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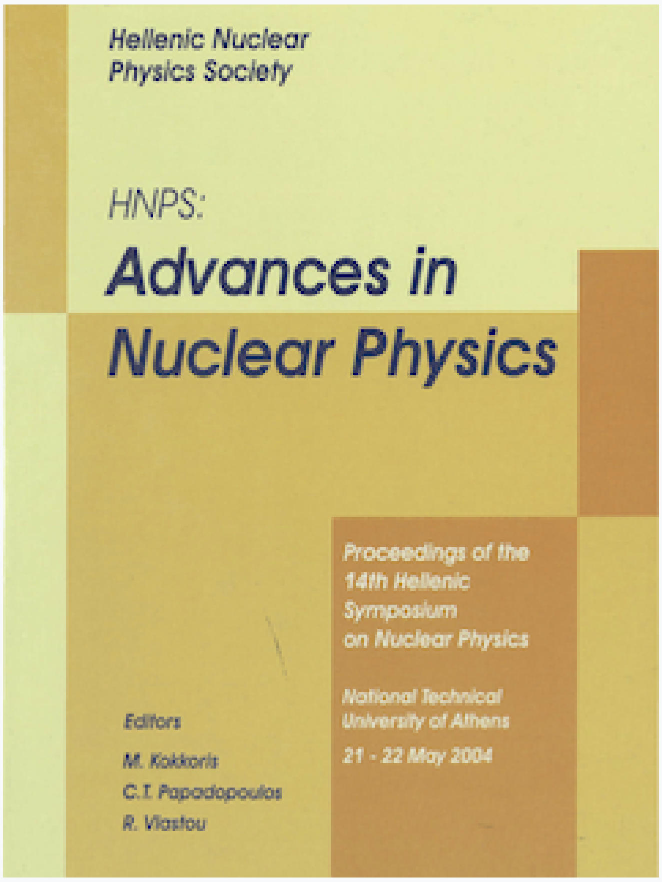

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Dependence of Information Entropy of Uniform Fermi Systems on Correlations and Thermal Effects

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Abstract

The influence of correlations of uniform Fermi systems (nuclear matter, electron gas and liquid ^{3}He) on Shannon's information entropy, S, is studied. It is found that, for three different Fermi systems with different particle interactions, the correlated part of S (S_{cor}) depends on the correlation parameter of the systems or on the discontinuity gap of the momentum distribution through two parameter expressions. The values of the parameters characterize the strength of the correlations. A two parameter expression also holds between S_{cor} and the mean kinetic energy (K) of the Fermi system. The study of thermal effects on the uncorrelated electron gas leads to a relation between the thermal part of S ($S_{thermal}$) and the fundamental quantities of temperature, thermodynamical entropy and the mean kinetic energy. It is found that, in the case of low temperature limit, the expression connecting $S_{thermal}$ with K is the same to the one which connects S_{cor} with K. Thus, regardless of the reason (correlations or thermal) that changes K, S takes almost the same value.

Key words: Information theory, Fermi systems, Momentum distribution
PACS: 05.30.Fk, 21.65.+f, 67.55.-s, 89.70.+c, 65.40.Gr

1 Introduction

Information theoretical methods have in recent years played an important role in the study of quantum mechanical systems [1–8] in two cases: first in the clarification of fundamental concepts of quantum mechanics and second in the synthesis of probability densities in position and momentum space. An important step was the discovery of an entropic uncertainty relation [1] which for a three-dimensional system has the form

$$S = S_r + S_k \geq 3(1 + \ln \pi) \simeq 6.434, \tag{1}$$

where

$$S_r = -\int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r}, \qquad S_k = -\int n(\mathbf{k}) \ln n(\mathbf{k}) d\mathbf{k} \tag{2}$$

are Shannon's information entropies (IE) in position- and momentum-space and $\rho(\mathbf{r})$, $n(\mathbf{k})$ are the density distribution (DD) and momentum distribution (MD), respectively, normalized to unity.

The physical meaning of S_r and S_k is that it is a measure of quantum-mechanical uncertainty and represents the information content of a probability distribution, in our case of various fermionic systems density and momentum distributions. Inequality (1) provides a lower bound for S which is attained for Gaussian wave functions [1]. It is mentioned that the sum $S = S_r + S_k$ is invariant to uniform scaling of coordinates, while the individual entropies S_r and S_k are not.

The motivation of the present work is to extend our previous study of IE in nuclei, atomic clusters and correlated bosonic systems to the direction of various uniform fermionic systems and to connect it with the interaction of the particles and the temperature. In uniform systems the density $\rho = N/V$ is a constant and the interaction of the particles is reflected to MD which deviates from the *theta* function form of the ideal Fermi-gas model. It is important to study how the interaction affects the MD as well as the IE. An attempt is also made to relate the IE with fundamental quantities such as the temperature, the thermodynamical entropy and the mean kinetic energy of the fermionic system (electron gas).

The quantum systems which are examined in the present work are nuclear matter, electron gas and liquid ^{3}He. The inter-particle interactions of these systems generally differ by many orders of magnitude in their strengths and ranges. If the potentials are scaled with suitable energy and length measures for the different systems, i.e. Fermi energy and inverse Fermi momentum, the potentials still differ by orders of magnitude. The helium system is the most strongly interacting, with an almost-hard-core interaction, and the electron gas the most weakly interacting [9]. The nuclear case lies somewhere between. In all these cases the strength of the interaction may be gauged by the depletion of the Fermi sea. Quantitatively, one examines the deviation of Z_F from unity, where Z_F is the discontinuity gap of the momentum distribution $n(k)$ at $k = k_F$ in an uniform Fermi system [10].

The paper is organized as follows. The method leading to the expression of Shannon's information entropy sum in finite Fermi systems is presented in Section II. Applications of that expression to nuclear matter, electron gas, and liquid ^{3}He are made in the three subsections of Section II. In the same subsections numerical results are also reported and discussed. In Section III the study of the influence of thermal effects on the information entropy sum is made.

2 Information entropy for an infinite Fermi system

The key quantity for the description of the MD both in infinite and finite quantum systems is the one-body density matrix (OBDM). The OBDM is defined as

$$\rho(\mathbf{r}_1, \mathbf{r}_1') = \int \Psi^*(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\Psi(\mathbf{r}_1', \mathbf{r}_2, ..., \mathbf{r}_N)d\mathbf{r}_2...d\mathbf{r}_N \qquad (3)$$

The diagonal elements $\rho(\mathbf{r_1}, \mathbf{r_1})$ of the OBDM yields the local density distribution, which is just a constant ρ in the uniform infinite system. Homogenity and isotropy of the system require that $\rho(\mathbf{r}_1, \mathbf{r}_1') = \rho(\mid \mathbf{r}_1 - \mathbf{r}_1' \mid) \equiv \rho(r)$. In the case of noninteractive Fermi systems the associated OBDM is

$$\rho(r) = \rho l(k_F \mid \mathbf{r}_1 - \mathbf{r}_1' \mid),$$

where

$$l(x) = 3x^{-3}(\sin x - x\cos x)$$

and $\rho = N/V$ is the constant density of the uniform Fermi system.

The density, normalized to 1 ($\int \rho_0 d\mathbf{r} = 1$), is given by the relation

$$\rho_o = \frac{1}{NV_o} = \frac{1}{N\frac{4}{3}\pi r_o^3} \qquad (4)$$

where the volume $V_o = \frac{4}{3}\pi r_o^3$ corresponds to the effective volume of the Fermi particle and N is the number of fermions.

The MD for fermions, having single-particle level degeneracy ν, is defined by

$$n(k) = \nu^{-1}\int \rho(r)e^{i\mathbf{k}\mathbf{r}}d\mathbf{r} \qquad (5)$$

The MD, normalized to 1 ($\int n(k)d\mathbf{k} = 1$), is given by the relation

$$n(k) = \frac{1}{V_k}\tilde{n}(k) = \frac{1}{V_k}\begin{cases} \tilde{n}_-(k), \ k < k_F \\ \tilde{n}_+(k), \ k > k_F \end{cases} \tag{6}$$

where $V_k = \frac{4}{3}\pi k_F^3$. The Fermi wave number k_F is related with the constant density $\rho = N\rho_0 = 3/(4\pi r_0^3)$ as follows

$$k_F = \left(\frac{6\pi^2\rho}{\nu}\right)^{1/3} = \left(\frac{9\pi}{2\nu}\frac{1}{r_0^3}\right)^{1/3} \tag{7}$$

where $\nu = 2$ for electron gas and liquid ^{3}He and $\nu = 4$ for nuclear matter. In the case of an ideal Fermi gas the MD has the form

$$n_0(k) = \frac{1}{V_k}\theta(k_F - k) \tag{8}$$

The information entropy in coordinate space (for density ρ_0 normalized to 1) for a correlated or uncorrelated Fermi system is given by the relation

$$S_r = -\int \rho_o \ln \rho_o d\mathbf{r} = \ln V. \tag{9}$$

Considering that $V = NV_o$, S_r becomes

$$S_r = \ln\left(\frac{4}{3}\pi r_o^3\right) + \ln N. \tag{10}$$

The information entropy in momentum space (for n(k) normalized to 1) is given by the relation

$$S_k = -\int n(k)\ln n(k)d\mathbf{k}. \tag{11}$$

S_k for an ideal Fermi gas, using Eq. (8), becomes

$$S_k = \ln V_k = \ln\left(\frac{6\pi^2}{\nu}\frac{1}{r_0^3}\right) \tag{12}$$

From Eq. (10) and (12) the information entropy sum $S = S_r + S_k$ for an uncorrelated infinite Fermi system becomes

$$S_0 = S_r + S_k = \ln\left(\frac{8\pi^3}{\nu}\right) + \ln N \tag{13}$$

It turns out that the functional form

$$S_0 = a + b \ln N$$

for the entropy sum as a function of the number of particles N holds for the ideal infinite Fermi systems. The same function has been found in Ref. [2] for atoms and in Ref. [8] for nuclei and atomic clusters. That expression has been found also in Ref. [11] for the ideal electron gas. It is well known that relation (1) ($S_r + S_k \geq 3(1 + \ln \pi)$) holds always. We found that for N large relation (13) holds. Relation (13) for $N = 1$ violates relation (1), but this is hardly a problem because (13) holds only for large N and we do not expect to agree with (1), e.g. relations holding for nuclear matter cannot lead to relations holding for finite nuclei with a few nucleons.

In the case of correlated Fermi systems, the IE in coordinate space is given again by Eq. (10) while the IE in momentum space can be found from Eq. (11) replacing $n(k)$ from Eq. (6). S_k is written now

$$S_k = \ln V_k - \frac{4\pi}{V_k}\left(\int_0^{k_F^-} k^2 \tilde{n}_-(k) \ln \tilde{n}_-(k) dk + \int_{k_F^+}^{\infty} k^2 \tilde{n}_+(k) \ln \tilde{n}_+(k) dk\right). \quad (14)$$

The correlated entropy sum has the form

$$S = S_r + S_k = S_0 + S_{cor} \quad (15)$$

where S_0 is the uncorrelated entropy sum of Eq. (13) and S_{cor} is the contribution of the particles correlations to the entropy sum. That contribution can be found from the expression

$$S_{cor} = -3\left(\int_0^{1^-} x^2 \tilde{n}_-(x) \ln \tilde{n}_-(x) dx + \int_{1^+}^{\infty} x^2 \tilde{n}_+(x) \ln \tilde{n}_+(x) dx\right), \quad (16)$$

where $x = k/k_F$.

Another quantity expected to be related with the IE is the mean kinetic energy K, defined by

$$K = \frac{\hbar^2}{2m}\int n(k) k^2 d\mathbf{k} = 3\epsilon_F \int_0^{\infty} x^4 \tilde{n}(x) dx$$

$$= 3\epsilon_F \left(\int_0^{1^-} x^4 \tilde{n}_-(x)dx + \int_{1^+}^{\infty} x^4 \tilde{n}_+(x)dx \right) \tag{17}$$

where $\epsilon_F = \hbar^2 k_F^2/(2m)$ is the Fermi energy.

From the above analysis it is clear that in order to calculate the IE sum in uniform Fermi systems, the knowledge of the MD is required.

In the present work we apply the low order approximation (LOA) for the calculation of the MD in nuclear matter [12–14]. For liquid ^{3}He we use the results of Moroni et al. [15], while the MD for the electron gas is taken from a work of P. Gori-Giorgi et al. [16].

2.1 Nuclear matter

The model we study is based on the Jastrow ansatz for the ground state wave function of nuclear matter

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \prod_{1 \leq i \leq j \leq N} f(r_{ij}) \Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \tag{18}$$

where $r_{ij} = \mid \mathbf{r}_i - \mathbf{r}_j \mid$, Φ is a Slater determinant (here, of plane waves with appropriate spin-isospin factors, filling the Fermi sea) and $f(r)$ is a state-independent two-body correlation function. In the present work the correlation function is taken to be the Jastrow function [17]

$$f(r) = 1 - \exp[-\beta^2 r^2] \tag{19}$$

where β is the correlation parameter. A cluster expansion for the one-body density matrix $\rho(\mathbf{r}_1, \mathbf{r}_1')$ has been derived by Gaudin, Gillespie and Ripka [12–14] for the Jastrow trial function (18).

In the LOA the momentum distribution is constructed as [14]

$$n_{LOA}(k) = \theta(k_F - k)\left[1 - k_{dir} + Y(k, 8)\right] + 8\left[k_{dir} Y(k, 2) - [Y(k, 4)]^2\right] \tag{20}$$

where

$$c_\mu^{-1} Y(k, \mu) = \frac{e^{-\tilde{k}_+^2} - e^{-\tilde{k}_-^2}}{2\tilde{k}} + \int_0^{\tilde{k}_+} e^{-y^2} dy + \mathrm{sgn}(\tilde{k}_-) \int_0^{|\tilde{k}_-|} e^{-y^2} dy \tag{21}$$

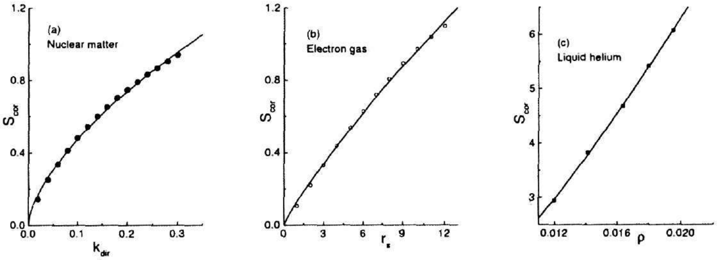

Fig. 1. The correlated part of the information entropy, S_{cor}, for nuclear matter (a), electron gas (b), and liquid ^{3}He (c) versus the wound parameter k_{dir}, the effective radius r_s, and the density ρ, respectively. The lines in the tree cases correspond to the fitted expressions $S_{cor}(k_{dir}) = sk_{dir}^{\lambda}$, $S_{cor}(r_s) = sr_s^{\lambda}$ and $S_{cor}(\rho) = s\rho^{\lambda}$, respectively. For the values of the parameters s and λ see text.

and

$$c_\mu = \frac{1}{8\sqrt{\pi}}\left(\frac{\mu}{2}\right)^{3/2}, \quad \tilde{k} = \frac{k}{\beta\sqrt{\mu}}, \quad \tilde{k}_\pm = \frac{k_F \pm k}{\beta\sqrt{\mu}}, \quad \mu = 2, 4, 8. \tag{22}$$

and $\mathrm{sgn}(x) = x/ \mid x \mid$. The normalization condition for the momentum distribution is

$$\int_0^\infty n_{LOA}(k)k^2 dk = \frac{1}{3}k_F^3 \tag{23}$$

A rough measure of correlations and of the rate of convergence of the cluster expansion is given by the dimensionless Jastrow wound parameter

$$k_{dir} = \rho \int [f(r) - 1]^2 d\mathbf{r} \tag{24}$$

where $\rho = 2k_F^3/(3\pi^2)$ is the density of the uniform nucleon matter.

The calculated values of S_{cor} for nuclear matter versus the wound parameter k_{dir} are displayed by points in Fig.1a. It is seen that S_{cor} is an increasing function of k_{dir}. The function $S_{cor}(k_{dir})$ is equal to zero for $k_{dir} = 0$ (no correlations) and the dependence of S_{cor} on k_{dir} is not very far from a linear dependence. Thus we fitted the numerical values of S_{cor} with the two parameters formula

$$S_{cor}(k_{dir}) = sk_{dir}^{\lambda} \tag{25}$$

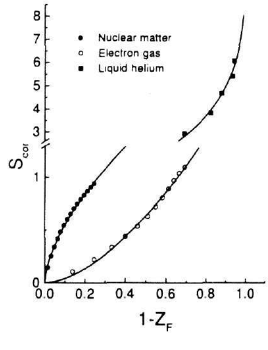

Fig. 2. The correlated part of the information entropy for nuclear matter, electron gas, and liquid ^{3}He versus the discontinuity parameter $1 - Z_F$. The lines in nuclear matter and electron gas correspond to the fitted expression $S_{cor}(Z_F) = s(1 - Z_F)^\lambda$ while in ^{3}He liquid to the fitted expression $S_{cor}(Z_F) = s(1 - Z_F^\lambda)$. For the values of the parameters s and λ see text.

That simple formula, with the best fit values of the parameters

$$s = 2.0575, \qquad \lambda = 0.6364$$

reproduces the numerical values of S_{cor} very well.

Another characteristic quantity which is used as a measure of the strength of correlations of the uniform Fermi systems is the discontinuity, Z_F, of the MD at $k/k_F = 1$. It is defined as

$$Z_F = n(1^-) - n(1^+).$$

For ideal Fermi systems $Z_F = 1$, while for interacting ones $Z_F < 1$. In the limit of very strong interaction $Z_F = 0$ there is no discontinuity on the MD of the system. The quantity $(1 - Z_F)$ measures the ability of correlations to deplete the Fermi sea by exciting particles from states below it (hole states) to states above it (particle states) [14].

The dependence of S_{cor} on the quantity $(1 - Z_F)$ is shown in Fig. 2. It is seen that S_{cor} is an increasing function of $(1-Z_F)$. For the same reasons mentioned before we fitted the numerical values of S_{cor} to the two parameters formula

$$S_{cor}(Z_F) = s(1 - Z_F)^\lambda \tag{26}$$

As before, the above simple formula, with the best fit values of the parameters

$$s = 2.2766, \qquad \lambda = 0.6164$$

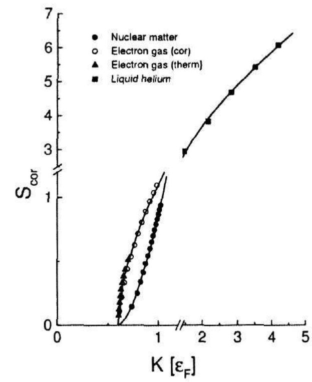

Fig. 3. The correlated part of the information entropy for various Fermi systems and its thermal part for electron gas versus the mean kinetic energy in units of Fermi energy. The lines in the various cases correspond to the fitted expression $S_{cor}(K) = s(\frac{K}{\epsilon_F} - 0.6)^{\lambda}$. For the values of the parameters s and λ see text.

reproduces the numerical values of S_{cor} very well.

From the above analysis we can conclude that the correlated part of the information entropy sum can be used as a measure of the strength of correlations in the same way the wound parameter and the discontinuity parameter are used.

An explanation of the above behaviour of S_{cor} is the following: The effect of nucleon correlations is the departure from the step function form of the MD (ideal Fermi gas) to the one with long tail behaviour for $k > k_F$. The diffusion of the MD leads to a decrease of the order of the system (in comparison to the ordered step function MD), thus it leads to an increase of the information content of the system.

Concluding we should state that, the increase of information entropy sum of the nuclear matter is due to the increase of the number of nucleons of the system, as it is seen from Eq. (13) and also to the increase of correlations.

Finally, the dependence of the IE on the kinetic energy K, which is given by Eq. (17), is also examined. The calculated values of the correlated part of IE, S_{cor}, versus K is shown in Fig. 3. S_{cor} is an increasing function of K. It should be noted that S_{cor} is equal to 0 for $K = \frac{3}{5}\epsilon_F$. For that reason we fitted the numerical values of S_{cor} to the formula

$$S_{cor}(K) = s\left(\frac{K}{\epsilon_F} - 0.6\right)^{\lambda}. \tag{27}$$

That simple formula, with the best fit values of the parameters

$$s = 3.7413, \qquad \lambda = 1.5911$$

reproduces the numerical values of S_{cor} very well.

2.2 Electron gas

We consider the electron gas as a system of fermions interacting via a Coulomb potential. The electron gas is a model of the conduction electrons in a metal where the periodic positive potential due to the ions is replaced by a uniform charge distribution. The density of the uniform electron gas (Jellium) is $\rho = 3/(4\pi r_o^3)$ and the momentum distribution is $n(x, r_s)$, where $x = k/k_F$ and $r_s = r_o/a_B$ (with $a_B = \hbar^2/me^2$, the Bohr radius).

The momentum distribution of the unpolarized uniform electron gas in its Fermi-liquid regime, $n(x, r_s)$ is constructed with the help of the convex Kulik function $G(\chi)$ [16]. It is assumed that $n(0, r_s)$, $n(1^{\pm}, r_s)$, the on-top pair density $g(0, r_s)$, and the kinetic energy $K(r_s)$ are known (respectively, from accurate calculations for $r_s = 1, \ldots, 5$, from the solution of the Overhauser model, and from quantum Monte Carlo calculations via the virial theorem) [16].

We examined the dependence of the correlated part of the IE for the electron gas on the correlation parameter r_s, (or $\rho = 3/(4\pi r_o^3)$), the discontinuity parameter $(1 - Z_F)$ and the mean kinetic energy K. The dependence of S_{cor} on those parameters are shown in Fig. 1b, 2, 3. It is seen that, as in the case of nuclear matter, S_{cor} depends on those quantities through two parameter expressions of the form

$$S_{cor}(r_s) = s r_s^{\lambda} \tag{28}$$

with

$$s = 0.1312, \qquad \lambda = 0.8648,$$

$$S_{cor}(Z_F) = s(1 - Z_F)^{\lambda} \tag{29}$$

with

$$s = 2.0381, \qquad \lambda = 1.6899$$

and

$$S_{cor}(K) = s\left(\frac{K}{\epsilon_F} - 0.6\right)^{\lambda} \tag{30}$$

with

$$s = 2.0786, \qquad \lambda = 0.6601.$$

The values of the parameters s and λ have been found by least squares fit of the above expressions to the calculated values of S_{cor}.

2.3 Liquid ^{3}He

The helium interaction potential is very strong at small distances, its core repulsion being very hard (but not infinite). As a consequence there is a Fermi-surface discontinuity of roughly $Z_F \sim 0.3$. This small value supports the view that liquid ^{3}He is the most strongly interacting Fermi system we have considered.

In the case of liquid ^{3}He the calculation of the momentum distribution is performed from diffusion Monte Carlo (DMC) simulations using trial functions, optimized via the Euler Monte Carlo (EMC) method [15].

As in the cases of nuclear matter and electron gas, we examined the dependence of the correlated part of the IE for the liquid ^{3}He on the density $\rho = 3/(4\pi r_o^3)$, the discontinuity parameter $(1 - Z_F)$ and the mean kinetic energy K. The dependence of those parameters are shown in Figures 1c, 2 and 3, respectively. As in the previous two cases, S_{cor} depends on those parameters through simple two parameter formulae of the form

$$S_{cor}(\rho) = s\rho^{\lambda} \tag{31}$$

with

$$s = 2032.56, \qquad \lambda = 1.4757$$

$$S_{cor}(Z_F) = s(1 - Z_F^{\lambda}) \tag{32}$$

with

$$s = 13.0640, \qquad \lambda = 0.2070$$

and

$$S_{cor}(K) = s\left(\frac{K}{\epsilon_F} - 0.6\right)^{\lambda} \tag{33}$$

with

$$s = 3.0993, \qquad \lambda = 0.5236.$$

The values of the parameters s and λ have been found by least squares fit of the above expressions to the calculated values of S_{cor}. The values of the parameters of expressions (31) and (32) indicate the strong character of the interaction of liquid ^{3}He. That character is also indicated by the expression of $S_{cor}(Z_F)$ (Eq. (32)). That expression differs from the corresponding expressions of the electron gas and nuclear matter.

3 Thermal effects in electron gas

The electrons of the electron gas, at temperature $T = 0$, occupy all the lower available states up to a highest one, the Fermi level. As the temperature increases the electrons of the gas tend to become excited into states of energy of order kT higher than the Fermi energy. However, the electrons with the lower energy cannot be excited as there are not available states for them to be excited. Only a small fraction of the gas, of order T/T_F, with energy about kT lower than the Fermi energy have any chance to be excited. The rest remain unaffected in their zero-degree situation. The net result is that the mean occupation number becomes slightly blurred compared to its sharp, step function form at $T = 0$ [18]. In general the occupation number of the electron gas is given by the Fermi-Dirac formula

$$n(\epsilon) = \frac{1}{\exp\left[\frac{1}{k_B T}(\epsilon - \mu)\right] + 1} \tag{34}$$

where $\epsilon = \frac{p^2}{2m}$ ($p = \hbar k$), k_B is the Boltzmann's constant and μ is the chemical potential. The chemical potential of a gas at absolute zero ($T = 0$) coincides with the Fermi energy ϵ_F. This is the characteristic energy for a Fermi gas and is by definition the energy of the highest single-particle level occupied at $T = 0$. The Fermi energy is given by the relation

$$\epsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2\rho\right)^{2/3} \tag{35}$$

while the Fermi temperature is defined by

$$\epsilon_F = k_B T_F \tag{36}$$

We will examine how the IE sum of the electron gas is affected when the temperature starts to increase above zero. Our study will include the cases of low temperature and high temperature limit, separately.

3.1 Thermal effects in electron gas for $T \ll T_F$

Since there is only one characteristic temperature, the Fermi temperature, by the term low energy we will mean the limit $T \ll T_F$. It is easy to see that for electron gas, i.e. in copper, $T_F \sim 8.5 \times 10^4$ ^{o}K, while the melting point is of the order of 10^3 ^{o}K. Thus, at all temperatures at which copper is a solid, the condition $T \ll T_F$ is satisfied; the electron gas is in its low-temperature limit. For $T \ll T_F$ the chemical potential, in a first approximation, is [18–20]

$$\mu = \epsilon_F \left[1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2\right] \tag{37}$$

and so Eq. (34) becomes

$$n(x) = \frac{1}{\exp\left[\frac{1}{\xi}\left(x^2 - 1 + \frac{\pi^2}{12}\xi^2\right)\right] + 1} \tag{38}$$

where $x = (\epsilon/\epsilon_F)^{1/2} = k/k_F$ and $\xi = T/T_F \ll 1$. The normalization of $n(x)$ is $\int_0^\infty x^2 n(x)dx = 1/3$.

Following the same steps as in Section 2, the information entropy sum of the electron gas at temperature $T \ll T_F$ is written

$$S = S_0 + S_{thermal} \tag{39}$$

where S_0 is given by Eq.(13) and

$$S_{thermal} = -3\int_0^\infty x^2 n(x) \ln n(x) dx \tag{40}$$

It is worthwhile to notice that the correlations between the fermi particles invoke discontinuity to the MD at $k = k_F$ while the thermal effect causes just

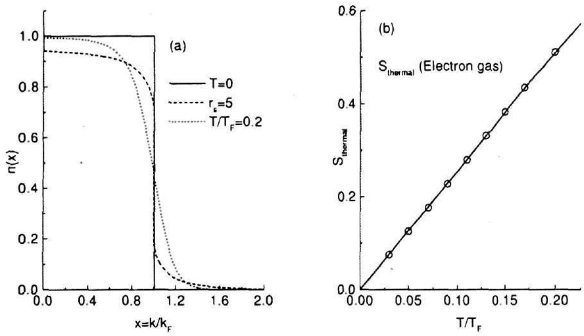

Fig. 4. a) The momentum distribution for correlated electron gas with effective radius $r_s = 5$ and the uncorrelated one for temperature $T = 0$ and $T = 0.2T_F$ versus the ratio $x = k/k_F$. b) The thermal part of the information entropy versus the temperature T in units of T_F.

a slight deviation from the sharp step function form at $T = 0$. That is shown in Fig. 4a, where the MD for a correlated electron gas with $r_s = 5$ and for an ideal electron gas at temperature $T = 0$ and $T/T_F = 0.2$ have been plotted versus k/k_F. The two cases of the figure ($r_s = 5$ and $T/T_F = 0.2$) give the same value for the information entropy. Thus, even though the origin of the two effects (correlations and temperature) is different and they influence in a different way the MD, the two information entropies S_{cor} and $S_{thermal}$ are almost the same.

The calculated values of $S_{thermal}$ for various values of the temperature (for $T \ll T_F$) are shown in Fig. 4b. It is seen that $S_{thermal}$ is an increasing function of the temperature and depends linearly on it. The line

$$S_{thermal} = \alpha \left(\frac{T}{T_F}\right), \qquad \alpha = 2.5466 \tag{41}$$

reproduces very well all the calculated values of $S_{thermal}$. That expression of the information entropy is similar to the expression which gives the thermodynamical entropy, S_{TE}, for $T \ll T_F$. S_{TE} in the low temperature limit has the form [18,20]

$$S_{TE} = \frac{\pi^2}{2} N k_B \frac{T}{T_F} \tag{42}$$

Comparing Eqs. (41) and (42), a relation between the two entropies could be found in the case $T \ll T_F$. That relation has the form

$$S_{thermal} = \frac{2\alpha}{\pi^2} \frac{S_{TE}}{Nk_B}, \qquad \alpha = 2.5466 \tag{43}$$

while the information entropy sum is written

$$S_{IE} = \ln N + \ln 4\pi^3 + \frac{2\alpha}{\pi^2} \frac{S_{TE}}{Nk_B} \tag{44}$$

Thus, the information entropy of a Fermi gas, which is a measure of the information content of the system, depends on the number of fermions as well as on the thermodynamical entropy of the system.

The increase of the temperature changes also the mean kinetic energy K of the ideal electron gas. For $T \ll T_F$, K is given by [20]

$$K = \frac{3}{5}\epsilon_F \left[1 + \frac{5}{12}\pi^2 \left(\frac{T}{T_F}\right)^2\right] \tag{45}$$

In the examined range of T, K changes about 15 %. As K appears both in correlated and uncorrelated Fermi systems, and a relation of the form $S_{cor} = S_{cor}(K)$ was already found in Sec. 2, it is of interest to examine the existence of a relation between $S_{thermal}$ and K.

That relation can be easily found writing Eq. (45) in the form

$$\frac{T}{T_F} = \frac{2}{\pi}\left(\frac{K}{\epsilon_F} - 0.6\right)^{1/2}$$

and replacing T/T_F into Eq. (41). The expression connecting $S_{thermal}$ and K is

$$S_{thermal} = s\left(\frac{K}{\epsilon_F} - 0.6\right)^{\lambda} \tag{46}$$

with

$$s = \frac{2a}{\pi} = 1.6212, \qquad \lambda = 0.5$$

Expression (46) is the same with the corresponding expression of $S_{cor}(K)$ which is given by Eq. (30). The values of the parameter s and λ ($s = 2.0786$

and $\lambda = 0.6601$) of Eq. (30) are close to the constants $s = 1.6212$ and $\lambda = 0.5$ of Eq. (46). For that reason we should expect that the same values of K corresponding either to the temperature or to the electron correlation lead to similar values for the two entropies $S_{thermal}$ and S_{cor}. The calculated values of $S_{thermal}$, for the uncorrelated Fermi gas, versus K are shown in Fig. 3. From that figure, it is seen that for the same values of K, $S_{thermal}$ and S_{cor} take similar values, as expected. From the above analysis it is seen that the information entropy sum and the thermal part of it are related with fundamental quantities, such as, the temperature, the thermodynamical entropy and the mean kinetic energy of the system.

3.2 *Thermal effects in electron gas for $T \gg T_F$*

A relation can also be established between the IE and the thermodynamical entropy in the classical case when it is assumed that $n(k) \ll 1$. That condition is valid when the density is low and/or the temperature is high. In that case the MD has the gaussian form [19]

$$n(k) = \left(\frac{a}{\pi}\right)^{3/2} e^{-ak^2}, \qquad a = \frac{\hbar^2}{2mk_BT} \tag{47}$$

and is normalized as $\int n(k)d\mathbf{k} = 1$. The thermodynamical entropy of the system is given by the relation [18,19]

$$\frac{S_{TE}}{Nk_B} = \ln V - \ln N + \frac{5}{2} + \frac{3}{2}\ln\frac{mk_BT}{2\pi\hbar^2} \tag{48}$$

Following the steps of Section 2, the information entropy sum for the above system is written

$$S_{IE} = \ln V + \frac{3}{2} + 3\ln 2\pi + \frac{3}{2}\ln\frac{mk_BT}{2\pi\hbar^2} \tag{49}$$

Comparing Eqs. (49) and (48) and using Eq.(13) a relation between S_{TE} and S_{IE} can also be found in the case $T \gg T_F$. That relation has the form

$$\begin{aligned} S_{IE} &= S_0 + (\ln 2 - 1) + \frac{S_{TE}}{Nk_B} \\ &= \ln N + (3\ln 2\pi - 1) + \frac{S_{TE}}{Nk_B} \end{aligned} \tag{50}$$

while the thermal part of the information entropy depends on S_{TE} through the relation

$$S_{thermal} = (\ln 2 - 1) + \frac{S_{TE}}{Nk_B} \tag{51}$$

Thus the information entropy sum as well the thermal part of it, in the limit $T \gg T_F$ depends also on the number of electrons as well as on the thernodynamical entropy of the system. Those relations are similar to the ones which have been found in the limit case $T \ll T_F$, only the two constants are different.

From Eqs. (51) and (48) a relation connecting $S_{thermal}$ with the temperature can be found. That relation has the form

$$S_{thermal} = \frac{3}{2} + \ln\frac{3\pi^{1/2}}{4} + \frac{3}{2}\ln\frac{T}{T_F} \tag{52}$$

Finally, from the well known result

$$K = \frac{\hbar^2}{2m}\int n(k)k^2 d\mathbf{k} = \frac{3}{2}k_B T \tag{53}$$

and Eq. (52) a relation connecting $S_{thermal}$ and K can be found. That relation has the form

$$S_{thermal} = \frac{3}{2} + \frac{1}{2}\ln\frac{\pi}{6} + \frac{3}{2}\ln\left(\frac{K}{\epsilon_F}\right) \simeq 1.1765 + \frac{3}{2}\ln\left(\frac{K}{\epsilon_F}\right) \tag{54}$$

We can conclude that, at the classical limit, the IE as well as its thermal part is related to S_{TE}, T and K, as in the low temperature limit.

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