(2)}) \dots \rho_0(R_k^{(M-1)}, q_{Pk})$, $(q)_N = \{q_1, \dots, q_N\}$, $(Pq)_N = \{q_{P1}, \dots, q_{PN}\}$. Here the passage to the limit of $M \rightarrow \infty$ results in the integral over the Wiener measure. Then the partition function in a grand canonical ensemble is equal to

$$\Psi(z) = \sum_{N=1}^{\infty} z^N \frac{Q_N}{N!}. \quad (1)$$

The analogous expressions in the ‘fixed-node approximation’ look like

$$\text{Tr}(\rho_\beta)_+ = N!^{-1} Q_N^+ = N!^{-1} \sum_{P^+} \int \cdots \int_{\Omega} \tilde{\rho}((q)_N, (P^+q)_N) d(q)_N dR^{(1)} \cdots dR^{(M-1)}$$

$$(-1)^{\kappa P^+} \equiv 1.$$

Here $\chi_N(P^+) = \chi [(q)_N, R^{(1)}, R^{(2)}, \dots, R^{(M-1)}, (P^+q)_N]$ is the smoothed or discontinuous characteristic function of the domain Ω_{P^+} (χ is equal to one inside the domain, where the ‘trial density matrix’ is positive and is equal to zero otherwise) and $\tilde{\rho}((q)_N, (P^+q)_N) \equiv \chi_N(P^+) \prod_{k=1}^N \rho_{k, P^+k}$. So, in the ‘fixed-node approximation’ the passage to the limit of $M \rightarrow \infty$ results in the integral over the modified Wiener measure. Then

$$\Psi_{\text{FNA}}(z) = \sum_{N=1}^{\infty} z^N \frac{Q_N^+}{N!}. \tag{2}$$

As is known [24] any permutation can be split into a composition of several cyclic permutations, so we are going to present the sum over all permutations as the sum over cyclic permutations. For example, for one, two and three fermions we have

$$|\rho_{11}| = \overbrace{\tilde{\rho}_{11}}^{C_1^1} = \tilde{\rho}(C_1^1)$$

$$\begin{vmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{vmatrix} = \overbrace{\tilde{\rho}_{11}}^{C_1^1} \overbrace{\tilde{\rho}_{22}}^{C_2^2} - \overbrace{\tilde{\rho}_{12}\tilde{\rho}_{21}}^{C_2^1} = \tilde{\rho}(C_2^2) + \tilde{\rho}(C_1^1)\tilde{\rho}(C_1^2)$$

$$\begin{vmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{vmatrix} = \overbrace{\tilde{\rho}_{11}}^{C_1^1} \overbrace{\tilde{\rho}_{22}}^{C_2^2} \overbrace{\tilde{\rho}_{33}}^{C_3^3} + \overbrace{\tilde{\rho}_{12}\tilde{\rho}_{23}\tilde{\rho}_{31}}^{\tilde{C}_3^1} + \overbrace{\tilde{\rho}_{13}\tilde{\rho}_{32}\tilde{\rho}_{21}}^{\tilde{C}_3^2}$$

$$- \overbrace{\tilde{\rho}_{22}}^{C_1^1} \overbrace{\tilde{\rho}_{13}\tilde{\rho}_{31}}^{C_2^1} - \overbrace{\tilde{\rho}_{11}}^{C_2^1} \overbrace{\tilde{\rho}_{23}\tilde{\rho}_{32}}^{C_2^2} - \overbrace{\tilde{\rho}_{33}}^{C_1^3} \overbrace{\tilde{\rho}_{12}\tilde{\rho}_{21}}^{C_2^2}$$

$$= \underbrace{\tilde{\rho}(C_3)}_{\text{two terms}} + \underbrace{\Sigma \tilde{\rho}(C_1)\tilde{\rho}(C_2)}_{\text{three terms}} + \underbrace{\tilde{\rho}(C_1)\tilde{\rho}(C_1)\tilde{\rho}(C_1)}_{\text{one term}}.$$

Here Σ means all renumbering, $\tilde{\rho}_{C_1} = \rho_{i_1, i_1}$, and for $\nu > 1$ C_ν means ordered ($i_1 < i_2 < \dots < i_\nu$) cyclic permutation of length ν and $\tilde{\rho}_{C_\nu^i}(i_1, i_2, \dots, i_\nu)$ is the sum of the contributions of all cyclic permutations \tilde{C}_ν^i of length ν related to C_ν :

$$\tilde{\rho}_{C_\nu}(i_1, i_2, \dots, i_\nu) \equiv \tilde{\rho}(C_\nu) = \sum_{\tilde{C}_\nu^i} (-1)^{\nu+1} \rho_{i_1, i_2} \rho_{i_2, i_3} \cdots \rho_{i_\nu, i_1} = \sum_{\tilde{C}_\nu^i} \rho(\tilde{C}_\nu^i).$$

Here the sum over \tilde{C}_ν^i contains $\nu!/ \nu$ terms. For example, for $\nu = 2, 3$ we have $\tilde{\rho}(C_2) = \rho_{i_1 i_2} \rho_{i_2 i_1}$, $i_1, i_2 \in C_2$, and $\tilde{\rho}(C_3) = \rho_{i_1 i_2} \rho_{i_2 i_3} \rho_{i_3 i_1} + \rho_{i_1 i_3} \rho_{i_3 i_2} \rho_{i_2 i_1}$, where $i_1, i_2, i_3 \in C_3$.

In the ‘fixed-node approximation’ given above expressions have the following form (underlined terms are not taken into account as the related characteristic functions are equal to zero for odd permutations):

$$|\rho_{11}|_+ = \rho_{11} = \rho(\tilde{C}_1^1)$$

$$\begin{vmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{vmatrix}_+ = \chi_2(\tilde{C}_1^1 \tilde{C}_1^2) \rho(\tilde{C}_1^1) \rho(\tilde{C}_1^2) + \underline{\chi_2(\tilde{C}_2^1) \rho(\tilde{C}_2^1)}$$

$$\begin{aligned}
 \left. \begin{array}{ccc} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{array} \right|_+ &= \chi_3(\tilde{C}_1^1 \tilde{C}_1^2 \tilde{C}_1^3) \overbrace{\rho_{11}}^{\tilde{C}_1^1} \overbrace{\rho_{22}}^{\tilde{C}_1^2} \overbrace{\rho_{33}}^{\tilde{C}_1^3} + \chi_3(\tilde{C}_3^1) \overbrace{\rho_{12} \rho_{23} \rho_{31}}^{\tilde{C}_3^1} + \chi_3(\tilde{C}_3^2) \overbrace{\rho_{13} \rho_{32} \rho_{21}}^{\tilde{C}_3^2} \\
 &- \chi_3(\tilde{C}_1^1 \tilde{C}_2^1) \overbrace{\rho_{22}}^{\tilde{C}_1^1} \overbrace{\rho_{13} \rho_{31}}^{\tilde{C}_2^1} - \chi_3(\tilde{C}_1^2 \tilde{C}_2^2) \overbrace{\rho_{11}}^{\tilde{C}_1^2} \overbrace{\rho_{23} \rho_{32}}^{\tilde{C}_2^2} - \chi_3(\tilde{C}_1^3 \tilde{C}_2^3) \overbrace{\rho_{33}}^{\tilde{C}_1^3} \overbrace{\rho_{12} \rho_{21}}^{\tilde{C}_2^3} \\
 &= \sum \chi_3(\tilde{C}_3) \rho(\tilde{C}_3) + \sum \chi_3(\tilde{C}_1 \tilde{C}_2) \rho(\tilde{C}_1) \rho(\tilde{C}_2) \\
 &+ \chi_3(\tilde{C}_1^1 \tilde{C}_1^2 \tilde{C}_1^3) \rho(\tilde{C}_1^1) \rho(\tilde{C}_1^2) \rho(\tilde{C}_1^3).
 \end{aligned}$$

4. Algebraic approach

Let us consider the main ideas of the algebraic approach, developed by Ruelle [22, 23] to simplify the derivations of cluster expansions. Let us define a linear vector space A of infinite sequences of integrable functions,

$$\vec{\Psi} = (\Psi(q)_N)_{N \geq 0}.$$

Let us remark that the zero component Ψ_0 of a vector $\vec{\Psi}$ is a constant. It is also convenient to use the following notation:

$$\Psi(q)_N = \Psi(Q) = \Psi(q_1, q_2, \dots, q_N) = \Psi(1, 2, \dots, N).$$

Let us define the product of two vectors $\vec{\vartheta}, \vec{\omega} \in A$ by the following definition:

$$\vec{\vartheta} \times \vec{\omega} = \vec{\Psi} \Rightarrow \left. \begin{array}{c} \vartheta(0) \\ \vartheta(1) \\ \vartheta(12) \\ \vartheta(123) \\ \vdots \end{array} \right\} \times \left. \begin{array}{c} \omega(0) \\ \omega(1) \\ \omega(12) \\ \omega(123) \\ \vdots \end{array} \right\} = \left. \begin{array}{l} \vartheta(0)\omega(0) = \Psi(0) \\ \vartheta(0)\omega(1) + \vartheta(1)\omega(0) = \Psi(1) \\ \vartheta(0)\omega(12) + \vartheta(1)\omega(2) \\ \quad + \vartheta(2)\omega(1) + \vartheta(12)\omega(0) = \Psi(12) \\ \vartheta(0)\omega(123) + \sum \vartheta(0)_1 \omega(0)_2 \\ \quad + \sum \vartheta(0)_2 \omega(0)_1 + \vartheta(123)\omega(0) = \Psi(123) \\ \vdots \end{array} \right\}.$$

For an arbitrary component of a vector $\vec{\Psi}$ we have

$$\Psi(1 \dots N) = \Psi(q)_N = \sum_{k=0}^N \sum_{Q'_k} \vartheta(Q'_k) \omega((q)_N - Q'_k).$$

Here the summation extends over all ordered subsequences, $Q'_k = (i_1 < i_2 < \dots < i_k) = \{q_{i_1} q_{i_2}, \dots, q_{i_k}\}$ of the lengths k ($k = 0, 1, 2, \dots, N$) of the sequence $1, 2, \dots, N$ and contains $N!/k!(N-k)!$ terms for each k .

Obviously, due to this product the vector space A is a commutative algebra with unit element $\vec{1} = \{1(0), 0, 0, \dots\}$. It can be readily checked that the homomorphism of algebra A in an algebra of formal power series:

$$\begin{aligned}
 \text{if } \vec{\vartheta} \in A &\Rightarrow \vartheta(z) = \sum_{N=0}^{\infty} z^N \frac{\vartheta_N}{N!} & \vartheta_N &= \int \dots \int d(q)_N \vartheta(1 \dots N) \\
 \text{if } \vec{\Psi} = \vec{\vartheta} * \vec{\omega} &\Rightarrow \Psi(z) = \vartheta(z) \omega(z).
 \end{aligned}$$

Elements of algebra A with elements u_0 equal to zero form the closed subspace A_+ , being an ideal in A :

$$\vec{u} \in A_+ \quad \text{if} \quad u(0) = 0 \quad \vec{u} = \{0, u(1), u(12), \dots, u(1 \dots N), \dots\}$$

$$\text{if} \quad \vec{u} \in A_+ \quad \Rightarrow \quad u * u \in A_+ \quad A_+ \subset A.$$

The power-series expansion of the exponential yields a well defined mapping $\vec{\Gamma}$ of A_+ onto $\vec{1} + A_+$. If

$$\vec{u} = \begin{pmatrix} 0 \\ u(1) \\ u(12) \\ u(123) \\ u(1234) \\ \vdots \end{pmatrix}$$

then

$$\vec{\Gamma}(\vec{u}) = \vec{1} + \vec{u} + \frac{1}{2!} \vec{u} \times \vec{u} + \frac{1}{3!} \vec{u} \times \vec{u} \times \vec{u} + \frac{1}{4!} \vec{u} \times \vec{u} \times \vec{u} \times \vec{u} + \dots$$

$$\vec{\Gamma}(\vec{u}) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ u(1) \\ u(12) \\ u(123) \\ u(1234) \\ u(12345) \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ u(1)u(2) \\ \sum u(0)_1 u(0)_2 \\ \sum u(0)_1 u(0)_3 + \sum u(0)_2 u(0)_2 \\ \sum u(0)_1 u(0)_4 + \sum u(0)_2 u(0)_3 \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ u(1)u(2)u(3) \\ \sum u(0)_1 u(0)_1 u(0)_2 \\ \sum u(0)_1 u(0)_1 u(0)_3 + \sum u(0)_1 u(0)_2 u(0)_2 \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ u(1)u(2)u(3)u(4) \\ \sum u(0)_1 u(0)_1 u(0)_1 u(0)_2 \\ \vdots \end{pmatrix} + \dots$$

Let us note that the components of a vector $\vec{\Gamma}(\vec{u})$ are the finite sums of all possible products of components of a vector \vec{u} related to all possible renumberings [22, 23].

5. Cluster expansions

Let us introduce an unknown vector \vec{u} by the relation $\vec{1} + \vec{\Psi} = \vec{\Gamma}(\vec{u})$, where the vector $\vec{\Psi}$ is a vector with components equal to the determinants of density matrices of ideal fermions, then we have

$$\vec{1} + \vec{\Psi} = \vec{\Gamma}(\vec{u}) = \vec{1} + \vec{u} + \frac{\vec{u} \times \vec{u}}{2!} + \frac{\vec{u} \times \vec{u} \times \vec{u}}{3!} + \dots$$

The components of this vector are equal to

$$u(0) = 0 = \Psi(0)$$

$$u(1) = \bar{\rho}_0(C_1) = \Psi(1)$$

$$u(12) + u(1)u(2) = \bar{\rho}_0(C_2) + \bar{\rho}_0(C_1)\bar{\rho}(C_1) = \Psi(12)$$

$$u(123) + \sum u(0_1)u(0_2) + u(1)u(2)u(3) = \bar{\rho}_0(C_3) + \sum \bar{\rho}_0(C_1)\bar{\rho}(C_2) + \bar{\rho}_0(C_1)\bar{\rho}_0(C_1)\bar{\rho}_0(C_1) = \Psi(123)$$

$$u(1234) + \sum u(0_1)u(0_3) + \sum u(0_2)u(0_2) + \sum u(0_1)u(0_1)u(0_2) + u(1)u(2)u(3)u(4) = \Psi(1234)$$

$$= \bar{\rho}_0(C_4) + \sum \bar{\rho}_0(C_1)\bar{\rho}_0(C_3) + \sum \bar{\rho}_0(C_2)\bar{\rho}_0(C_2)$$

$$+ \sum \bar{\rho}_0(C_1)\bar{\rho}_0(C_1)\bar{\rho}_0(C_2) + \bar{\rho}_0(C_1)\bar{\rho}_0(C_1)\bar{\rho}_0(C_1)\bar{\rho}_0(C_1)$$

⋮

These relations can be considered as a system of algebraic equations defining the components of an unknown vector \vec{u} . The inverse mapping $\vec{\Gamma}^{-1}$ gives us a unique solution of this system of algebraic equations,

$$\vec{u} = \vec{\Gamma}^{-1}(\vec{1} + \vec{\Psi}) = \vec{\Psi} - \frac{\vec{\Psi} \times \vec{\Psi}}{2} + \frac{\vec{\Psi} \times \vec{\Psi} \times \vec{\Psi}}{3} - \dots$$

For components of this expression we have

$$u(0) = 0$$

$$u(1) = \Psi(1) = \bar{\rho}_0(C_1)$$

$$u(12) = \Psi(12) - u(1)u(2) = \bar{\rho}_0(C_2)$$

$$u(123) = \Psi(123) - \sum u(0_1)u(0_2) - u(0_1)u(0_1)u(0_1) = \bar{\rho}(C_3)$$

$$u(1234) = \Psi(1234) - \sum u(0_1)u(0_3) - \sum u(0_2)u(0_2) - \sum u(0_1)u(0_1)u(0_2) - u(1)u(2)u(3)u(4) = \bar{\rho}(C_4)$$

⋮

Let us note that in the ‘fixed-node approximation’ contributions of odd permutations are equal to zero, therefore in the analogous relations written below the underlined terms are not taken into account:

$$\vec{\Gamma}\vec{u} = \vec{1} + \vec{\Psi}.$$

The component-wise form of this expression has the form:

$$\begin{aligned}
\tilde{u}(0) &= 0 = \tilde{\Psi}(0) \\
\tilde{u}(1) &= \rho(\tilde{C}_1) = \tilde{\Psi}(1) \\
\tilde{u}(12) + \tilde{u}(1)\tilde{u}(2) &= \chi_2(\tilde{C}_2)\rho(\tilde{C}_2) + \chi_2(\tilde{C}_1\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1) = \tilde{\Psi}(12) \\
\tilde{u}(123) + \sum \tilde{u}(0_1)\tilde{u}(0_2) + \tilde{u}(1)\tilde{u}(2)\tilde{u}(3) &= \Sigma\chi_3(\tilde{C}_3)\rho(\tilde{C}_3) + \Sigma\chi_3(\tilde{C}_1\tilde{C}_2)\rho(\tilde{C}_1)\rho(\tilde{C}_2) \\
&\quad + \chi_3(\tilde{C}_1\tilde{C}_1\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1) \\
&= \tilde{\Psi}(123) \\
\tilde{u}(1234) + \sum \tilde{u}(0_1)\tilde{u}(0_3) + \sum \tilde{u}(0_2)\tilde{u}(0_2) + \sum \tilde{u}(0_1)\tilde{u}(0_1)\tilde{u}(0_2) + \tilde{u}(1)\tilde{u}(2)\tilde{u}(3)\tilde{u}(4) &= \tilde{\Psi}(1234) \\
&= \Sigma\chi_4(\tilde{C}_4)\rho(\tilde{C}_4) + \sum \chi_4(\tilde{C}_1\tilde{C}_3)\rho(\tilde{C}_1)\rho(\tilde{C}_3) + \sum \chi_4(\tilde{C}_2\tilde{C}_2)\rho(\tilde{C}_2)\rho(\tilde{C}_2) \\
&\quad + \sum \chi_4(\tilde{C}_1\tilde{C}_1\tilde{C}_2)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_2) \\
&\quad + \chi_4(\tilde{C}_1\tilde{C}_1\tilde{C}_1\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1).
\end{aligned} \tag{3}$$

The unique vector \vec{u} is defined by the inverse mapping $\vec{\Gamma}^{-1}$:

$$\vec{u} = \vec{\Gamma}^{-1}(\vec{1} + \vec{\Psi}).$$

Therefore, the vector \vec{u} in the ‘fixed-node approximation’ does not coincide with the initial exact vector \vec{u} . The component-wise form of \vec{u} is

$$\begin{aligned}
\tilde{u}(0) &= \tilde{\Psi}(0) = 0 \\
\tilde{u}(1) &= \tilde{\Psi}(1) = \rho(\tilde{C}_1) \\
\tilde{u}(12) &= \tilde{\Psi}(12) - \tilde{u}(1)\tilde{u}(2) = (\chi_2(\tilde{C}_1\tilde{C}_1) - 1)\rho(\tilde{C}_1)\rho(\tilde{C}_1) \\
\tilde{u}(123) &= \tilde{\Psi}(123) - \sum \tilde{u}(0_1)\tilde{u}(0_2) - \tilde{u}(1)\tilde{u}(2)\tilde{u}(3) \\
&= \sum \chi_3(\tilde{C}_3)\rho(\tilde{C}_3) - \sum (\chi_2(\tilde{C}_1\tilde{C}_1) - 1)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1) \\
&\quad - (\chi_3(\tilde{C}_1\tilde{C}_1\tilde{C}_1) - 1)\rho(\tilde{C}_1)\rho(\tilde{C}_1)\rho(\tilde{C}_1) \\
\tilde{u}(1234) &= \tilde{\Psi}(1234) - \sum \tilde{u}(0_1)\tilde{u}(0_3) - \sum \tilde{u}(0_2)\tilde{u}(0_2) \\
&\quad - \sum \tilde{u}(0_1)\tilde{u}(0_1)\tilde{u}(0_2) - \tilde{u}(1)\tilde{u}(2)\tilde{u}(3)\tilde{u}(4) \\
&= \dots
\end{aligned} \tag{4}$$

By taking advantage of the homomorphism, we shall consider the formal power series of a new independent variable z corresponding to vectors $\vec{1} + \vec{\Psi}$ and $\vec{1} + \vec{\Psi}$. These formal power series have a simple physical meaning of the grand partition functions of fermions, while the mapping $\vec{\Gamma}$ allows one to present a logarithm of the grand partition function $\ln(1 + \Psi(z))$ as the sum of the contributions of the linked diagrams related to the cyclic permutations. The independent complex variable z on a positive semiaxis has the physical meaning of activity. Expressions $pV/k_B T = \ln(1 + \Psi(z))$ and $N\lambda^3/V = z\partial \ln(1 + \Psi)/\partial z$ ($\lambda^2 = 2\pi\hbar^2\beta/m$) determine the equation of state in a grand canonical ensemble and the dependence of a density versus z , respectively. Excluding from these relations the variable z , it is possible to obtain the equation of a state in the canonical ensemble.

For ideal fermions the logarithm of the grand partition function is the well known fermi function with index $\frac{5}{2}$, which can be easily derived from the above obtained expressions:

$$\vec{1} + \vec{\Psi} = \vec{\Gamma}\vec{u} \Rightarrow 1 + \Psi(z) = 1 + \sum_{N=1}^{\infty} z^N \frac{\Psi_N}{N!} = \exp[u(z)] = \exp\left[\sum_{\nu=1}^{\infty} z^{\nu} \frac{u_{\nu}}{\nu!}\right]. \tag{5}$$

For ideal fermions the cluster integrals can be calculated analytically:

$$u_v = \int \cdots \int_{\Omega} d(q)_v u(1 \dots v) = \int \cdots \int_{\Omega} d(q)_v \bar{\rho}(C_v) = u_v = (-1)^{v+1} (v-1)! \frac{V}{\lambda^3 v^{3/2}}.$$

As result the equation of state in a grand canonical ensemble is described by the fermi function:

$$\frac{pV}{k_B T} = \ln(1 + \Psi(z)) = \frac{V}{\lambda^3} \sum_{v=1}^{\infty} \frac{(-1)^{v+1} z^v}{v^{5/2}}. \quad (6)$$

The analogous consideration in the ‘fixed-node approximation’ results in another equation of state, i.e.

$$\vec{1} + \vec{\Psi} = \vec{\Gamma} \vec{u} \Rightarrow 1 + \tilde{\Psi}(z) = 1 + \sum_{N=1}^{\infty} z^N \frac{\tilde{\Psi}_N}{N!} = \exp[\tilde{u}(z)] = \exp\left[\sum_{v=1}^{\infty} z^v \frac{\tilde{u}_v}{v!}\right]. \quad (7)$$

The analytical calculations of cluster integrals, except \tilde{u}_2 , are now impossible due to the presence of the characteristic functions. Now \tilde{u}_2 depends on the choice of the ‘trial density matrix’ and M , as the Trotter formula for the matrix elements of the density matrix is not satisfied. Here:

$$\tilde{u}_v = \int \cdots \int_{\Omega} d(q)_v \tilde{u}(1 \dots v).$$

For the equation of state we have

$$\frac{\tilde{p}V}{k_B T} = \ln(1 + \tilde{\Psi}(z)) = \sum_{v=1}^{\infty} \frac{z^v \tilde{u}_v}{v!}.$$

Thus, the inequality of vectors $\tilde{u} \neq \vec{u}$ results in the difference in the equations of state. Due to the uniqueness of an analytic continuation this inequality is valid over the entire complex plane of variable z ,

$$pV/k_B T = \ln(1 + \Psi(z)) \neq \ln(1 + \tilde{\Psi}(z)) = \tilde{p}V/k_B T.$$

As follows from the presented derivation for ideal fermions, the difference between the exact equation of state and the equation of state in the ‘fixed-node approximation’ is a pure combinatorial property and does not depend on a modification of the domain of integration by an appropriate choice of a ‘trial density matrix’. Excluding z from the equation of state $pV/k_B T = \ln(1 + \Psi(z))$ and the expression for density $N\lambda^3/V = z \ln(1 + \Psi)/\partial z$, it is possible to prove the analogous statement in the canonical ensemble. The incorrectness of the cluster expansion in the ‘fixed-node approximation’ is also connected with the fact that some terms related to the definite cluster integral can be proportional to V^n , where $n > 1$, while other terms are proportional to V , for example, the term $\sum (\chi_2(\tilde{C}_1 \tilde{C}_1) - 1) \rho(\tilde{C}_1) \rho(\tilde{C}_1) \rho(\tilde{C}_1)$ in (4). Let us note that $\rho(\tilde{C}_3)$ is going to zero, while $\chi_2(\tilde{C}_1 \tilde{C}_1)$ is going to one, when the characteristic distances between trajectories of fermi particles are greater than the thermal wavelength.

6. Interacting fermions

The most reliable and complete results in the ‘fixed-node approximation’ are obtained for a hydrogen plasma in [3, 4, 21], which is a mixture of classical (N_i protons) and Fermi particles (N_e electrons, $N_e = N_i$). As is well known the thermodynamic properties of a quantum system are fully determined by the related derivatives of partition function Z :

$$Z(N_e, N_i, V, \beta) = \frac{Q(N_e, N_i, \beta)}{N_e! N_i!} \quad \text{with} \quad Q(N_e, N_i, \beta) = \sum_{\sigma} \int_{\Omega} dq dr \rho(q, r, \sigma; \beta). \quad (8)$$

Here $q \equiv \{q_1, q_2, \dots, q_{N_i}\}$ comprises the coordinates of the protons, and $\sigma = \{\sigma_1, \dots, \sigma_{N_e}\}$ and $r \equiv \{r_1, \dots, r_{N_e}\}$ are the electron spins and coordinates, respectively. The density matrix ρ in equation (8) is represented in standard way by a path integral [11],

$$\rho(q, r, \sigma; \beta) = \frac{1}{\lambda_i^{3N_i} \lambda_\Delta^{3N_e}} \int_{\Omega} dr^{(1)} \dots dr^{(n)} \times \sum_P (\pm 1)^{\kappa_P} \rho(q, r, r^{(1)}; \Delta\beta) \dots \rho(q, r^{(n)}, \hat{P}r^{(n+1)}; \Delta\beta) \mathcal{S}(\sigma, \hat{P}\sigma') \quad (9)$$

where $\Delta\beta \equiv \beta/(n+1)$ and $\lambda_\Delta^2 = 2\pi\hbar^2\Delta\beta/m_e$. Furthermore, $r^{(n+1)} \equiv r$ and $\sigma' = \sigma$, i.e. the particles are represented by fermionic loops with the coordinates (beads) $[r] \equiv [r, r^{(1)}, \dots, r^{(n)}, r]$. The electron spin gives rise to the spin part of the density matrix \mathcal{S} , whereas exchange effects are accounted for by the permutation operator \hat{P} and the sum over the permutations with parity κ_P .

In this paper, following [7, 25], we shall take into account all permutations and shall integrate over the initial domain Ω . Following [7, 25, 26], we use a modified representation of the high-temperature density matrices on the right-hand side of equation (9) which is suitable for efficient direct fermionic PIMC simulations of plasmas. With the error of order $\epsilon \sim (\beta Ry)^2 N_e \lambda_e^3 / V(n+1)$ vanishing with growing numbers of beads we obtain the approximation

$$\begin{aligned} \sum_{\sigma} \rho(q, r, \sigma; \beta) &= \frac{1}{\lambda_i^{3N_i} \lambda_\Delta^{3N_e}} \sum_{s=0}^{N_e} \rho_s(q, [r], \beta) \\ \rho_s(q, [r], \beta) &= \frac{C_{N_e}^s}{2^{N_e}} e^{-\beta U(q, [r], \beta)} \prod_{l=1}^n \prod_{p=1}^{N_e} \phi_{pp}^l \det |\psi_{ab}^{n,1}|_s \\ U(q, [r], \beta) &= U^i(q) + \sum_{l=0}^n \frac{U_l^e([r], \beta) + U_l^{ei}(q, [r], \beta)}{n+1} \end{aligned} \quad (10)$$

where U^i , U_l^e and U_l^{ei} denote the sum of the binary interaction Kelbg potentials [27, 28] Φ^{ab} between protons, between electron beads ('l'), and between electron beads ('l') and protons, respectively.

In equation (10), $\phi_{pp}^l \equiv \exp[-\pi |\xi_p^{(l)}|^2]$ arises from the kinetic energy density matrix ρ^K of the electron with index p , and we introduced dimensionless distances $\xi^{(1)}, \dots, \xi^{(n)}$ between neighbouring beads on the loop, then explicitly, $[r] \equiv [r; r + \lambda_\Delta \xi^{(1)}; r + \lambda_\Delta (\xi^{(1)} + \xi^{(2)}); \dots]$. The exchange matrix is given by

$$\|\psi_{ab}^{n,1}\|_s \equiv \|e^{-(\pi/\lambda_\Delta^2) |(r_a - r_b) + y_a^n|^2}\|_s \quad (11)$$

where $y_a^n = \lambda_\Delta \sum_{k=1}^n \xi_a^{(k)}$. As a result of the spin summation, the matrix has the block structure and carries a subscript s denoting the number of electrons having the same spin projection.

Furthermore, as an example, we present the equation of state, $\beta p = \partial \ln Q / \partial V = [\alpha / 3V \partial \ln Q / \partial \alpha]_{\alpha=1}$,

$$\begin{aligned} \frac{\beta p V}{N_e + N_i} &= 1 + \frac{(3Q)^{-1}}{N_e + N_i} \sum_{s=0}^{N_e} \int dq dr d\xi \rho_s(q, [r], \beta) \\ &\times \left\{ \sum_{p < t}^{N_i} \frac{\beta e^2}{|q_{pt}|} - \sum_{p < t}^{N_e} |r_{pt}| \frac{\partial \Delta\beta \Phi^{ee}}{\partial |r_{pt}|} - \sum_{p=1}^{N_i} \sum_{t=1}^{N_e} |x_{pt}| \frac{\partial \Delta\beta \Phi^{ie}}{\partial |x_{pt}|} \right\} \end{aligned}$$

$$\begin{aligned}
& - \sum_{l=1}^n \left[\sum_{p<t}^{N_e} A_{pt}^l \frac{\partial \Delta\beta\Phi^{ee}}{\partial |r_{pt}^l|} + \sum_{p=1}^{N_i} \sum_{t=1}^{N_e} B_{pt}^l \frac{\partial \Delta\beta\Phi^{ie}}{\partial |x_{pt}^l|} \right] + \frac{\alpha}{\det |\psi_{ab}^{n,1}|_s} \frac{\partial \det |\psi_{ab}^{n,1}|_s}{\partial \alpha} \Bigg\} \\
& \text{with } A_{pt}^l = \frac{\langle r_{pt}^l | r_{pt}^l \rangle}{|r_{pt}^l|} \quad B_{pt}^l = \frac{\langle x_{pt}^l | x_{pt}^l \rangle}{|x_{pt}^l|}. \quad (12)
\end{aligned}$$

Here, $\Phi^{ee} = e^2/|r_{pt}|$, α is a length scaling, $\alpha = L/L_0$, $\langle \dots | \dots \rangle$ denotes the scalar product, and q_{pt} , r_{pt} and x_{pt} are differences of two coordinate vectors: $q_{pt} \equiv q_p - q_t$, $r_{pt} \equiv r_p - r_t$, $x_{pt} \equiv r_p - q_t$, $r_{pt}^l = r_{pt} + y_{pt}^l$, $x_{pt}^l \equiv x_{pt} + y_p^l$ and $y_{pt}^l \equiv y_p^l - y_t^l$. Other thermodynamic quantities exhibit an analogous form¹.

The important advantage of expression (12) is that the sum over all permutations has been taken into account by the determinant, which can be calculated by the direct methods of linear algebra. Moreover, in the limit when the number of beads is going to infinity $n \rightarrow \infty$ all terms in (12) are bounded, which improves the convergence of calculations using the Monte Carlo method.

Expressions of the type (12) are convenient for calculations using a Monte Carlo method as they allow one to use the effective procedure for calculations of the ratio of determinants of the two-successor state of a Markov chain $R = \det |\psi_{ab}^{n,1}|_{\text{new}} / \det |\psi_{ab}^{n,1}|_{\text{old}}$. In our calculations the probability of acceptance of a new configuration of particles was proportional to an absolute value R , while the sign of the determinants was taken into account by the weight function of the current configuration of particles. Moreover, effective calculations using formulae (12) require fast calculations of derivatives of a determinant. All of these problems were effectively solved due to calculations of an inverse exchange matrix. To generate a new configuration of particles the elementary algorithm was used, in which one bead of the electronic trajectory or one of the plasma particles (electron or proton) as whole were shifted. Due to these elementary Monte Carlo steps the trivial modifications of an exchange matrix (modifications of only one line or column) have been related, which increased the efficiency of the calculations. Calculations were mainly performed for $N_e = N_p = 50$ in a Monte Carlo cell, that allowed one to take in the sum over s only one main term related to $s = N_e/2$. The test calculations were performed for an ideal plasma of non-interacting classical protons and ideal fermi electrons as the thermodynamic quantities of an ideal plasma has well known analytical expressions [5]. Good agreement with the analytical estimates was obtained [19, 20].

The results obtained here for a strongly coupled plasma were compared with analogous results by Militzer and Ceperley [21] for hydrogen and deuterium plasma in the ‘fixed-node approximation’. These results for pressure and energy at fixed density $2N_e/V = 2.5 \times 10^{23} \text{ cm}^{-3}$ are presented in table 1. At temperatures above 100 000 K, where the degeneration parameter $n_e \lambda_e^3 \leq 2$ (λ_e is a thermal wavelength of an electron, $\lambda_e^2 = 2\pi \hbar^2 \beta / m_e$) the agreement is rather good. However, at temperatures lower than 100 000 K the difference starts to rapidly grow, which is due to the increase of the exchange effects and the appearance of atoms and molecules.

7. Conclusions

This work is devoted to the treatment of correlated proton–electron systems with degenerate electrons. We compared our direct PIMC simulations with independent restricted PIMC results of Militzer and Ceperley for one isochor corresponding to $r_s = 1.86$ and temperatures

¹ The approach [16] does not take into account the sign of the determinant (11), which results in essential errors for strongly degenerate systems. We underline that, in contrast, our method rigorously takes into account the sign of the determinant of each Monte Carlo configuration in the calculation of all thermodynamic averages.

Table 1. Pressure p (Mbar) and energy E (2NRyd) of a dense plasma. Upper line, present work; bottom line, the ‘fixed-node approximation’. Coupling parameter $\Gamma = (4\pi n_e/3)^{1/3} e^2/k_B T$, $2N_e/V = 2.5 \times 10^{23} \text{ cm}^{-3}$.

T (1000 K)	$n\lambda_e^3$	Γ	p (Mbar)	E (2NRyd)
1000	0.10	0.169	67.74 ± 0.02	9.050 ± 0.005
			66.86 ± 0.08	9.018 ± 0.015
500	0.29	0.339	32.85 ± 0.03	4.169 ± 0.003
			32.13 ± 0.05	4.114 ± 0.007
250	0.83	0.679	15.37 ± 0.01	1.654 ± 0.005
			14.91 ± 0.03	1.629 ± 0.007
125	2.33	1.350	6.98 ± 0.01	0.412 ± 0.005
			6.66 ± 0.02	0.404 ± 0.004
62.5	6.58	2.701	3.07 ± 0.02	-0.248 ± 0.005
			2.99 ± 0.04	-0.140 ± 0.007
31.25	18.48	5.376	2.20 ± 0.01	-2.377 ± 0.005
			1.58 ± 0.07	-0.360 ± 0.010
15.625	52.26	10.75	1.46 ± 0.05	-2.937 ± 0.08
			1.01 ± 0.05	-0.44 ± 0.007
10.000	103.6	16.96	1.39 ± 0.06	-2.52 ± 0.3
			0.80 ± 0.08	-0.49 ± 0.02

in the range $10\,000 \text{ K} \leq T \leq 10^6 \text{ K}$, where $\Gamma < 20$ and $n_e \lambda_e^3 < 100$. This region is particularly complicated as here the pressure and temperature ionization occur and, therefore, an accurate and consistent treatment of scattering and bound states is crucial. Results of the direct path integral Monte Carlo simulation performed here have shown that the ‘fixed-node approximation’ describes the thermodynamic properties of the strongly coupling fermions rather well at ‘weak and moderate’ degeneracy. To analyse the reasons for the increasing difference between the ‘fixed-node approximation’ and the results of the direct path integral Monte Carlo simulations for highly degenerate fermions the correctness of the ‘fixed-node approximation’ for ideal Fermi systems has been analysed by analytical methods. A rigorous proof has been given to the fact that the exact Fermi function with index $\frac{5}{2}$ describing the logarithm of the grand partition function of ideal fermions cannot be reproduced in the ‘fixed-node approximation’, which means that the ‘fixed-node approximation’ does not have the correct limit of an ideal Fermi gas.

Acknowledgments

The author expresses his deep gratitude for stimulating discussions and valuable notes to Professor W D Kraeft, D Kremp, M Schlanges and Drs M Bonitz and J Ortner. The author expresses thanks to Professor D Ceperley and Dr B Militzer for discussions and providing data [21] prior to publication. The author thanks the Deutsche Forschungsgemeinschaft (Mercator-Programm) for financial support and NIC Jülich for computer time for calculations.

References

- [1] Lifshiz E M and Pitaevskii L D 1978 Theory of a condensed matter *Statistical Physics, part 2 (Theoretical Physics, vol IX) Science* (in Russian)
- [2] Tilley D R and Tilley J 1974 *Superfluidity and Superconductivity* (London: Van Nostrand Reinhold)
- [3] Kalman G 1998 (ed) *Strongly Coupled Coulomb Systems* (Oxford: Pergamon)

- [4] Kraeft W D and Schlanges M (ed) 1996 *Proc. Int. Conf. on Strongly Coupled Plasmas* (Singapore: World Scientific)
- [5] Kraeft W D, Kremp D, Ebeling W and Röpke G 1986 *Quantum Statistics of Charged Particle Systems* (Berlin: Akademie)
- [6] Bonitz M (ed) 2000 *Progress in Nonequilibrium Green's Functions* (Singapore: World Scientific)
- [7] Zamalin V M, Norman G E and Filinov V S 1977 *The Monte Carlo Method in Statistical Thermodynamics* (Moscow: Nauka) (in Russian)
- [8] Binder K and Cicotti G (ed) 1996 *The Monte Carlo and Molecular Dynamics of Condensed Matter Systems* (Bologna: SIF)
- [9] Berne B J, Cicotti G and Coker D F (ed) 1998 *Classical and Quantum Dynamics of Condensed Phase Simulation* (Singapore: World Scientific)
- [10] Egger R, Häusler W, Mak C H and Grabert H 1999 *Phys. Rev. Lett.* **82** 3320 and references therein
- [11] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
- [12] Ceperley D 1996 *The Monte Carlo and Molecular Dynamics of Condensed Matter Systems* ed K Binder and G Cicotti (Bologna: SIF) pp 447–82
- [13] Ceperley D 1991 *J. Stat. Phys.* **63** 1237–48
- [14] Ceperley D 1992 *Phys. Rev. Lett.* **69** 331–6
- [15] Militzer B and Pollock R *Phys. Rev. E* 2000 **61** 3470–81
- [16] Imada R 1984 *J. Phys. Soc. Japan.* **53** 2861–7
- [17] Filinov V S, Levashov P R, Fortov V E and Bonitz M 2000 *Progress in Nonequilibrium Green's functions* ed M Bonitz (Singapore: World Scientific)
(Filinov V S, Levashov P R, Fortov V E and Bonitz M 1999 *Preprint cond-mat/9912055*)
- [18] Filinov V S and Bonitz M 2000 *Progress in Nonequilibrium Green's functions* ed M Bonitz (Singapore: World Scientific)
(Filinov V S and Bonitz M 1999 *Preprint cond-mat/9912049*)
- [19] Filinov V S, Bonitz M and Fortov V E 2000 *JETP Lett.* **72** 245–8
- [20] Filinov V S, Fortov V E, Bonitz M and Kremp D 2000 *Phys. Lett. A* **274** 228–35
- [21] Militzer B and Ceperley D 2000 *Phys. Rev. Lett.* **85** 1890
Militzer B and Ceperley D 2000 *Phys. Rev. Lett.* **85** 1893
- [22] Ruelle D 1969 *Statistical Mechanics, Rigorous Results* (New York: Benjamin-Cummings)
- [23] Zelener B V, Norman G E, Filinov V S 1981 *Perturbation Theory and Pseudopotential in Statistical Thermodynamics* (Moscow: Nauka) (in Russian)
- [24] Kurosh A G 1962 *Algebra* (State Publishing House of the Physical and Mathematical Literature) (in Russian)
- [25] Filinov V S 1975 *High Temp.* **13** 1065–71
Filinov V S 1976 *High Temp.* **14** 225–36
- [26] Zelener B V, Norman G E and Filinov V S 1975 *High Temp.* **13** 650–9
- [27] Kelbg G 1963 *Ann. Phys., Lpz.* **12** 219–30
Kelbg G 1964 *Ann. Phys., Lpz.* **13** 354–361
Kelbg G 1964 *Ann. Phys., Lpz.* **14** 394–402
- [28] Ebeling W, Hoffmann H J and Kelbg G 1967 *Contr. Plasma Phys.* **7** 233–41