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LETTER TO THE EDITOR

Form of first-order density matrix for jellium near to the diagonal

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Abstract. Kimball's work on the momentum distribution of electrons is utilized to establish the form of the expansion of the first-order density matrix for jellium around the diagonal. There is non-analytic behaviour and the connection between the present result and the analytic form for non-interacting electrons is established.

In a very recent paper Kimball (1975) has pointed out that for any system of non-relativistic electrons and nuclei, the large-wavevector limit of the momentum distribution $n(k)$ is proportional to k^{-8}.

We consider in this letter the implications of this for the form of the first-order density matrix $\gamma(\boldsymbol{r}, \boldsymbol{r}')$ for the special case of jellium, near to the diagonal. Our starting point is the form of γ for non-interacting fermions in a volume Ω, namely

$$\gamma_{\text{free}}(\boldsymbol{r}, \boldsymbol{r}') = \frac{2}{\Omega} \sum_{k<k_f} \exp\left[i\boldsymbol{k} \cdot (\boldsymbol{r}-\boldsymbol{r}')\right] \tag{1}$$

k_f being the Fermi momentum. Replacing the summation by an integration, we have the well known result

$$\gamma_{\text{free}}(\boldsymbol{r}, \boldsymbol{r}') = \frac{k_f^3}{\pi^2} \frac{j_1(k_f|\boldsymbol{r}-\boldsymbol{r}'|)}{k_f|\boldsymbol{r}-\boldsymbol{r}'|} \qquad j_1(x) = \frac{\sin x - x\cos x}{x^2}. \tag{2}$$

Expanding this result around the diagonal we find

$$\gamma_{\text{free}}(\boldsymbol{r}, \boldsymbol{r}') = \frac{k_f^3}{3\pi^2}\left(1 - \frac{k_f^2 R^2}{10} + \frac{k_f^4 R^4}{280} + O(R^6)\right) \tag{3}$$

where we have written $R = |\boldsymbol{r}-\boldsymbol{r}'|$.

But when we turn to interacting jellium, $n(k)$ is no longer 1 inside k_f and zero outside, since the interactions lead to occupation of momentum space outside k_f and the first-order density matrix is given by

$$\gamma(\boldsymbol{r}, \boldsymbol{r}') = \frac{2}{8\pi^3} \int n(k)\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\, d\boldsymbol{k} \qquad \int n(k)\, d\boldsymbol{k} = \tfrac{4}{3}\pi k_f^3 \qquad k_f r_s = (9\pi/4)^{1/3}, \tag{4}$$

where we have introduced the usual jellium interparticle spacing r_s in the last part of (4).

We now use Kimball's result that for large k

$$n(k) = Bg(0, r_s)/k^8 \tag{5}$$

where he has determined the quantity B and $g(r, r_s)$ is the jellium pair function for the interacting system at the appropriate density. Known Fourier transform theory (see, for example, Lighthill 1958) now tells us that the asymptotic result (5) heralds a term proportional to R^5 in the expansion of γ in equation (4) about its diagonal. Hence, for the interacting case, equation (3) must be modified to read

$$\gamma(r, r') = \frac{k_f^3}{3\pi^2}(1 + t_2(r_s)R^2 + t_4(r_s)R^4 + t_5(r_s)R^5 + O(R^6)). \tag{6}$$

The physical significance of the quantity $t_2(r_s)$ is that, essentially, it measures the kinetic energy per electron (cf equation (3) for non-interacting electrons) while Kimball's result (5) leads us to conclude that $t_5(r_s)$ represents the zero-range correlations in the electron assembly. Explicitly, from equations (4)–(6) we find

$$t_5(r_s) = -\frac{Bg(0, r_s)\pi}{480k_f^3}. \tag{7}$$

The physical significance of $t_4(r_s)$ is merely its relation to the fourth moment of $n(k)$. Having established the form (6) the rest of this letter is concerned with what we can learn about the quantities t_2, t_4 and t_5 in limiting cases. We begin with the high-density limit.

Small-r_s limit. In this limit of small r_s, the many-body perturbation theory of Gell-Mann and Brueckner (1957) leads to the total energy E which can be combined with the virial theorem to yield the kinetic energy (March 1958). Hence $t_2(r_s)$ is readily obtained as

$$t_2(r_s) = -\frac{k_f^2}{10}\left(1 - \frac{A \ln r_s}{\bar{E}_f} - \frac{A + C}{\bar{E}_f} + \ldots\right) \tag{8}$$

where we have written $\bar{E}_f$ for the mean Fermi energy $2{\cdot}21/r_s^2$. The constants A and C were determined by Gell-Mann and Brueckner as $A = (2/\pi^2)(1 - \ln 2)$ and $C = -0{\cdot}096$ respectively.

The form of t_4 as $r_s \to 0$ is immediately obtained in lowest order as $k_f^4/280$ by comparing equations (6) and (3). Also to lowest order we find t_5 from equation (7) by using (subscript FH stands for Fermi hole)

$$g_{FH}(R) = 1 - \frac{9}{2}\left(\frac{j_1(k_f R)}{k_f R}\right)^2 \qquad g_{FH}(0, r_s) = \tfrac{1}{2}. \tag{9}$$

From this form plus equation (5), it can be readily shown that if we use new variables $k_f R$ and r_s in equations (6) and (3), then the term involving t_5 in equation (6) tends to zero as r_s tends to zero and we have established the connection of (6) with the non-interacting case.

Large-r_s limit. It seems of some interest to discuss the off-diagonal form of γ in the large-r_s limit; that is beyond the Wigner transition. Here, it is certain that for sufficiently large r_s, $t_2(r_s) \sim r_s^{-3/2}$. If the first-order density matrix is constructed approximately from the Wigner harmonic oscillator orbitals, then we find (see Care and March 1975)

$$\gamma(r, r') = \frac{k_f^3}{3\pi^2} \exp\left(-\frac{R^2}{4r_s^{3/2}}\right). \tag{10}$$

The change from oscillatory behaviour in (2) to real exponential decay in (10) is due to

the fact that the discontinuity in $n(k)$ at k_f has disappeared following Wigner crystallization. The approximate form (10) suggests that $t_4 \backsim r_s^{-3}$ as r_s tends to infinity. Using the same Wigner orbitals to build the pair function $g(r)$, the value $g(r = 0, r_s)$ is simply determined by the tails of these orbitals from the Wigner body-centred cubic lattice sites leaking into the origin and $g(0, r_s)$ is expected to decrease exponentially as r_s increases. Thus, for most practical purposes, we anticipate that t_5 will be numerically unimportant in the Wigner regime.

In summary, the first-order density matrix of interacting jellium has been established as having the form (6) near the diagonal. The properties of the coefficients $t_2(r_s)$, $t_4(r_s)$ and $t_5(r_s)$ are known precisely in certain limits.

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