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PERIODIC GROUND STATES AND THE MANY-BODY PROBLEM*

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In a recent Letter, Overhauser[1] proposed that the description of the ground state of nuclear matter start with spatially periodic Hartree-Fock functions. The periodic state has been proposed in other many-body problems, and may occur widely in nature. Examples that have been worked out in some detail are Vlasov's classical theory of "solids,"[2] Fröhlich's one-dimensional model of superconductivity,[3] and the author's theory of interacting bosons.[4] The physical idea of these theories is that when attractive interactions outweigh repulsions at a characteristic distance, the system may pay the cost in kinetic energy to establish space periodicity. Except for close collisions, a particle moves freely through the entire volume of the system, in contrast to the localization in a solid state. Yet there is long-range order involving a self-consistent density variation. This Letter first reports a general method to describe systems in which the periodic state forms the correct starting point. It enables one to determine the excitations and thermodynamic properties, as well as to calculate modifications of the self-consistent field produced by close collisions. Second, we note some qualitative and unusual features of such periodic states. These have been studied in some detail in I and II for bosons. Since the present approach embraces both fermions and bosons, the features are general possibilities. Because of the difficulties of making quantitative predictions in many-body theory, the qualitative ideas suggest a general search for experimental evidence for the features.

Consider, for simplicity, spinless bosons or fermions, described by a quantized field $\psi(\vec{x}) = \sum_f a_f \varphi_f(\vec{x})$. The $\varphi_f(\vec{x})$ form a complete set of one-body functions; we are mainly concerned with a plane wave basis or a set of solutions to a periodic potential problem in extended zone correspondence with the plane waves. The basic units are the operators $c(\vec{f}\,|\,\vec{f}') = a_f^\dagger a_{f'}$, i.e., components of the density matrix $\rho(\vec{x}, \vec{y}) = \psi^\dagger(\vec{x})\psi(\vec{y})$. They obey the commutation rules

$$[c(\vec{f}\,|\,\vec{f}'), c(\vec{g}\,|\,\vec{g}')] = c(\vec{f}\,|\,\vec{g}')\delta_{f',g} - c(\vec{g}\,|\,\vec{f}')\delta_{f,g'},$$

for both Bose and Fermi systems. The Hamiltonian is

$$H = \sum_{f,g} T(\vec{f}\,|\,\vec{g})c(\vec{f}\,|\,\vec{g}) + \sum_{f,g,f',g'} V(\vec{f}\vec{g}\,|\,\vec{f}'\vec{g}')c_2(\vec{f}\vec{g}\,|\,\vec{f}'\vec{g}'),$$

with

$$T(\vec{f}\,|\,\vec{g}) = (\hbar^2/2M)\int \nabla\varphi_f^* \cdot \nabla\varphi_g\, d^3x,$$

$$V(\vec{f}\vec{g}\,|\,\vec{f}'\vec{g}') = \tfrac{1}{2}\iint \varphi_f^*(\vec{x})\varphi_g^*(\vec{y})V(\vec{x}-\vec{y})\varphi_{f'}(\vec{x})\varphi_{g'}(\vec{y})\,d^3x\,d^3y,$$

$$c_2(\vec{f}\vec{g}\,|\,\vec{f}'\vec{g}') = a_f^\dagger a_g^\dagger a_{f'} a_{g'}.$$

c_2 can be broken into products of c operators. The $c(\vec{f}\,|\,\vec{f}')$ thus form a complete description.

The elementary Hartree theory consists in

assigning values to the number operators $c(\vec{f}\,|\,\vec{f})$, neglecting off-diagonal elements and contributions of $c(\vec{f}\,|\,\vec{f}\,')$ with $\vec{f}\,' \neq \vec{f}$. The choice $c(0\,|\,0) = N$, $c(\vec{f}\,|\,\vec{f}) = 0$ for $\vec{f} \neq 0$ yields the semi-classical boson theory of I. $c(\vec{f}\,|\,\vec{f}) = 1$ for $|\vec{f}|$ less than the wave vector in correspondence with the Fermi momentum, for fermions leads, for example, to Overhauser's ground state for nuclear matter. One obtains a set of equations for $\varphi_f(\vec{x})$ by functionally varying the energy with respect to $\varphi_f^*(\vec{x})$. The plane wave basis makes the energy stationary, but when attractive forces are vital, a spatially periodic basis yields a minimum energy.

It is important that there are other periodic solutions of the Hartree equations (different lengths or symmetries) of higher energy than the lowest solution, but lower in energy than the plane wave solutions. As discussed in II, the various periodic states are mutually orthogonal as $N \to \infty$. They have a different energy per particle and so determine the properties at a finite temperature. In fact, the correlation function should be periodic at absolute zero and lose the long-range order, as the temperature is raised, because of admixture of other periodicities.

To describe the low-lying excitations, one linearizes the equations of motion for $c(\vec{f}\,|\,\vec{f}\,')$ by breaking down $c_2(\vec{f}\vec{g}\,|\,\vec{f}\,'\vec{g}\,')$ and retaining only terms containing one number operator. This is a "random phase" approximation, but it is important that it is basis dependent. We obtain a set of linear equations for $c(\vec{f}\,|\,\vec{f}\,')$, an associated excitation spectrum, and a lowering of the ground-state energy from the zero-point shift of the excitations. When one uses a plane wave basis, the resulting theory includes Bogolyubov's theory of bosons and Sawada's theory of fermions. For periodic bases there are new results, most importantly, gaps in the excitation spectra at absolute zero. With rising temperature the other periodic solutions, with gaps in their excitation spectra at different places, come into play. The observed gaps should therefore narrow and ultimately disappear. This effect should be looked for, e.g., by studying inelastic neutron scattering at very low temperatures in liquid helium.

To include the effects of close collisions, c_2 is left unaltered in the equation of motion of c. One writes an equation for the time dependence of c_2. This involves $c_3(\vec{f}\vec{g}\vec{h}\,|\,\vec{f}\,'\vec{g}\,'\vec{h}\,')$, which is broken to a sum of products of c_2 and c. Terms containing vacuum expectation values of either of the operators are retained. Elimination of c_2 leads to a new, consistent field as modified by collisions. The above scheme is in the spirit of much recent work in many-body theory. The main point of difference is the recognition of the importance of a non-plane-wave basis even in absence of external fields.

One objects immediately that this violates the translational invariance of the Hamiltonian. For every basis $\varphi_f(\vec{x})$, we get a corresponding theory for a basis $\varphi_f(\vec{x}+\vec{\epsilon})$, where $\vec{\epsilon}$ is any real vector. This point has been studied in II. There, a formalism involving linear combinations of creation and annihilation operators was used. A translationally invariant ground state is constructed by superposing wave functions for different $\vec{\epsilon}$. The ground-state energy per particle is unaltered as $N \to \infty$. Corresponding results are obtained for fermions using Bogolyubov's variational method.[5]

A second point is that the periodic state is not a solid. The solid[4] is described by using a set of $\varphi_f(\vec{x})$, localized at different points in space, and can be treated in the above scheme. A check is obtained by examining the excitation spectrum for long waves. The solid has transverse branches in contrast to the periodic state under consideration. By rewriting the theory in terms of the Wigner distribution, one can show that Vlasov's theory[2] is not a theory of a solid. It is interesting that the solid also has periodic solutions with different periodicities from the one realized at absolute zero. In accordance with the above ideas, these solutions are to be used in the theory of the thermal expansion, for example, of solid He^4.

The above scheme has been used by the author and Vail[6] to extend Fröhlich's one-dimensional model of superconductivity. To Fröhlich's consideration of the static self-consistent state one adds the dynamical interactions of electrons and lattice. This extends the validity of his theory to more reasonable coupling strengths. Fröhlich places the wave vector of the periodicity at twice the Fermi momentum. In three dimensions it is not likely that one can gain energy with such a small periodicity because of the irregular shape of the Fermi surface. But the possibility of a range of long-wavelength periodicities has not been sufficiently explored. This leads back to earlier, abortive theories of superconductivity referred to by Bardeen.[7] Even if the self-consistent superlattice concept is com-

pletely irrelevant to superconductivity, it may be needed in other solid state problems. In particular, Slater[8] has used the idea in an interesting way to give a qualitative explanation of a number of anomalous effects. The self-consistent periodic state is such a general notion that experimental investigation, further exploration of its limitations, or perhaps theoretical refutation seems to be called for.

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LINKED CLUSTER EXPANSION APPLICABLE TO NONSPHERICAL SITUATIONS*

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The Brueckner-Goldstone[1] or linked cluster expansion for the ground-state energy of a many-fermion system has recently been criticized by Kohn and Luttinger[2] and Luttinger and Ward,[3] who have shown by using statistical mechanics, that the formula obtained starting from a spherical unperturbed state is correct, in general, only for systems with complete spherical symmetry. It is the purpose of this note to exhibit a generalized linked cluster expansion applicable also to situations lacking such symmetry.

To illustrate our viewpoint, we consider for simplicity a system of spinless fermions interacting via two-body forces as described by the Hamiltonian

$$H = H_0 + \lambda H_1 = \sum_{\vec{p}} a^\dagger(\vec{p}) a(\vec{p}) p^2 + \frac{\lambda}{2\Omega} \sum_{\vec{p},\vec{p}',\vec{q}} a^\dagger(\vec{p}+\vec{q}) a^\dagger(\vec{p}'-\vec{q}) a(\vec{p}') a(\vec{p}) v(\vec{q}), \quad (1)$$

where p^2 is the kinetic energy of a free particle, Ω is the volume of the system, and the potential $v(\vec{q})$ is assumed not to be spherically symmetric. As is customary, we shall be interested in a system of N particles in the limit in which N and $\Omega \to \infty$, but, of course, $\rho = (N/\Omega)$ remains fixed and finite.

It is first essential to inquire about which element of the Goldstone proof can fail in the present situation. Putting aside questions of convergence, direct examination shows that the formal derivation can fail only if we start the adiabatic switching-on process with an unperturbed state which is orthogonal to the actual ground state. The procedure described below is designed specifically to avoid this dilemma and to yield a series which should represent the lowest normal state.

Let $M(\vec{p}, p_0, \rho)$ be the proper self-energy operator[4] for a single fermion of four-momentum $(\vec{p}, p_0)$ moving through the medium at density ρ. For a normal system, the minimum single-particle excitation energy is required to coincide with the chemical potential, μ, and to be the unique real solution of the equation[5]

$$\mu = p^2 - M(\vec{p}, \mu; \rho). \quad (2)$$

Since in our present example M depends on the direction of $\vec{p}$, for given μ, the real solutions $\vec{p} = \vec{p}_F$ of Eq. (2) define a surface in $\vec{p}$ space, $\mu = \epsilon(\vec{p}_F)$, the perturbed Fermi surface. It is essential for our further considerations to suppose that ρ is itself a single-valued functional of this surface. We may thus write

$$\epsilon(\vec{p}) = p^2 - M(\vec{p}, \epsilon(\vec{p}), \rho[\vec{p}]) \equiv p^2 + \mathcal{U}(\vec{p}), \quad (3)$$

where we have dropped the subscript F to emphasize that we now wish to consider the