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MOMENTUM DISTRIBUTION OF NON-INTERACTING FERMIONS ENCLOSED IN A BOX

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ABSTRACT

We study the finite size effect on the momentum distribution $n(\vec{k})$ of an ensemble of A non-interacting fermions enclosed in a box. Analytical expressions are obtained in the two limiting cases $\frac{k}{k_F} \gg 1$ and $\frac{k}{k_F} \ll 1$ (k_F being the Fermi momentum). It allows us to analyze the convergence of $n(\vec{k})$ toward the standard step function in the infinite medium. Applying our results to the nuclear case, we compare the changes in $n(\vec{k})$ generated by the finite size of actual nuclei to those due to short range correlations. Both effects are shown to be of same order of magnitude. The next step should be to take into account the short range correlations directly in finite systems.

1. INTRODUCTION

The nuclear interaction is responsible for the departure of the actual distribution of momentum in the nuclei $n(\vec{k})$ from the step function limit $\theta(k-k_F)$ (case of the uncorrelated nuclear matter). In first approximation the effect of the interaction can be divided into two parts i) a selfconsistent average field ; ii) the short range correlations (SCR). In a further simplification one can i) mock up the average field by confining non-interacting nucleons inside a Hill and Wheeler box of length a and ii) simulate the SCR by replacing the point particles by hard spheres of core radius c. By doing so, one can get analytical expansions of $n(\vec{k})$, the small parameters being respectively $(ak_F)^{-1}$ and ck_F. In this work

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we will first calculate $n(\vec{k})$ for free point particles in a box, then derive simple expressions in the two limiting cases $\frac{k}{k_F} \ll 1$ and $\frac{k}{k_F} \gg 1$. The structure of our formulae resembles that of Belyakov [1] who has calculated n(k) for a gas of hard spheres ; we are then able to compare the role of the finiteness of the nuclei to that of the finiteness of the nucleons.

2. BACKGROUND AND NOTATIONS

The particles move freely inside an infinite cubic potential well. The individual wave functions are

$$\begin{aligned} \Psi_{\ell mn} &= \varphi_\ell(x)\varphi_m(y)\varphi_n(z) \\ \varphi_\ell(x) &= \sqrt{\frac{2}{a}}\sin \pi \frac{\ell}{a} x \qquad 0 < x < a \\ \varphi_\ell(x) &= 0 \qquad \text{otherwise} \end{aligned} \tag{1}$$

Like in the r-space, the Fourier transform of the wave functions can be factorized. Therefore the momentum distribution is

$$\rho(\vec{k}) = \sum_{\ell,m,n} \left|\tilde{\varphi}(k_x)\right|^2 \left|\tilde{\varphi}_m(k_z)\right|^2 \left|\tilde{\varphi}_n(k_z)\right|^2 . \tag{2}$$

In the ground state, the summation entering (2) runs for ℓ, m and n positive integers , with the condition $\ell^2 + m^2 + n^2 < N$. N and E (the energy of the A particles of the system) are related by

$$E = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\sum_{\ell mn}(\ell^2 + m^2 + n^2) \tag{3}$$

The energy of the last particle being $\frac{\hbar^2}{2m}\frac{\pi^2}{a^2} N$, it is natural to define the Fermi momentum by

$$k_F = \frac{\pi}{a}\sqrt{N} . \tag{4}$$

Let us now relate N to the number of states A (we assume one particle for each state). Eq.(3) identifies A with the number of points of integer coordinates inside the octant of the sphere of radius $\sqrt{N}$. For large N

$$A \approx \frac{1}{8}\frac{4}{3}\pi(\sqrt{N})^3 \quad . \tag{5}$$

The precise counting is known as the lattice remainder problem [2] and surface and curvature terms can be obtained.

To deal with dimensionless quantities we introduce $\vec{\kappa} = \frac{\vec{k}}{k_F}$ (κ will stand for $|\vec{\kappa}|$) and replace $\rho(\vec{k})$ by $n(\vec{\kappa}) = \frac{\rho(\vec{k})}{\rho_o}$ where $\rho_o = (\frac{a}{2\pi\hbar})^3$. In the thermodynamic limit (a and $A \to \infty$ with a finite matter density)

$$\begin{aligned} n(\vec{\kappa}) &= 1 \qquad && \kappa < 1 \\ &= 0 && \kappa > 1 \quad . \end{aligned} \tag{6}$$

3. RESULTS

We are interested in understanding how $n(\vec{\kappa})$ tends to its limit (6). For sake of simplicity let us explain the calculation when $\kappa = 0$. In that case, it is easy to show that

$$\begin{aligned} \left|\tilde{\varphi}_\ell(\rho)\right|^2 &= \frac{4a}{\pi^3\hbar}\ \frac{1}{\ell^2} \qquad , \quad && \ell \text{ odd} \\ &= 0 \qquad , && \ell \text{ even} \end{aligned} \tag{7}$$

Therefore $n(0)$ reduces to $(\frac{8}{\pi^2})^3 \sum \frac{1}{\ell^2 m^2 n^2}$ with ℓ,m and n being odd. The result is

$$\sum \frac{1}{\ell^2 m^2 n^2} = (\frac{\pi^2}{8})^3 \left[1 - \frac{12}{\pi^2\sqrt{N}} + \dots \right]$$

One cannot derive compact formula for any κ , but in the two limiting cases $\kappa \ll 1$ and $\kappa \gg 1$. After some straightforward if tedious calculations one can write, up to first order in $(ak_F)^{-1}$ and κ^2

$$n(\vec{\kappa}) = 1 - \frac{12}{\pi}(ak_F)^{-1}\ (1 + \frac{5}{9}\kappa^2) \qquad \kappa \ll 1 \tag{8}$$

For $\kappa \gg 1$, the distribution is highly anisotropic (and depends on the shape of the potential). For instance, in the cube,

$$n(\vec{\kappa}) = \left(\frac{2}{\pi}\right)^5 \frac{1}{945} \left[\pi\,(ak_F)^{-1}\right]^3 \quad \frac{1}{(\kappa_x\,\kappa_y\,\kappa_z)^4} \qquad \kappa_q \gg 1 \quad q=1,2,3 \tag{9}$$

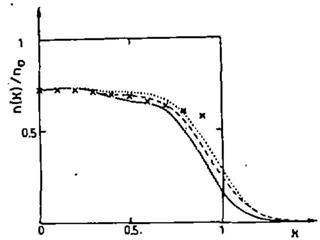

FIG.1 - $n(\vec{\kappa})$ as function of κ in the cubic case (A=26). The full line corresponds to $\kappa_x = \kappa_y = \kappa_z = \frac{\kappa}{\sqrt{3}}$, the dashed line to $\kappa_y = \kappa_z = \frac{\kappa}{\sqrt{2}}$ and $\kappa_x = 0$, the dotted line to $\kappa_x = \kappa_y = 0$ and $\kappa_z = \kappa$. The approximation (8) is represented by the crosses.

4. DISCUSSION

4.1 Role of the shape of the infinite well

We have replaced the cubic shaped domain by a parallelepipedic or a spherical one and shown that $n(0)$ is still given by eq.(8) provided that the size of the cube, a, is replaced by $6\frac{V}{S}$ (V and S are the volume and the surface of the box). Therefore we believe that eq.(8) holds for $\kappa = 0$ irrespective of the shape of the domain. Now for large values of κ , the behaviour of $n(\vec{\kappa})$ is strongly affected by the shape of the potential. In contrast to the cubic case, for instance, in a spherical potential (all magnetic substates being filled) $n(\vec{\kappa})$ is spherical symmetric and decreases to zero like $\frac{1}{\kappa^6}$.

4.2 Role of the depth of the potential

We have obtained analytical formulae in the case of a finite square potential in one dimension. As expected, if the well is far from being filled, the situation resembles that of the infinite case. Now when all the bound states are occupied, $n(\vec{\kappa})$ shows large shell oscillations and, on the average, $n(0)$ increases while the plateau for $\kappa < 1$ is decreasing more rapidly. We believe that the same trend remains true in 3 dimensions.

5. COMPARISON WITH THE EFFECTS DUE TO THE SCR

The momentum distribution has been calculated by Belyakov [1] in a gas of hard spheres. By expanding his formula up to the first order, one finds

$$n^c(\kappa) \approx 1 - \frac{\nu-1}{3}\, 0.40\, (ck_F)^2 \, [1 + 1.07 \, \kappa^2] \quad \kappa << 1 \qquad (10)$$

ν is the spin-isospin degeneracy ($\nu = 4$ for symmetric nuclear matter) which plays here a key role.

In the nuclear case $ck_F \approx 0.7$ and $(ak_F)^{-1}$ varies from 0.12 to 0.052 from A = 16 to A = 108. From eqs.(8) and (10) one sees that both finite size effects are of the same order of magnitude.

Concerning the energy per particle, for point particles in a box

$$\frac{E/A}{(E/A)_o} = 1 + \frac{3}{8} \left(\frac{ak_F}{\pi}\right)^{-1} + \ldots \qquad (11)$$

for the hard sphere gas

$$\frac{E/A}{(E/A)_o} = 1 + \frac{10}{3} \left(\frac{ck_F}{\pi}\right) \frac{\nu - 1}{3} + \ldots \qquad (12)$$

where $(E/A)_o = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2$.

Although similar, both formulae have different meanings : the first corrective term of (12) is generated by the (pseudo) potential, whereas it is of course of kinetic origin in eq.(11). In the infinite medium the SCR produce an increase of 75 % of the energy while in nuclei the finite size effect on E/A varies from 29 % to 12 % from light to heavy nuclei.

Despite its schematic character, our study can help disentangle the various effects entering the actual n(k) : i) the finite size effect smoothly varying with A, ii) the shell effects caused by the filling of the orbits, iii) the SCR effects. An interesting extension of this work is to consider SCR directly in finite system within the same framework, using the technique of the pseudo potential [3].

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6. REFERENCES

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