Density fluctuations in infinite Fermi systems

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(Received 28 June 1982)

Within the framework of many-body theory, a generalized Hartree-Fock equation is derived assuming a periodic density fluctuation. In a one-dimensional model, self-consistent solutions are calculated. A band structure of the single-particle spectrum and several minima of the total energy appear as novel features.

[NUCLEAR MATTER Static density fluctuations, generalized Hartree-Fock method.]

Static density fluctuations of the ground state of Fermi systems have been known for some time. The Wigner lattice[1] of the electron system is one example. Overhauser[2] considered an oscillatory density constructed from the eigenfunctions of a translationally invariant Hartree-Fock Hamiltonian for an infinite Fermi system and showed that the total energy of the state so obtained is lower than the total energy of the traditional plane wave solution which leads to a uniform density. More recent extensions[3] of this idea were applied to the problem of α clusters in the nuclear surface[4] and density fluctuations in nuclear matter[5] using realistic forces.

The method applied in the quoted papers proceeds from a given form of the wave function which is determined by a variational principle. Our point of departure is the equation of motion of the single particle operator in an infinite system ($\hbar = 1$)

$$-i\dot{c}_k^\dagger = [H, c_k^\dagger] = \epsilon_k c_k^\dagger + \sum_{k'q} V_q c_{k-q}^\dagger c_{k'}^\dagger c_{k'-q} \quad (1)$$

which is linearized in the usual fashion by the approximation

$$c_{k-q}^\dagger c_{k'}^\dagger c_{k'-q} \cong c_{k-q}^\dagger \langle c_{k'}^\dagger c_{k'-q} \rangle - c_{k'}^\dagger \langle c_{k-q}^\dagger c_{k'-q} \rangle \ , \quad (2)$$

where the brackets denote the expectation value with respect to a ground state yet to be determined.

Note that the assumption of a uniform density distribution of the ground state yields the traditional Hartree-Fock (HF) equation when Eq. (2) is inserted into Eq. (1). In the following we assume that such a HF calculation has been carried out and that it leads to a stable ground state. Hence the $c_k^\dagger$ in Eq. (1) refer to HF quasiparticle creation operators with corresponding HF single particle energies ϵ_k. Consequently V_q in Eq. (1) represents the Fourier transform of the residual two-particle interaction.

Physically, nonvanishing expectation values such as those appearing in Eq. (2) would arise in the presence of an *external* perturbation $U_Q \sum_k c_k^\dagger c_{k-Q}$, for fixed Q. In particular

$$\rho_s(Q) = \sum_{k'} \langle c_{k'}^\dagger c_{k'-sQ} \rangle \ , \quad s = 0, \pm 1, \pm 2, \ldots \quad (3)$$

would then not vanish. As a consequence, the density distribution would be a periodic function in space,

$$\rho(x) = \langle \psi^\dagger(x) \psi(x) \rangle = \sum_{s-0}^{\infty} \rho_s(Q) \cos(sQx) \ . \quad (4)$$

By calculating the total energy $E = \langle H \rangle$ we now investigate the question as to whether the system favors the state of nonuniform density distribution even when the external potential is switched off and, if this happens, as to what values of Q give rise to the lowest total energy.

To simplify the discussion we consider a short range interaction V, i.e., we ignore the q dependence of V_q. Taking the sums over spins into account the direct and exchange term in (2) can be combined and we finally obtain

$$-i\dot{c}^\dagger{}_k = \epsilon_k c^\dagger{}_k + 2V \sum_{s=-\infty}^{\infty} \rho_s(Q) c^\dagger{}_{k-sQ} \ . \quad (5)$$

In the following we consider a one dimensional model. Then it is obvious from Eq. (5) that only the Brillouin range $-Q/2 \leq k \leq Q/2$ needs to be con-

sidered; we denote values from this reduced zone by $\bar{k}$. The "ansatz" $c_k^\dagger(t) = c_k^\dagger \exp(i\omega_{\bar{k}} t)$ yields the eigenvalue equation

$$\omega_{\bar{k}} c_k^\dagger = \epsilon_k c_k^\dagger + 2V \sum_{s=-\infty}^{\infty} \rho_s(Q) c_{k-sQ}^\dagger \ . \tag{6}$$

We now introduce the quasiparticle operators

$$\psi_{\bar{k},n}^\dagger = \sum_{r=-\infty}^{\infty} \alpha_r^{(n)}(\bar{k}) c_{\bar{k}+rQ}^\dagger \tag{7}$$

with $\alpha_r^{(n)}(\bar{k})$ being the eigenvectors of the coupled system (6), viz.,

$$\omega_{\bar{k}}^{(n)} \alpha_r^{(n)}(\bar{k}) = \epsilon_{\bar{k}+rQ} \alpha_r^{(n)}(\bar{k}) + 2V \sum_{s=-\infty}^{\infty} \rho_s(Q) \alpha_{r-s}^{(n)}(\bar{k}) \tag{8}$$

The transformation (7) is canonical as the $\alpha_r^{(n)}(\bar{k})$ are complete and orthogonal for each value of $\bar{k}$. Thus we retrieve the usual anticommutation relations $[\psi_{\bar{k},n}^\dagger, \psi_{\bar{k}',n'}]_+ = \delta_{nn'}\delta(\bar{k}-\bar{k}')$, and zero for the other anticommutators. Therefore the ground state can be constructed in the usual way from the vacuum by application of the $\psi_{\bar{k},1}^\dagger$ to fill up all states in the range $|\bar{k}| \leq Q/2$, then by $\psi_{\bar{k},2}^\dagger$ and so forth until a given total number density is reached. From this we obtain

$$\rho_s(Q) = \int_{-Q/2}^{Q/2} d\bar{k} \sum_{r=-\infty}^{\infty} \sum_{n=1}^{N_F} \alpha_r^{(n)}(\bar{k}) \alpha_{r-s}^{(n)}(\bar{k}) + \int_{-\alpha Q/2}^{\alpha Q/2} d\bar{k} \sum_{r=-\infty}^{\infty} \alpha_r^{(N_F+1)}(\bar{k}) \alpha_{r-s}^{(N_F+1)}(\bar{k}) \tag{9}$$

with $0 < \alpha < 1$. The second term occurs if the last zone is only partially filled; if the first zone is only partially filled, $N_F = 0$. Denoting the given density by $2k_F$, we have $2k_F = \rho_0 = (N_F + \alpha)Q$.

Equations (8) and (9) constitute a self-consistent nonlinear eigenvalue problem which is solved numerically by iteration. We used parameter values $0 < 2k_F \leq 3$ and $|V| \leq 2.5(\hbar^2/2m = 1)$. We now record the main qualitative features of the one-dimensional model calculation:

(i) A consistent solution is only obtainable for attractive ($V < 0$) interactions.

(ii) If $Q > 2k_F (N_F = 0)$ there is a critical interaction strength below which a consistent solution cannot be attained. Its value depends on the total density. The lower the density, the stronger the critical interaction must be. For $Q \leq 2k_F$ there is always a consistent solution ($V < 0$).

(iii) The total energy per particle

$$\frac{E}{N} = \frac{1}{4k_F}\left[\int_{-Q/2}^{Q/2} d\bar{k} \sum_{n=1}^{N_F} \left\{\omega_{\bar{k}}^{(n)} + \sum_{r=-\infty}^{\infty} \epsilon_{\bar{k}+rQ}[\alpha_r^{(n)}(\bar{k})]^2\right\} + \int_{-\alpha Q/2}^{\alpha Q/2} d\bar{k}(n \to N_F + 1)\right] \tag{10}$$

is illustrated as a function of $2k_F/Q$ for fixed k_F in Fig. 1. Not only does a minimum occur at $Q = 2k_F$ that is in fact lower than the corresponding value of the plane wave solution, if the interacting is strong enough, but a remarkable second local minimum also occurs at $Q = 2k_F/2$. We conjecture that further local minima are present at $Q = 2k_F/m$, $m = 3, 4, \ldots$. Remark that the total energy has changed due to effects of the residual interaction that go beyond traditional HF theory. It is doubtful whether the HF ground state itself would support a permanent density fluctuation in nuclear matter.[6]

(iv) The single particle spectrum $\omega_{\bar{k}}^{(n)}$ shows the same pattern as the one obtained from the band model in solid state physics[7] with $\bar{k}$ being a wave number in a Brillouin zone. There is a gap between $\omega_{\bar{k}}^{(1)}, \omega_{\bar{k}}^{(2)}, \ldots$ which decreases with increasing n while for large n the unperturbed energies $\epsilon_{\bar{k}\pm nQ}$ are approached. Note, however, that this is brought about by a self-consistent density distribution in the present case.

(v) Typical self-consistent density deistributions [Eq. (4)] are plotted in Fig. 2 for the $Q = 2k_F$ and $Q = k_F$ states. While the former resembles the pat-

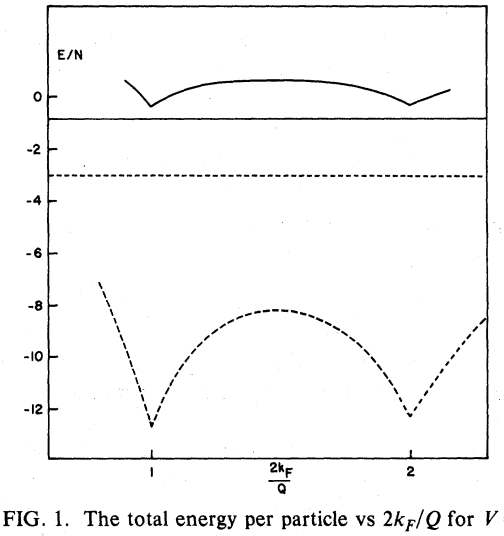

FIG. 1. The total energy per particle vs $2k_F/Q$ for $V = -1$ (solid curve) and $V = -2.5$ (dashed curve) for $2k_F = 3$. The horizontal lines indicate the corresponding energies of the respective plane wave solutions. If the interaction is weaker than a certain critical value, all points of the curves lie above the corresponding energy of the plane wave solution.

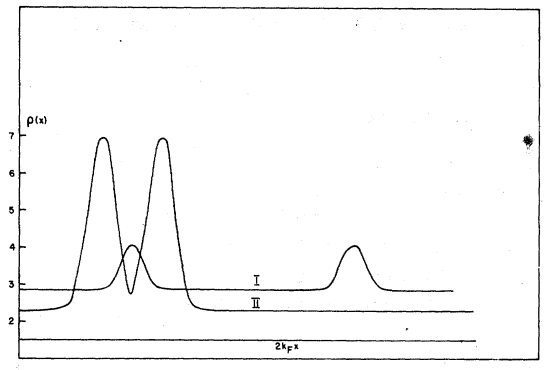

FIG. 2. Periodic density fluctuations around the average value $\rho_0 = 2k_F = 3$ for $V = -2.5$. Two periods are shown for the state with $Q = 2k_F$ (I) to allow the display of one full period of the state with $Q = k_F$ (II).

tern obtained previously by other authors,[5] the latter shows a remarkably different structure.

(vi) There is no sharp Fermi momentum in the single particle density

$$n(k) = \langle c_k^\dagger c_k \rangle = \sum_{n=1}^{N_F} [\alpha_r^{(n)}(\bar{k})]^2 \ . \qquad (11)$$

This function looks rather like the distribution of a superconducting state, i.e., there is a drop at $k = k_F$ but the function is smooth and extends to infinity. Obviously, $\int n(k)\, dk = 2k_F$.

While we could reproduce known facts on generalized Hartree-Fock solutions with periodic density distributions, we have gained considerable additional insight by our procedure. The band structure of the single particle spectrum and the "higher" states at $mQ = 2k_F$ are the most interesting features. In view of the simplicity of our model, a definite physical assessment of these findings is premature. However, we mention the possible analogy with the various possible antiferromagnetic orderings of spins on a common basic lattice.[8] Also, at this stage, our model does not contain a driving mechanism which "arranges" the appropriate Q value for a given total density. We expect more insight when extending the random phase approximation along the same lines. Work towards this aim is in progress.

The authors gratefully acknowledge the assistance of Mrs. H. C. Marais who wrote the computer program.

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