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Generalized Fermi sea for plane-wave Hartree-Fock theory: One dimensional model calculation

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The Hartree-Fock theory for many fermions with plane-wave orbitals but with abnormal occupation is studied. A one-dimensional problem with an interparticle interaction of finite range which saturates the N body system at a fixed density and finite binding energy is solved explicitly. A direct variation of the resulting Hartree-Fock energy with respect to the additional variational parameters introduced is carried out numerically and results reminiscent of a gas-to-liquid phase transition are found.

[NUCLEAR STRUCTURE plane-wave Hartree-Fock; model calculation; nuclear matter.]

I. INTRODUCTION

The exact solution, analytically or numerically, of an N-fermion problem with realistic interparticle interactions is apparently still far away. Two general microscopic approaches to the problem exist: (1) variational,[1] of the Jastrow-type, Fermi-hypernetted-chain approximation methods, etc., and (2) perturbation theory,[2] based mainly on diagrammatic methods of the "ladder," "ring," or other infinite partial summations.

Both of these general approaches begin with an assumed unperturbed one-particle state, about which one then perturbs in one manner or another. The usual such state is a single Slater determinant of plane-wave one-particle "orbitals" with occupied $\vec{k}$ vectors spanning a sphere (the "Fermi sphere") in $\vec{k}$ space. As a Slater determinant of plane waves is a Hartree-Fock (HF) state *regardless of which N single-particle states are occupied*, we wish to examine the possibility of achieving a "better" (i.e., stabler or lower-energy) HF state, with a different (or "abnormal") occupancy of the plane-wave orbitals.

II. DEFINITION OF THE PROBLEM: ANY DIMENSIONALITY

The Hartree-Fock (HF) approximation for the ground state consists in writing, for the ground state of the N-particle Hamiltonian,

$$H=\sum_{i=1}^{N} T_i+\sum_{i<j}^{N} v_{ij}, \quad T_i \equiv -\frac{\hbar^2}{2m}\nabla_i{}^2, \tag{1}$$

a *single* Slater determinant

$$\begin{aligned}&\Phi_0=(N!)^{-1/2}\det_{n_k}[\varphi_k(x_i)],\\ &n_k=0 \text{ or } 1,\\ &\sum_k n_k=N,\end{aligned} \tag{2}$$

of as yet unknown single-particle orbitals $\varphi_k(x_i)$, labeled by the state index k which takes on N different values. The *occupation* in that determinant is, of course, specified by the set of numbers (of value 0 or 1) n_k called the "occupation numbers." Extremizing[3] the expectation value of (1) with (2), with respect to the functions $\varphi_k(x_i)$, and subject to the restriction that these functions be normalized during the variation finally leads to the N coupled, nonlinear, integro-differential HF equations for the unknown orbitals $\varphi_k(x_i)$:

$$\begin{aligned}T_i\varphi_k(x_1)&+\sum_l n_l\int dx_2\,|\varphi_l(x_2)|^2 v_{12}\varphi_k(x_1)\\ &-\sum_l n_l\int dx_2\varphi_l^*(x_2)v_{12}\varphi_l(x_1)\varphi_k(x_2)=\epsilon_k\varphi_k(x_1),\end{aligned} \tag{3}$$

where the N Lagrange multipliers ϵ_k play the role of eigenvalue energies, and where the occupation numbers of the problem *have been explicitly displayed*.

Placing the N particles in a box of "volume" V and applying periodic boundary conditions to this box along all "d" dimensions then, providing that the range of $(v_{12}) \ll V^{1/d}$ (a condition easily fulfilled by taking a large enough box) and if v_{12} is independent of the center of mass of the particle pair (1,2), one can easily show that the N orbitals

$$\varphi_k(x_1)=V^{1/2}e^{ikx_1}, \quad kx_1\equiv\vec{k}\cdot\vec{x}_1 \tag{4}$$

allowed to exist by the nonzero values of the relevant set n_k do indeed satisfy the HF equations (3). This is true *regardless* of what the set n_k is, subject only to the restrictions (2). Thus the n_k may be treated as separate variational parameters to find that set giving the *lowest* value for the HF energy,

$$E=\langle\Phi_0|H|\Phi_0\rangle$$
$$=\sum_k n_k\langle k|T_1|k\rangle$$
$$+\tfrac{1}{2}\sum_{k_1k_2} n_{k_1}n_{k_2}\langle k_1k_2|v_{12}|k_1k_2-k_2k_1\rangle . \tag{5}$$

In the present case "direct" and "exchange" matrix elements, respectively, are

$$\langle k_1k_2|v_{12}|k_1k_2\rangle \equiv V^{-2}\int_V dx_1\int_V dx_2\, e^{-ik_1x_1}e^{-ik_2x_2}v_{12}\times e^{ik_1x_1}e^{ik_2x_2}$$
$$=V^{-2}\int_V dx_1\int_V dx_2\, v_{12}$$
$$=V^{-1}\int dx\, v(x) , \tag{6}$$

$$\langle k_1k_2|v_{12}|k_2k_1\rangle \equiv V^{-2}\int_V dx_1\int_V dx_2\, e^{-ik_1x_1}e^{-ik_2x_2}v_{12}\times e^{ik_2x_1}e^{ik_1x_2}$$
$$=V^{-1}\int dx\, e^{-i(k_1-k_2)x}v(x) , \tag{7}$$

assuming that the interaction potential v_{12} is local. Writing the total HF energy as

$$E=\langle T\rangle+\langle v\rangle_D-\langle v\rangle_E \tag{8}$$

then

$$\langle v\rangle_D=\tfrac{1}{2}V^{-1}\int dx\, v(x)\Big(\sum_k n_k\Big)^2$$
$$=\tfrac{1}{2}N^2V^{-1}\int dx\, v(x) \tag{9}$$

regardless of what set of n_k's are used, subject only to (2).

The usual (or *normal*) set of n_k's employed are

$$n_k^0=\theta(k_0-|k|) , \tag{10}$$

which define the normal Fermi sea of "size" (length, radius, etc.) k_0 which determines the particle density of the system since

$$N=\sum_k n_k^0 \xrightarrow[\text{large } V]{} \frac{V}{(2\pi)^d}\int d^dk\, \theta(k_0-|k|) ,$$
$$\rho=\frac{N}{L}=(k_0/\pi)(\text{for one dimension}) . \tag{11}$$

The (normal) occupation number set (10), of course, gives the (absolute) minimum of the kinetic energy of the system, i.e., its ground state, and the Rayleigh-Ritz variational principle would give for *any* other set n_k the bound

$$\langle T\rangle_{n_k}\geq\langle T\rangle_{n_k^0}=\frac{\hbar^2}{2m}\Big(\sum_k n_k^0\Big)^{-1}\int d^dk\, k^2\theta(k_0-|k|)$$
$$=\frac{\hbar^2k_0^{\,2}}{6m} , \tag{12}$$

the last result being for $d=1$, and where $\langle k|T_1|k\rangle=\hbar^2k^2/2m$ was used.

Since from (12) the *normal* n_k^0 (10) minimizes the energy for the noninteracting N particle system, the question we address is whether one can find an *abnormal* $n_k\neq n_k^0$ which minimizes the (HF) energy, but within the plane waves (PW) orbital picture, of a *fully interacting system*, and gives a *lower* HF energy than the n_k^0 case would give. Obviously, this could only be accomplished by the "exchange," since

$$\langle v\rangle_{E,n_k}\neq\langle v\rangle_{E,n_k^0} \tag{13}$$

and since from (9)

$$\langle v\rangle_{D,n_k}=\langle v\rangle_{D,n_k^0} . \tag{14}$$

Clearly, the single-particle density

$$\rho(x)=\sum_k|\varphi_k(x)|^2n_k=N/V \tag{15}$$

would be space independent, or homogeneous, regardless of what the set n_k is, subject only to (2).

We finally note that for such a lower-energy, PW-HF state to be found, the two-particle potential *must* be finite-ranged, for if $v_{12}=v_0\delta(x_{12})$, and one has g species of fermions, one easily sees from (7) and (5) that

$$\langle v\rangle_{E,n_k}=g^{-1}\langle v\rangle_{D,n_k} , \tag{16}$$

so that using (14) one has *no dependence with* n_k in the total potential energy expectation value, and in view of (12) one finally arrives, in this case, at

$$E_{n_k}\geq E_{n_k^0} . \tag{17}$$

We must thus look to finite-range interactions.

III. ILLUSTRATION OF THE PROBLEM: ONE-DIMENSIONAL MODEL

Although a desired goal is to know the set n_k which minimizes the PW-HF energy of a *three*-dimensional system of particles interacting via *realistic* potentials, this undertaking is best preceded by an example simple enough so as to minimize heavy numerical work which often obscures the problem. For this purpose we propose a one-dimensional problem which has several realistic features: (a) It has a finite-range interaction, (b) the interaction is capable of *two*-body bound states, (c) the exact (so far unknown) N-body ground state is a self-bound condensed system which, moreover, (d) does *not* collapse, and thus (e) *saturates* at some fixed density. These properties make the model at least a suggestive one for studying numerous physical systems such as nuclear matter, liquid helium, liquid metals, etc.

We consider a one-dimensional system of N spinless ($g=1$) fermions in a box of length L (with periodic boundary conditions), with Hamiltonian given by (1) where ($x \equiv x_1 - x_2$)

$$v(x) = v_0 e^{-|x|/\gamma} \cos \bar{k}x, \quad v_0, \gamma, \bar{k} \geq 0 \tag{18}$$

which for sufficiently large v_0 will be capable of supporting a two-body bound state. The Fourier transform of (18) is then

$$\begin{aligned}\nu(q) &\equiv \int_{-\infty}^{\infty} dx\, e^{-iqx} v(x) \\ &= \gamma v_0 \{[\gamma^2(q-\bar{k})^2 + 1]^{-1} + [\gamma^2(q+\bar{k})^2+1]^{-1}\} \\ &\geq 0 \quad \text{for all } q\,.\end{aligned} \tag{19}$$

This condition, together with the fact that $v(0) \equiv v_0 < \infty$ (for finite v_0), allows the establishment[4] of a rigorous *lower* bound to the exact energy per particle of the system (for any d, in fact) given by

$$E_{\text{exact}}/N \geq C_d \rho^{2/d} + \tfrac{1}{2}\rho\nu(0) - \tfrac{1}{2}v(0), \quad C_1 \equiv \frac{\hbar^2\pi^2}{6m} \tag{20}$$

which ensures against collapse.

Next we propose a specific (abnormal) functional form for n_k given by

$$\begin{aligned} n_k &= \theta(\beta k_0 - |k|) + \theta(\alpha k_0 - |k|)\theta(|k| - (\alpha+\beta-1)k_0)\,, \\ \alpha &\geq 1, \quad 0 \leq \beta \leq 1, \quad \theta(x) \equiv \tfrac{1}{2}(1+\operatorname{sgn} x)\,,\end{aligned} \tag{21}$$

which becomes n_k^0 for $\alpha = \beta = 1$ and which is compared with the normal n_k^0 in Fig. 1. It clearly satisfies the conditions in (2). The parameters α and β will be additional variational parameters. This functional form ensures that n_k and n_k^0 will have the same particle density for fixed k_0.

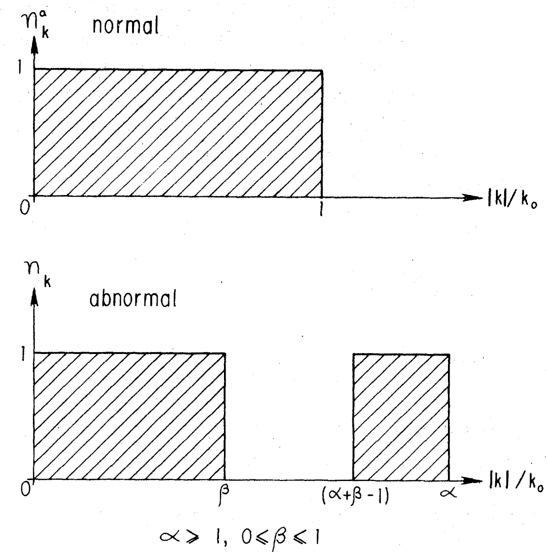

FIG. 1. "Normal" Fermi sea in one dimension (above) Eq. (10) and "abnormal" generalization thereof considered in this paper Eq. (21) (below), where the parameters α and β are to be varied numerically.

The kinetic energy will thus become, after simple integrations,

$$\langle T\rangle_{n_k} = N\frac{\hbar^2 k_0^2}{6m}[\alpha^3 + \beta^3 - (\alpha+\beta-1)^3]\,. \tag{22}$$

The "direct" potential energy, on the other hand, is

$$\langle v\rangle_{D,n_k} = N\tfrac{1}{2}\rho\nu(0) = N\rho\gamma v_0[\gamma^2\bar{k}+1]^{-1} \tag{23}$$

independent of α and β.

The calculation for the "exchange" potential energy is lengthy and tedious, though direct and analytical: It involves essentially integrals such as (a, b, c, and $d \equiv$ constants)

$$\int_a^b dk_1 \int_c^d dk_2 [\gamma^2(k_1 - k_2 \pm \bar{k})^2 + 1]^{-1} = \gamma^{-1}\int_a^b dk_1 [\tan^{-1}\gamma_y]_{k_1-c\pm\bar{k}}^{k_1-d\pm\bar{k}}\,,$$

TABLE I. Definitions of constants ω_i and functions f_i.

i	1	2	3	4	5	6	7	8	9
ω_i	−1	2	−2	−2	2	2	−1	−1	−2
f_i	2β	$\beta-\alpha$	$\beta+\alpha$	$1-\alpha$	$\alpha+2\beta-1$	$2\alpha+\beta-1$	$2(\alpha+\beta-1)$	2α	$\beta-1$

which in turn can be reduced to integrals such as ($K \equiv$ constant)

$$\int_{a-K\pm\bar{k}}^{a-K\pm\bar{k}} dz \tan^{-1}\gamma z = \left[z \tan^{-1}\gamma z - \frac{1}{2\gamma}\ln(1+\gamma^2 z^2)\right]_{a-K\pm\bar{k}}^{b-K\pm\bar{k}} .$$

One finally has

$$N^{-1}\langle v\rangle_{E,n_k} = -\frac{v_0\bar{k}}{4\pi k_0}\left(6\tan^{-1}\gamma\bar{k} - \frac{3}{\gamma\bar{k}}\ln(1+\gamma^2\bar{k}^2) + \sum_{i=1}^{9}\omega_i\left\{\left(\frac{k_0}{\bar{k}}f_i+1\right)\tan^{-1}\gamma\bar{k}\left(\frac{k_0}{\bar{k}}f_i+1\right) + \left(\frac{k_0}{\bar{k}}f_i-1\right)\tan^{-1}\gamma\bar{k}\left(\frac{k_0}{\bar{k}}f_i-1\right) - \frac{1}{2\gamma\bar{k}}\ln\left[1+\gamma^2\bar{k}^2\left(\frac{k_0}{\bar{k}}f_i+1\right)^2\right]\left[1+\gamma^2\bar{k}^2\left(\frac{k_0}{\bar{k}}f_i-1\right)^2\right]\right\}\right), \tag{24}$$

where the constants ω_i and functions f_i are defined in Table I.

For $\alpha = 1 = \beta$ we have $n_k = n_k^0$, and

$$N^{-1}\langle v\rangle_{E,n_k^0} = -\frac{v_0}{4\pi\gamma}\left\{2\bar{k}\tan^{-1}\gamma\bar{k} - (2k_0+\bar{k})\tan^{-1}\gamma(2k_0+\bar{k}) - (2k_0-\bar{k})\tan^{-1}\gamma(2k_0-\bar{k}) + \frac{1}{2\gamma}\ln\frac{[1+\gamma^2(2k_0+\bar{k})^2](1+\gamma^2 2k_0-\bar{k})}{(1+\gamma^2\bar{k}^2)^2}\right\} . \tag{25}$$

Putting Eqs. (22), (23), and (24) together one finally has the explicit function

$$\epsilon(\alpha,\beta;v_0,\gamma,\bar{k};k_0) \equiv E/N \geq E_{\text{exact}}/N , \tag{26}$$

which is a rigorous *upper* bound to the exact energy per particle of the problem.

Before proceeding to the numerical analysis of Eq. (26) let us note its large and small density behavior. For large k_0 one can verify, using the sum rule $\sum_{i=1}^{9}\omega_i f_i = -2$, that

$$N^{-1}\langle v\rangle_{E,n_k} \xrightarrow[k_0\to\infty]{} \tfrac{1}{2}v_0 + O(1/k_0) \tag{27}$$

independent of α and β, just as is $\langle v\rangle_{D,n_k}/N$. Hence, the minimum of (26) with respect to α,β at high density is just, from Eq. (22), the $\alpha=\beta=1$ total energy per particle. Since this, also being an upper bound, is identical with the lower bound Eq. (20), the exact energy per particle for the system is known exactly. [Indeed, this occurs[2] for any N-fermion system whose interparticle interaction satisfies the quite general restrictions (i) $|v(0)| < \infty$ and (ii) $\nu(q) \geq 0$ for all q.] For small k_0, on the other hand, one must Taylor-expand Eq. (24) and use the second sum rule $\sum_{i=1}^{9}\omega_i f_i^2 = -4$. One finally obtains

$$N^{-1}\langle v\rangle_{E,n_k} \xrightarrow[k_0\to 0]{} \langle v\rangle_{E,n_k^0}/N + O(k_0^3) , \tag{28}$$

or, that all the α,β dependence is of order k_0^3, and *not* k_0^2 as might be expected, so that since $\langle v\rangle_{D,n_k}/N$ is order k_0^2 while $\langle T\rangle_{n_k}/N$ is order k_0^2, the minimum in (26) with respect to α,β for small enough k_0 must occur for $\alpha=1=\beta$, independent of the dynamical parameters $v_0,\gamma,\bar{k}$.

A direct variation of Eq. (26) in α and β was carried out numerically for many values of $(v_0,\gamma,\bar{k})$ and of density $\rho = k_0/\pi$, and indeed we found that ($\hbar^2/6m \equiv 1$)

$$\min_{\alpha\geq 1,\, 0\leq\beta\leq 1} \epsilon(\alpha,\beta;v_0,\gamma,\bar{k};k_0) \equiv \epsilon(\alpha_0,\beta_0;v_0,\gamma,\bar{k};k_0) < \epsilon(1,1;v_0,\gamma,\bar{k};k_0) \tag{29}$$

for intermediate values of density and many families of $(v_0,\gamma,\bar{k})$. Figures 2, 3, and 4 are typical cases corresponding, respectively, to $\gamma\bar{k}$

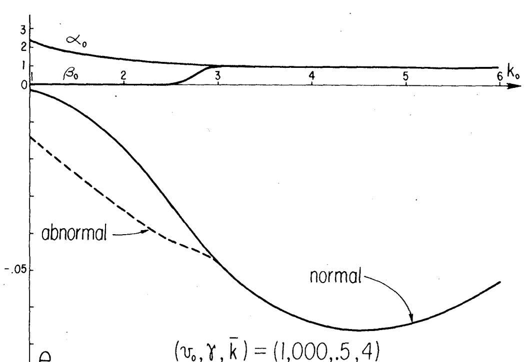

FIG. 2. Energy-per-particle, Eq. (29), divided by v_0, i.e., $e \equiv v_0^{-1}\epsilon$, as a function of $k_0 \equiv \pi\rho$ which results upon minimizing numerically in α and β, for each density for a typical value of the force parameters (v_0, γ, $\bar{k}$) shown. The dashed curve refers to the (lower energy) HF state obtained with the "abnormal" occupation, Eq. (21). The associated values of α and β which minimized Eq. (29), α_0 and β_0, are graphed above the k_0 axis.

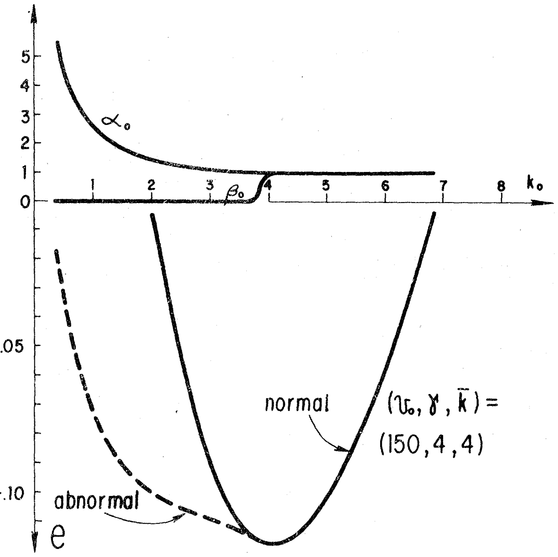

FIG. 3. Same as Fig. 2 for another set of force parameters $(v_0, \gamma, \bar{k})$.

$=2$, 16, and 144, for which the two-body interaction potential is shown in Figs. 5 and 6. Moreover, we also found that for some $(v_0, \gamma, \bar{k})$ the left-hand side of (29) can be *lower* for some k_0 than the lowest value of the right-hand side for *any* k_0: See Fig. 4. This is reminiscent of a gas-to-liquid phase transition but the rather large value of $\gamma\bar{k}=144$, meaning many oscillations in the two-body interaction potential, as seen in Fig. 6, was needed to achieve it with the present generalization of the Fermi sea.

IV. DISCUSSION

Although many oscillations in the two-body potential were needed to give a lower energy with the generalized Fermi sea than with the normal one, Eq. (10), the present study shows that even

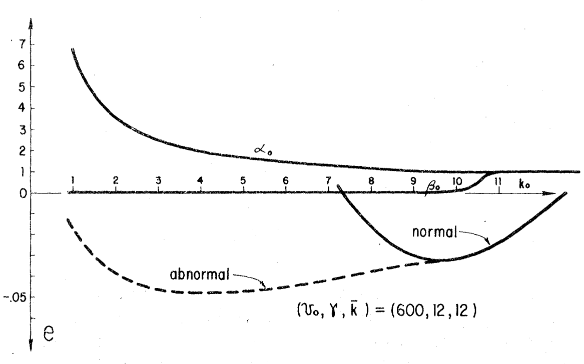

FIG. 4. Same as Fig. 2 for the set of force parameters $(v_0, \gamma, \bar{k})$ shown. Note that the minimum in k_0 of the abnormally occupied state is now *lower* than that for the normally occupied one.

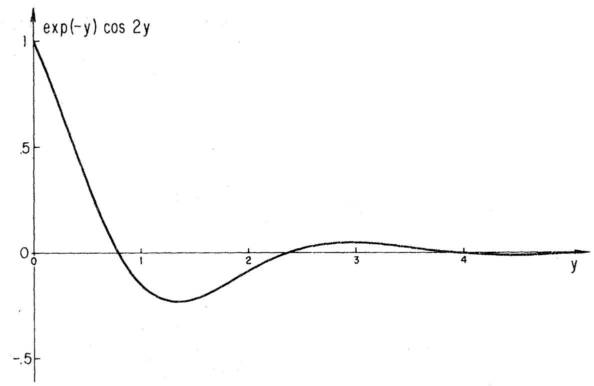

FIG. 5. The two-particle potential function Eq. (18) with $y \equiv x/\gamma$ for $\bar{k}\gamma = 2$.

with such a simple, two-part Fermi sea, Eq. (21), one obtains a new (plane-wave) HF state which is stabler at densities moderately lower than the normal Fermi sea saturation density. This in itself appears to be a stimulating invitation to further study of "abnormal" Fermi sea occupation functions for both one- and three-dimensional N-fermion systems.

Finally, let us consider the two-body correlation function $g(x_1, x_2)$ defined through

$$\langle v \rangle \equiv \tfrac{1}{2}\rho_0^2 \int dx_1 \int dx_2\, v(x_1 - x_2) g(x_1, x_2)\,.$$

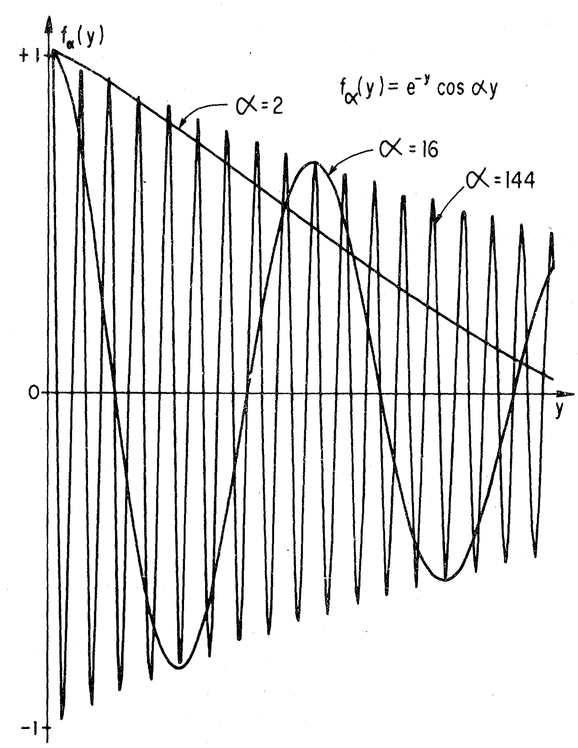

FIG. 6. Same as Fig. 5 but also for $\alpha \equiv \bar{k}\gamma = 16$ and 144.

For the problem at hand then

$$g(x_1, x_2) = 1 - \rho_0^{-2} |\rho(x_1, x_2)|^2,$$

where

$$\rho(x_1, x_2) \equiv \sum_k \varphi_k^*(x_1)\varphi_k(x_2)n_k .$$

Thus, if $x \equiv x_1 - x_2$ and using Eq. (21), one has

$$\begin{aligned} g(x) &\equiv g(x_1 - x_2) \\ &= 1 - (k_0 x)^{-2}[\sin\beta k_0 x + \sin\alpha k_0 x - \sin(\alpha+\beta-1)k_0 x]^2 \\ &\xrightarrow[k_0 x \to 0]{} \tfrac{1}{3}[\alpha^3 + \beta^3 - (\alpha+\beta-1)^3](k_0 x)^2 + O[(k_0 x)^3] . \end{aligned}$$

But since we know from Eq. (22) that the bracket coefficient of $\frac{1}{3}(k_0 x)^2$ is greater than or equal to unity (equality only for $\alpha = \beta = 1$), we arrive at the conclusion that *short-range correlations are suppressed* in the generalized Fermi sea considered here and that most likely it is the intermediate-range correlations which have been enhanced.

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