PHYSICAL REVIEW VOLUME 147, NUMBER 1 8 JULY 1966

Broken Symmetry, Sum Rules, and Collective Modes in Many-Body Systems*

H. STERN
Faculté des Sciences, Université Libre de Bruxelles, Bruxelles, Belgium
(Received 19 July 1965; revised manuscript received 24 January 1966)

An investigation is made of the relationship between long-wavelength, low-frequency normal modes and broken symmetry in nonrelativistic many-body systems. In particular, the relationship between broken symmetry as manifested through the so-called Goldstone pole and the normal-mode structure is examined. Through the study of various models, we show that the structure of the normal modes is correlated to the Goldstone pole either completely, partially, or not at all, according to the class of symmetry of the Hamiltonian of the system. For example, in the neutral superconductor, the Hamiltonian has such low symmetry that although the Anderson modes restore the symmetry of the ground state, they have no relationship at all to the Goldstone pole. It is observed that as the symmetry decreases, a dynamical sum rule takes the place of such a correlation and in all systems a sum rule gives the normal-mode frequency ω. These sum rules also give the ω distribution of states through the Huang–Klein dispersion relation.

I. INTRODUCTION

THE question of whether the Goldstone theorem[1] can be proved for nonrelativistic theories has been the subject of recent investigation. The theorem would say: A many-body system which displays order in some "direction," but which is nevertheless described by a "rotationally" invariant Hamiltonian, has collective modes which arise as a consequence of broken symmetry. The frequency of the collective mode tends to zero as its wave number tends to zero. No general proof of this theorem has yet been found, i.e., there is as yet no general proof that such collective modes are a *consequence* of broken symmetry.[2]

However, given the existence of long-wavelength, low-frequency normal modes in the presence of broken symmetry (in the absence of long-range forces), it is of interest to investigate the relationship between such modes and broken symmetry. It is this problem to which we direct our attention in this paper.

One relationship which exists in all cases and was originally pointed out by Anderson,[3] is the following. *Anderson's theorem*: If there exists a spectrum of collective modes with the end point $\omega\rightarrow 0$ as $q\rightarrow 0$, then the mode in that limit is the operator which connects the set of degenerate ground states, i.e. "rotates" the ground state. This is called the *symmetry-restoring operator*. It is obvious that the theorem is true for any system with broken symmetry since the ground state in such cases is degenerate.

On the other hand, the relationship between the normal modes and the Goldstone coordinates (defined below) is not obvious. We demonstrate in this paper how closely this relationship depends on the nature of the symmetry of the Hamiltonian.

$\chi_q(\omega)$, the response to an infinitesimal field with frequency ω and wave number q is, in general, a tensor. We choose as principal axes, those determined by the privileged direction given by the broken symmetry. The matrix, $\chi_{q=0}(\omega=0)$, in the frame of the principal axes, has at least one divergent element, on account of the broken symmetry of the ground state. *The Goldstone response function* is defined as the element of the matrix $\chi_q(\omega)$, in the frame of the principal axes, which has a singularity at ω, $q=0$. The singularity is known as the *Goldstone pole. The Goldstone coordinate* is defined as the principal-axis coordinate corresponding to the Goldstone response function. At $q=0$, the Goldstone coordinate is clearly the coordinate generated by the "rotating" ground state in the restoration of symmetry.

If the Goldstone response function is continuous in the limit $\omega,q\rightarrow 0$, (static limit) then a spectrum at small ω,q exists. This is obvious, because an infinite response to a field with given ω and q means that the system has a natural excitation with that ω and q. The proof of the spectrum hinges on the continuity. Since no general proof of this point has been established, we simply assume, in this paper, the existence of normal modes in the long-wavelength region.

We wish to investigate whether the Goldstone coordinate is reflected in the normal-mode structure, i.e. whether the Goldstone coordinate is a linear combination of normal modes at small q.

It is the central point of this paper that such a relationship depends closely on the symmetry of the Hamiltonian. For example, the neutral superconductor has such low symmetry, that the Anderson modes,[3] which indeed restore symmetry in the limit $\omega,q\rightarrow 0$, have no relationship at all with the Goldstone coordinate. In direct contrast, the isotropic ferromagnet has such high symmetry, that the Goldstone coordinate is itself the normal mode. In intermediate cases, the Goldstone coordinate is a linear combination of normal modes.

At the same time, we show how, as the symmetry decreases, a dynamical sum rule[4] takes the place of the

* This research was supported in part by the U. S. Air Force under Grant No. AF-EOAR 63-51 and monitored by the European Office, Office of Aerospace Research.

[1] S. Goldstone, A. Salam, and S. Weinberg, Phys. Rev. **127**, 965 (1962); S. Bludman and A. Klein, *ibid.* **131**, 2364 (1963).

[2] A. Klein and B. W. Lee, Phys. Rev. Letters **12**, 266 (1964); W. Gilbert, *ibid.* **12**, 713 (1964).

[3] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[4] The application of these sum rules to superfluid helium is found in Ref. 6.

relationship between normal-mode and Goldstone coordinate.

The clearest way to demonstrate the role of symmetry in the various cases is to work with spin models: the isotropic ferromagnet, the Anderson spin model[3] of the neutral superconductor, and an anisotropic ferromagnetic model[5] which is a prototype of the intermediate cases.

In all the systems, a sum rule[4] gives the frequency; the choice of sum rule depends on convenience and differs from a gas to a system of localized particles. By means of these sum rules, contact is made with the Huang and Klein[6] dispersion relation to give the ω distribution of states in the neutral superconductor.

We list here the many-body systems in question, the nature of their broken symmetry, and the collective modes which restore it. (See Ref. 7 for an account of these systems.)

(1) The isotropic Heisenberg ferromagnet. Orientation of spin alignment violates the rotational symmetry. Spin waves. (Bloch ferromagnet similar.)

(2) The crystal lattice. Position in space violates the translational and rotational symmetry of the free crystal. Phonons.

(3) Superfluid helium. Violation of gauge invariance. Phonons. (Bogoliubov particles.)

(4) The neutral superconductor. Violation of gauge invariance. Phonons. (Anderson modes.)

II. FERROMAGNETIC MODELS

1. The Goldstone Coordinate and the Isotropic Heisenberg Ferromagnet

The isotropic ferromagnet is the only many-body system for which the Goldstone coordinate is itself the normal mode. This relationship is seen as follows.

In the ground state, all the spins are aligned but their orientation is not determined in the absence of external field. We artificially choose a direction, say z. The response $\chi_\perp$ to a uniform static field in a direction normal to the broken symmetry is infinite in that direction. This is obvious, because whereas the initial broken symmetry is artificial, the applied field truly breaks the symmetry and so the total spin $\mathbf{R}$ turns completely in that direction. (e.g. a field in direction y gives $R_y=|\mathbf{R}|=NS$, $\chi_{yy}=\lim_{h_y\to 0}(NS/h_y)=\infty$.) Hence $\chi_\perp$ is the Goldstone response function.

The Goldstone coordinate is therefore $S_q^x+iS_q^y$. But at zero ω,q, the Goldstone coordinate, $S_0^x+iS_0^y$ is known to be the normal mode by the Anderson theorem. Hence $S_q^x+iS_q^y$ is in fact the normal mode, in agreement with the solution of the equations of motion. In other words, the Goldstone coordinate is the normal mode, because the operators which restore the symmetry (i.e., rotate the ground state) are also the operators generated by the rotating ground state. In this respect, the isotropic ferromagnet is unique among many-body systems.

For completeness, we indicate how the normal mode appears in the expression for $\chi_q^{+-}(\omega)$ and how the Goldstone pole arises. The expression for $\chi_q^{+-}(\omega)$ given in time-dependent perturbation theory[8] is

$$\chi_q^{+-}(\omega)=\sum_n\left[\frac{|\langle 0|S_q^-|n\rangle|^2}{\omega-\omega_{n0}+i\epsilon}-\frac{|\langle 0|S_{-q}^+|n\rangle|^2}{\omega+\omega_{n0}+i\epsilon}\right],$$

where $|n\rangle$ are the eigenstates and ω_{n0} their energy with respect to the ground state. Since a spectrum exists, this becomes

$$\chi_q^{+-}(\omega)=(\omega-\omega_q+i\epsilon)^{-1}.$$

In the static limit and with $q=0$, the pole arises trivially, $S_0^\pm$ connects the degenerate states, $\omega_{n0}=0$. Since $\lim_{q,\omega\to 0}\chi_q^{+-}(\omega)$ is continuous, however, the pole has dynamical significance.

Although not part of our main interest, we indicate here[7,9] how the spectrum totally vanishes in the limit of long-range forces. In the absence of long-range forces, a spectrum can exist at wavelengths λ far greater than the range of forces r because then no energy is expended well within the local regions of motion. ω therefore increases with decreasing λ. When $\lambda\ll r$ energy is expended in the motion of each individual spin and so there can be no collective motion. In the limit $r\to\infty$, therefore, there is no collective motion at all apart from the total rotation. The static response $\chi_{\perp q}(0)$ is therefore $(v_0)^{-1}$ (v_0S is the molecular field) for all finite q, no matter how small, and $\lim_{q\to 0}\chi_{\perp q}(0)$ is discontinuous.

2. The Goldstone Coordinate and an Anisotropic Model

A striking way of demonstrating the role of symmetry in the difference between the isotropic ferromagnet (I.F.), the Anderson spin model of the superconductor and the other many-body systems, is to invent an anisotropic ferromagnetic model (A.F.) with the symmetry properties of the latter systems. We take a model with Hamiltonian

$$H=-\sum v_{ij}(S_i^xS_j^x+S_i^yS_j^y).$$

The analogy to the many-body systems will be explained later.

The model has only axial symmetry, which means only one constant of motion, S_0^z. In the true ground state, the spins are aligned and confined to the x-y plane for minimum energy, but since S_0^z is a good quantum number, they precess about the z axis. The symmetry is broken by taking a wave packet with the total spin

[5] This model was suggested to the author by Professor R. Brout.
[6] K. Huang and A. Klein, Ann. Phys. **30**, 203 (1964).
[7] R. Brout, *Phase Transitions* (W. A. Benjamin, Inc., 1965).
[8] See, for example, R. Brout and P. Carruthers, *Lectures on the Many-Electron Problem* (Wiley-Interscience, New York, 1963).
[9] R. V. Lange, Phys. Rev. Letters **14**, 3 (1965).

in a fixed direction, say x. This wave packet is a good approximation to the true eigenstate as will be seen in a later subsection. That the broken symmetry is a wave packet is a consequence of the lower symmetry, but the most direct consequence of the lower symmetry for the relationship between Goldstone coordinate and normal mode is that there is only one symmetry-restoring operator S_0^z (the single constant of the motion), and so the operator generated by the rotating ground state, i.e., the Goldstone coordinate at $q=0$, must be different.

Thus, while the Anderson theorem gives S_0^z as the mode at $q,\omega \rightarrow 0$, the Goldstone coordinate is S_q^y. (The Goldstone response function is $\chi_q^{yy}(\omega)$.) The mode has the general form[10]

$$\eta_q = (A_q)^{-1} S_q^z \pm i A_q S_q^y, \quad \text{where} \quad \lim_{q\rightarrow 0} A_q = 0 \qquad \text{(II.1)}$$

If we wish to know A_q, we must find the sum rule given by the susceptibility in the z direction, χ^{zz}. Broken symmetry now plays no part. The molecular field, $v_0 S$, acts only in the x-y plane and so $\chi_q^{zz}(0)$ is $(v_0)^{-1}$ for all q. This gives us the sum rule

$$\chi_q^{zz}(0) = 2\sum\nolimits_n \left(|\langle n | S_q^z | 0\rangle|^2 / \omega_{n0} \right) = (v_0)^{-1}.$$

Substituting the mode (II.1) gives $(A_q)^2/\omega_q = (v_0)^{-1}$ and so we have the mode

$$\eta_q = (v_0/\text{two}\,\omega_q)^{1/2} S_q^z \pm i(\omega_q/\text{two}\,v_0)^{1/2} S_q^y. \qquad \text{(II.2)}$$

It is interesting to write down the expressions for the $\chi_q(\omega)$, given by this mode, to see how the limit $\lim_{q,\omega\rightarrow 0} \chi_q^{zz}(\omega) = (v_0)^{-1}$ and the Goldstone pole $\lim_{q,\omega\rightarrow 0} \chi_q^{yy}(\omega) \rightarrow \infty$ arise. The mode (II.2) is substituted into the expressions for $\chi_q(\omega)$ given by time-dependent theory (cf. isotropic ferromagnet). We obtain

$$\chi_q^{zz}(\omega) = (\omega_q/v_0)\left((\omega+\omega_q+i\epsilon)^{-1} - (\omega-\omega_q+i\epsilon)^{-1}\right),$$
$$\chi_q^{yy}(\omega) = (v_0/\omega_q)\left((\omega+\omega_q+i\epsilon)^{-1} - (\omega-\omega_q+i\epsilon)^{-1}\right).$$

The wave-packet nature of the broken symmetry means that the $q,\omega=0$ mode does restore the symmetry unlike the I.F. at $T=0$; (see below). Since the ground state is a wave packet its shape is modified by the zero-point motion of the modes, i.e. "dressed." The state "dressed" by mode q is given by $\eta_q|0\rangle = 0$. It is precisely such states $|0\rangle$ which appear in the general expression for $\chi_q(\omega)$ when η_q is substituted. The restoration of symmetry is seen by substituting η_q in $\langle 0|(S_q^z)^2|0\rangle$ and $\langle 0|(S_q^y)^2|0\rangle$. Then $\lim_{q\rightarrow 0}\langle 0|(S_q^z)^2|0\rangle = 0$ and $\lim_{q\rightarrow 0}\langle 0|(S_q^y)^2|0\rangle = \infty$.

In the I.F., the broken symmetry is a true ground state in the first place and contains the zero-point motion of all the modes in the form of the incoherent precession. At finite T, however, the symmetry is restored in thermal equilibrium. (See end of Appendix.)

A proof of the Goldstone theorem would be the proof of continuity of $\lim_{q,\omega\rightarrow 0} \chi_q^{yy}(\omega)$.[11] An alternative dynamical derivation of the spectrum would be to prove the continuity of $\lim_{q,\omega\rightarrow 0} \chi_q^{zz}(\omega)$ and the vanishing of $\langle 0|(S_q^z)^2|0\rangle$ with q.[11]

In a later subsection, contact is made with the many-body systems in question, by interpreting the motion as a coupled harmonic oscillation of massive particles. The above sum rule then tells us the "mass" of the particles. The existence of such "mass" is a feature of the lower symmetry.

3. The Frequency, ω_q

ω_q can be found using one more sum rule involving dynamics. The rule most convenient for systems with localized particles is $\langle 0|H-E_0|0\rangle = \frac{1}{2}\sum\omega_q$, the zero-point energy, where E_0 is the energy in the absence of zero-point motion.

In the I.F., putting $S_i^z = S - S_i^+ S_i^-$ for $S=\frac{1}{2}$, one gets

$$\sum\nolimits_q (v_0 - v_q)\langle 0|S_q^+ S_q^-|0\rangle = \tfrac{1}{2}\sum\omega_q,$$

and hence $\omega_q = (v_0 - v_q) \propto q^2$. In the limit of long-range forces, $\omega_q = 0$ for $q=0$ and $\omega_q = v_0$ for $q \neq 0$, as expected from previous considerations.

In the A.F., we put $S_i^x = \frac{1}{2}S - (S_i^{y2} - S_i^{z2})$ for $S=\frac{1}{2}$ and get

$$v_0\langle 0|S_q^z S_{-q}^z|0\rangle + (v_0 - v_q)\langle 0|S_q^y S_{-q}^y|0\rangle = \omega_q.$$

Employing the mode (II.2), to evaluate the averages, we get

$$\omega_q = [v_0(v_0 - v_q)]^{1/2} \propto q. \qquad \text{(II.3)}$$

The lower dependence on q is due to the "mixed" nature of the motion.

4. The Equations of Motion of the A.F.

The interpretation of the motion as a coupled harmonic oscillation of massive particles, mentioned previously, is easily made from the equations of motion.

The model is simple enough for an exact solution of the equations of motion about the approximate ground state originally chosen (i.e., the "bare" state). Of course, the modes are a good approximation only in so far as the "bare" state is. This is a common feature of all the systems where the broken symmetry is an approximation, and is quite independent of either the solubility of the equations of motion or the Goldstone theorem. The justification can only be found in the wave packet itself, that it be a very good approximation. This, we shall verify shortly.

---

[10] In excited states the motion is no longer uniform and the spins are not confined to the x-y plane. A coherent precession about the x axis occurs, with a phase difference between lattice sites like standard spin waves, but the precession is now elliptical, with the eccentricity in the z axis vanishing as $q,\omega \rightarrow 0$.

[11] This might be treated by "dressing" the "bare" state in a diagrammatic analysis. Continuity proofs of this kind are given in Ref. (18) for the normal fermion system and might be applicable to the neutral superconductor, in Nambu's (Ref. 17) formalism, and similarly to the condensed Bose gas.

The continuity of $\lim_{q,\omega\rightarrow 0} \chi_q^{zz}(\omega)$ alone is not a sufficient condition, e.g., in the limit of long-range forces, $\chi_q^{yy}(0) = (v_0)^{-1}$ and is discontinuous at $q \rightarrow 0$, whereas $\chi_q^{zz}(0)$ is unchanged. In fact "χ^{zz}" $= (v_0)^{-1}$ for nonwavelike fields also.

We define

$$\mathbf{S}_q=(N)^{-1/2}\sum_i \mathbf{S}_i e^{i\mathbf{q}\cdot\mathbf{i}},$$
$$v_q=\sum_{ij} v_{ij} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})},$$

and wish to calculate

$$\dot{\mathbf{S}}_q|0)=[H,\mathbf{S}_q]|0),$$

where $|0)$ is the "bare" state. Both classically and quantum-mechanically we get (always in the ground state)

$$\dot{S}_q^y=v_0 S_q^z,$$
$$\dot{S}_q^z=(v_0-v_q)S_q^y. \quad \text{(II.4)}$$

These equations are exact. This is because the operator S_q^x can always be placed on the extreme right due to the commutability of the operators, $(i\neq j)$, and then we have $S_q^x|0)=|0)\delta_{q,0}$.

The equations give the harmonic-oscillator equations

$$\ddot{S}_q^\alpha+v_0(v_0-v_q)S_q^\alpha=0, \quad \alpha=y,z, \quad \text{(II.5)}$$

and so $\omega_q=[v_0(v_0-v_q)]^{1/2}$, confirming (II.3).

The normal mode η_q obeys $\dot{\eta}_q=i\omega_q\eta_q$, with normalization $[\eta_q^\dagger,\eta_q]=1$. Our previous expression (II.2) is thus confirmed.

Contact is later made with the many-body systems by taking S_i^z as nothing but the canonical conjugate of S_i^y. The S_i^y execute a coupled harmonic motion, (II.5), and since $S_i^z=(v_0)^{-1}\dot{S}_i^y$, (II.4), the "mass" of the particles in motion is $(v_0)^{-1}$. The normal mode is

$$(v_0\omega_q)^{-1/2}(\dot{S}_q^y\pm i\omega_q S_q^y). \quad \text{(II.6)}$$

We now verify that $|0)$ is a good approximation. We find the time taken for the state to spread. Although we could choose for $|0)$ an unknown wave packet with a specified smudge for the total spins (cf. Anderson's[12] discussion of the antiferromagnet), it is more convenient to take the product of spinors pointing in the x direction. This corresponds to the BCS ground state. Apart from the spread, there is no motion in equilibrium, $(0|\dot{S}_0^x|0)=0$. The lifetime of the state, τ, however, is given by $(0|(\dot{S}_0^x)^2|0)=(\tau^2)^{-1}(0|(S_0^x)^2|0)$. Therefore, taking $v_{ij}=$ constant, v, for z neighbors and zero otherwise, we obtain $\tau=(N/z)^{1/2}(\hbar/v)$. (This result is also obtained from the energy uncertainty

$$N^{-1}[(0|H^2|0)-|(0|H|0)|^2]^{1/2},$$

the factor $(N)^{-1}$ being necessary because the zero-point motion of the spins in $|0)$ are independent.) The unknown wave packet would be a better approximation, $[\tau\sim(N/z)(\hbar/v)]$, because, with the zero-point motion of the spins not independent, it is closer to the true ground state. However, the differences are of no importance; the approximation is well justified in either case.

[12] P. W. Anderson, Phys. Rev. **86**, 694 (1952).

5. The Analogy of the A.F. to the Many-Body Systems

The characteristic feature of all the many-body systems, apart from the I.F., in the symmetry of their Hamiltonians, is that whereas the generalized coordinates of the I.F. are all coupled with equal coupling, so that the Hamiltonian has full symmetry in the space defined by the generalized coordinates, the other systems do not have all generalized coordinates coupled, and are invariant only in a subspace. This feature is made particularly transparent in the A.F. model.

In this subsection we point out the analogy of the A.F. to systems with identical symmetry, leaving to the next section the more complex superconductor.

Superfluid Helium

The constant of motion, the analog of S_0^z, is $\lim_{q\to 0}\rho_q=\sum_k a_k^\dagger a_k$ i.e. the total number of particles N. The broken symmetry is a wave packet $|0)$, such that $a_0^\dagger|0)=a_0|0)=(N_0)^{1/2}|0)$, where N_0 is the number of particles with $k=0$ in the true ground state, i.e. the phase symmetry of $a_0e^{i\phi}$ is broken, (broken-gauge invariance). Then $\rho_q|0)=(N_0)^{1/2}(a_q^\dagger+a_{-q})|0)$. The operator $\lim_{q\to0}\rho_q=(N_0)^{1/2}(a_0^\dagger+a_0)$ rotates $|0)$, and the rotating $|0)$ generates the operator at right angles, viz. $(N_0)^{1/2}(a_0^\dagger-a_0)$, the analog of S_0^y. χ^{zz}, which is $dN/d\mu$, equals $(N_0v_0)^{-1}$. The "mass" of the "particles" is therefore $(N_0v_0)^{-1}$, which is confirmed by the approximate equation of motion at small q,

$$(2N_0v_0)^{-1}\frac{d}{dt}(a_q-a_{-q}^\dagger)=(a_q+a_{-q}^\dagger)=\rho_q(N_0)^{-1/2}.$$

The correctly normalized Bogoliubov particle is given at small q by

$$(N_0v_0/2\omega_q)^{1/2}\rho_q(N_0)^{-\frac{1}{2}}+(\omega_q/2N_0v_0)^{1/2}(a_q-a_{-q}^\dagger)$$

or by

$$\left(\frac{1}{2N_0v_0\omega_q}\right)^{1/2}\left[\frac{d}{dt}(a_q-a_{-q}^\dagger)+\omega_q(a_q-a_{-q}^\dagger)\right].$$

This has precisely the form of the mode in the A.F., (II.2) and (II.6). (The velocity of ordinary sound, c, is given by $dN/d\mu=(mc^2)^{-1}$ where m is the mass of the true particles.)

The Crystal Lattice

The total momentum $\mathbf{P}$ is the good quantum number. The analogy of $\mathbf{P}$ to S_0^z and $\mathbf{Q}$ (position of the center of mass), to $S_0^\perp$, (total spin in x-y plane), is obvious. $|0)$ is now a wave packet fixing $\mathbf{Q}$ within a distance of order a (the lattice spacing). If $\mathbf{Q}_q$ and $\mathbf{P}_q$ are defined by $\mathbf{u}_i=(1/\sqrt{N})\sum_q \mathbf{Q}_q e^{iq\cdot i}$ and $m\dot{\mathbf{u}}_i=(1/\sqrt{N})\sum_q \mathbf{P}_q e^{iq\cdot i}$, where $\mathbf{u}_i$ is the deviation from the lattice site $\mathbf{i}$ during the motion, then $\mathbf{Q}_q$ is the analog of S_q^y, and $\mathbf{P}_q$ of

S_q^z. The phonon mode is given by

$$(1/2m\omega_q)^{1/2}\mathbf{P}_q \pm i(\tfrac{1}{2}m\omega_q)^{1/2}\mathbf{Q}_q,$$

like the A.F. (II.2). The particles executing the coupled harmonic motion are now the true particles with mass m. $\mathbf{P}_q = m\dot{\mathbf{Q}}_q$.

It is a common feature of these systems, including the neutral superconductor now to be discussed, that, unlike the I.F. the collective mode has the form $(m/2\omega_q)^{1/2}(\dot{x}_q + i\omega_q x_q)$, where $\lim_{q\to 0} m\dot{x}_q$ restores the symmetry. So far, it has also been the case that $\lim_{q\to 0} x_q$ is the operator generated by the ground state as it recovers its symmetry, i.e. that x_q is the Goldstone coordinate. However, this is only a consequence of the symmetry of the A.F. type systems. In the superconductor, where the symmetrv is lower, it fails to apply, and the Goldstone coordinate has nothing to do with collective motion.

III. THE NEUTRAL SUPERCONDUCTOR

In this discussion of the superconductor, we stick to the spin model of Anderson[3] even at finite q. This makes it easier to study the modes, especially in relation to the anisotropic ferromagnet.

The Hamiltonian is given by

$$H = \sum_k (\epsilon_k - \mu)(n_k + n_{-k}) + \sum_{k\neq k',\,-(k'+q)} V b_k^{q\dagger} b_{k'}^{q},$$

in which $n_k = a_k^\dagger a_k$ and $b_k^q = a_{k+q} a_{-k}$, where a_k is the destruction operator for momentum k and spin up, and a_{-k} for momentum $-k$ and spin down. The second summation is over a shell about the Fermi surface and we take constant V for simplicity. The full Hamiltonian also has interaction terms bilinear in operators $\rho_{k\sigma}^q = a_{k+q\sigma}^\dagger a_{k\sigma}$, where σ denotes spin. These terms, however, are relatively unimportant for the neutral superconductor and are therefore not included here. The restriction $k \neq k'$, $-(k'+q)$ in H is often unimportant and we shall drop it when it is so.

We begin with the description of the ground state and the $q=0$ mode.[3] Therefore we need consider for the moment only the $q=0$ part of H, i.e., the BCS reduced Hamiltonian, H_{red}.

The spin model interprets an empty level k as having spin up in a fictitious space, and a full level as spin down. Thus, in terms of spin, the BCS operators are given as

$$S_k^z = \tfrac{1}{2}(1 - n_k - n_{-k}),$$
$$S_k^x + iS_k^y = b_k^\dagger,\quad S_k^x - iS_k^y = b_k.$$

H_{red} becomes in this notation,[3] (apart from a constant term),

$$H_{\text{red}} = -2\sum_k (\epsilon_k - \mu) S_k^z - \sum_{k\neq k'} V(S_k^x S_{k'}^x + S_k^y S_{k'}^y),$$

where the second summation is over a shell about the Fermi surface. This model is clearly very similar to the A.F. but its difference proves to be of great significance. The difference is that, whereas the A.F. has no field (or a constant field) in the z direction, the superconductor has a varying field $(\epsilon_k - \mu)$.

In the true ground state, the spins precess in phase at varying orientation θ_k with the z axis. The molecular field I in the x-y plane is $I = V\sum S \sin\theta_k$, $(S=\tfrac{1}{2})$; therefore the total field acting on spin k is of magnitude $H_k = [(\epsilon_k - \mu)^2 + I^2]^{1/2}$, at angle θ_k given by

$$\sin\theta_k = I/H_k. \tag{III.1}$$

The symmetry is broken by taking all the spins to lie in the z-x plane.

Before considering the connection between broken symmetry and normal mode, we find the modes given by the equations of motion in the random-phase approximation (R.P.A.).[3,13]

1. The Equations of Motion in R.P.A.

The equations of motion about the approximate ground state are (both classically and quantum-mechanically)

$$\dot{S}_k^y = H_k S_k^{||}$$
$$\dot{S}_k^{||} = -H_k S_k^y + V \sum_{k\neq k'} S_{k'}^y, \tag{III.2}$$

where $S_k^{||}$ is in the z-x plane in the direction perpendicular to the equilibrium position. This motion gives S_k^y and $S_k^{||}$ even in $\epsilon_k - \mu$, which is the motion of the $\omega=0$ mode; thus the term $V\cos\theta_k \sum S_k^x$, which appears in general in $\dot{S}_k^y$, vanishes.

The collective modes η_ω are found by substituting

$$\eta_\omega = \sum_k (A_k^\omega S_k^{||} + B_k^\omega S_k^y)$$

in (III.2), with the requirement $\dot{\eta}_\omega = i\omega\eta_\omega$, and equating the coefficients of S_k^y and $S_k^{||}$ respectively. We obtain

$$\begin{aligned} A_k^\omega &= (H_k V/(H_k^2 - \omega^2))\sum A_k^\omega \\ B_k^\omega &= (i\omega V/(H_k^2 - \omega^2))\sum A_k^\omega. \end{aligned} \tag{III.3}$$

The condition $\sum A_k^\omega \neq 0$ in (III.3) gives the dispersion equation for ω,

$$1 = V\sum (H_k/(H_k^2 - \omega^2)),$$

with solutions $\omega \sim H_k$ and $\omega = 0$. The collective mode η_ω is given by

$$\eta_\omega = \left[2\omega \sum \frac{H_k}{(H_k^2 - \omega^2)^2}\right]^{-1/2} \sum \frac{H_k S_k^{||} + i\omega S_k^y}{H_k^2 - \omega^2}. \tag{III.4}$$

This has the same form as (II.2).

The $\omega=0$ mode is $\sum (S_k^{||}/H_k)$. Let us check that this is identical to the symmetry restoring mode, $\sum S_k^z$, which rotates the spins about the z axis. Semiclassically, the operator $\mathbf{S}_k$ is interpreted as the small deviation from equilibrium, and its component in the x-z plane is

[13] G. Rickayzen, Phys. Rev. **115**, 795 (1959).

$S_k^{||}$. Hence $\sum S_k^z = \sum S_k^{||} \sin\theta_k$, which from (III.1) is precisely $I\sum(S_k^{||}/H_k)$, as required. We now give the quantum-mechanical argument. The $\omega=0$ mode is $\sum S_k^z$ only when the ground state is expressed in the x,y,z system of coordinates, i.e. the BCS ground state. This is not the system of coordinates in (III.2), however, and S_k^z is given by $S_k^z = S_k^{||}\sin\theta_k + S_k^{x'}\cos\theta_k$, where the x' axis is parallel to the spin in the ground state. A rotation of the spin through ϕ about the z axis is, therefore $\prod_k\{\exp[i\phi(S_k^{||}\sin\theta_k + S_k^{x'}\cos\theta_k)]\}|0)$. Since the operator $\exp(i\phi S_k^{x'}\cos\theta_k)$ merely introduces a phase factor, the symmetry-restoring mode is $\sum S_k^{||}\sin\theta_k$.

In the absence of the collective term in (III.2), η_ω is $S_k^{||}+iS_k^y$ and $\omega=H_k$, i.e. the excitations are individual spin flips equivalent to the Bogoliubov-excitations, $\alpha_{k1}\alpha_{k0}$. Extending these considerations to finite q, we define $S_{k||}^q$ and S_{ky}^q by $S_{k||}^q + iS_{ky}^q = \alpha_{k1}\alpha_{k+q,0}$, $S_{k||}^q - iS_{ky}^q = \alpha_{k+q,0}^\dagger\alpha_{k1}^\dagger$. In the absence of collective terms, $S_{k||}^q + iS_{ky}^q$ is an individual excitation of energy $H_{k+q}+H_k$, which we shall denote by H_k^q.

The equations of motion in R.P.A.[3,13] for the neutral gas are

$$\dot{S}_{ky}^q = H_k^q S_{k||}^q,$$

$$\dot{S}_{k||}^q = H_k^q S_{ky}^q - \cos\tfrac{1}{2}(\theta_k-\theta_{k+q})V \times \sum_{k'\neq k}\cos\tfrac{1}{2}(\theta_{k'}-\theta_{k'+q})S_{k'y}^q. \quad \text{(III.5)}$$

These are the generalization to finite q of the equations (III.2). We are considering only the motion which gives even solutions at $q\to 0$, and for small q we have therefore neglected a term in $\dot{S}_{ky}^q$.

We seek a solution of the form

$$\eta_\omega^q = \sum_k (A_k^q S_{k||}^q + B_k^q S_{ky}^q)$$

where $\dot{\eta}_\omega^q = i\omega\eta_\omega^q$. Substituting into (III.5) and equating coefficients of $S_{k||}^q$ and S_{ky}^q, respectively, we get

$$A_k^q = \frac{V\cos\frac{1}{2}(\theta_k-\theta_{k+q})H_k^q}{(H_k^q)^2-\omega^2}\sum_{k'}\cos\tfrac{1}{2}(\theta_{k'}-\theta_{k'+q})A_{k'}^q$$

$$B_k^q = (i\omega/H_k^q)A_k^q. \quad \text{(III.6)}$$

The dispersion equation for ω is the condition $\sum\cos\frac{1}{2}\times(\theta_{k'}-\theta_{k'+q})A_{k'}^q \neq 0$ in (III.6), i.e.,

$$1 = \sum_k [H_k^q \cos^2\tfrac{1}{2}(\theta_k-\theta_{k+q})/((H_k^q)^2-\omega^2)]. \quad \text{(III.7)}$$

The collective modes are given by

$$\eta_\omega^q = \left(\omega\sum_k \frac{H_k^q\cos^2[\frac{1}{2}(\theta_k-\theta_{k+q})]}{((H_k^q)^2-\omega^2)^2}\right)^{-1/2} \times\sum_k \frac{\cos[\frac{1}{2}(\theta_k-\theta_{k+q})]}{(H_k^q)^2-\omega^2}(H_k^q S_{k||}^q + i\omega S_{ky}^q). \quad \text{(III.8)}$$

(III.7) has two types of solutions[3]; the large ω, which are the independent-particle excitations, and the low-lying ω, viz. $\omega=(v_F/\sqrt{3})q$ at small q, where v_F is the Fermi velocity.

It has not been proved whether the R.P.A. is a good approximation. Of course, at $q=0$ the mode is exact. The equations of motion are exact because $k\neq k'$ in H_{red}, which does not however hold in general. Moreover, no possibility exists of handling the problem by comparison with the exactly soluble A.F. This is because contact between the models can only be made by taking[14] $\epsilon_k-\mu$ as zero in the shell or as constant. However, this passage is discontinuous since the ground state is given a translational symmetry.

In this paper, we continue to assume the existence of a spectrum at small q, but caution the reader on the incomplete character of the subsequent development.

2. The Goldstone Coordinate and Sum Rules

We now attempt to repeat the discussion of the broken symmetry and the normal mode along the lines given for the A.F., but we shall see that the Goldstone coordinate has no connection with the normal mode.

By the Anderson theorem, the mode at $q,\omega\to 0$ is $\sum_k S_{kz}$. Since the Goldstone coordinate is $\sum_k S_{ky}^q$, one would expect $\sum_k S_{ky}^q$ to be a linear combination of η_q. Thus, since $\sum_k S_{kz} = I\sum_k(S_k^{||}/H_k)$, (paragraph following III.4), the correctly normalized mode expected, in analogy to the I.F., would be

$$\eta_q = [\sum_k (S_{k||}^q/H_k) \pm iA_q\sum_k S_{ky}^q]/|(A_q\sum H_k^{-1})^{-1/2}$$

where

$$\lim_{q\to 0} A_q = 0. \quad \text{(III.9)}$$

(The normalization is correct because $[S_{ky}^q, S_{k||}^q] = iS$.) However, trouble arises when we go to χ^{zz} to find A_q.

The response is to a field h_k acting on each spin in the positive z direction; its magnitude may vary with k but must be even in $\epsilon_k-\mu$. Such a field gives rise to no collective effect, and each spin responds independently. Each spin therefore points parallel to the resultant of the fields h_k and H_k, i.e. at angle $\delta\theta_k = (h_k\sin\theta_k/H_k)$ to the direction of H_k, the original direction of the spin. The increment of the spin in the z direction is $\delta\theta_k\sin\theta_k$, and so

$$\chi^{zz} = \sum_k (\sin^2\theta_k/H_k) = I^2\sum_k (H_k^3)^{-1}.$$

The formal expression for $\lim_{q\to 0}\chi_q^{zz}(0)\,k$, then gives a sum rule. On substituting the mode (III.9), we get

$$\lim_{q\to 0}\frac{A_q}{\omega_q}\sum_k (H_k)^{-1} = \sum_k (H_k^3)^{-1}.$$

But, since the H_k are independent, A_q is k dependent, i.e. $\lim_{q\to 0} A_q/\omega_q = H_k^{-2}$ and so $\sum_k S_{ky}^q$ does not con-

[14] The identification $\Sigma b_k^q = S_q^-$, etc. is then made and H_k^q is constant. η_q and the dispersion equation for ω_q become those of A.F., with $S_q^{||}$ instead of S_q^z if the field is finite.

tribute to η_q. One obtains, therefore, instead of (III.9)

$$\eta_q=[\sum_k H_{k\|}{}^{-1}S_k{}^q \pm i\omega_q \sum_k H_k{}^{-2}S_{ky}{}^q] \times(\omega_q \sum H_k{}^{-3})^{-1/2} \quad \text{(III.10)}$$

which agrees with the R.P.A. (III.8), to lowest order in q.

The Goldstone coordinate $\sum_k S_{ky}{}^q$, therefore, has nothing to do with the collective motion. This is because the system does not have $\lim_{q\to 0}\sum_k \dot{S}_{ky}{}^q$ as its symmetry restoring operator. The reason for the failure lies in the lower symmetry of this system, but cannot be ascertained independently of the dynamics.

There will be a singularity in the Goldstone response function, $\chi_q{}^{yy}(\omega)$, at $q,\omega=0$, as a consequence of the broken symmetry. In the present model, it is impossible that this pole is also the terminus of a continuous spectrum. The conditions for a spectrum would have to be sought by the alternative way given for the A.F. viz. in the continuity of $\lim_{q,\omega\to 0}\chi_q{}^{zz}(\omega)=(v_0)^{-1}$ and the condition that $\lim_{q\to 0}\langle 0|(\sum H_k{}^{-1}S_{k\|}{}^q)^2|0\rangle\to 0$, (cf. A.F. and Ref. 11). The necessity for the latter relation is seen as follows, on recalling that

$$\lim_{q\to 0}\sum_k (S_{k\|}{}^q/H_k)=\sum_k S_{kz}=-\lim_{q\to 0}\rho_q.$$

At $q=0$, the restored symmetry of the "dressed" state requires $\langle 0|(\rho_0)^2|0\rangle=N^2$. However, when we go to the limit $q\to 0$, we are finding $\langle 0|(\rho_0)^2|0\rangle-(\langle 0|\rho_0|0\rangle)^2$, which is zero.

In a charged superconductor, $\lim_{q,\omega\to 0}\chi_q{}^{zz}(\omega)$ is not continuous on account of the discontinuity in the Coulomb interaction due to the background, and the usual plasma effect occurs.[3,8]

The Frequency ω_q

The sum rule most convenient for a gas is the well-known relation[8]

$$\langle 0|[\rho_q,\rho_q]|0\rangle=q^2/2m.$$

Substituting η_q, (III.10), at small q, $(\sum(S_{k\|}{}^q/H_k)\to -\rho_q$ as $q\to 0)$, we get $\omega_q{}^2=(q^2/2m)/\sum(I^2/H_k{}^3)$ at small q.

$\sum(I^2/H_k{}^3)=\chi^{zz}$ is alternatively written as $(mc^2)^{-1}$, where c is the velocity of ordinary sound, since $\chi^{zz}\equiv dN/d\mu$ and $dN/d\mu=(mc^2)^{-1}$. Hence

$$\omega_q=cq$$

and the collective modes are truly phonons. As a first approximation, (independent of V), the free-gas value for $dN/d\mu$ can be taken, viz. $g(\epsilon_F)$,[15] giving $c=v_F/\sqrt{3}$, (the R.P.A. value).

In a normal fermion gas, there is no broken symmetry, and $\lim_{q\to 0}\rho_q$ is no mode. The neutral gas has modes of zero sound.[8]

The ω Distribution of States

Since at $q\to 0$, $\sum(S_{k\|}{}^q/H_k)\to -\rho_q$ and

$$\sum(I^2/H_k{}^3)=\chi^{zz}\equiv dN/d\mu=(mc^2)^{-1},$$

the sum rules and continuity conditions are exactly the same as for superfluid helium (cf. Sec. II.5). Huang and Klein[6] have found the shape of the ω distribution of states by means of a dispersion relation, employing only these sum rules with the assumption of continuity. The procedure is identical for the superconductor. We quote the result.

The distribution curve, defined by

$$\mathcal{S}_q(\omega)=\sum_n|\langle n|\sum(IS_{k\|}{}^q/H_k)|0\rangle|^2\delta(\omega-\omega_{n0})\to \sum_n|\langle n|\rho_q|0\rangle|^2\delta(\omega-\omega_{n0}),$$

is found, in the small q limit and near the peak $\omega\sim cq$, to be

$$\mathcal{S}_q(\omega)=\langle 0||\rho_q|^2|0\rangle(\pi)^{-1}\Gamma_q/((\omega-cq)^2+\Gamma_q{}^2),$$

where Γ_q approaches 0 faster than q. At $q\to 0$, it reduces to the δ function required.

ACKNOWLEDGMENTS

It is a pleasure to express my gratitude to Professor R. Brout for introducing me to this problem, for his numerous suggestions and ideas, and for his helpful criticism of the manuscript. I wish also to thank Professor F. Englert for some valuable discussions.

I gratefully acknowledge the financial support of a CIBA Fellowship and the partial support of a NATO Science Fellowship.

APPENDIX

We describe a proof due to Professor R. Brout of the existence of the Goldstone pole at finite temperature. It is a generalization of similar proofs at $T=0$ given in Ref. (1). The proof gives the pole at $q=0$, $\omega=0$ only. The extension to finite q,ω is complicated by the fact that the modes are hydrodynamic at small q,ω, (see the work of Hohenberg and Martin[16] on superfluid helium).

We work in the isotropic Heisenberg ferromagnet. Consider it to have magnetization $\mathbf{R}$ in a field $\mathbf{H}$, and consider the free energy as a function of $\mathbf{R}$ and $\mathbf{H}$, $F(\mathbf{R},\mathbf{H})$. (The partition function is $Z(\mathbf{R},\mathbf{H})=\mathrm{Tr}_{\mathbf{R}} \times\exp[-\beta(H+\mathbf{H}\cdot\sum\mathbf{S}_i)]$ with the trace restricted to give $\mathbf{R}$.) The dependence of $\mathbf{R}$ on $\mathbf{H}$ is fixed by minimization, $\partial F/\partial\mathbf{R}=0$.

However, let us first consider $\partial F/\partial\mathbf{R}$ for independent

[15] This result is also obtained directly from $\Sigma(I^2/H_k{}^3)$, by noting that its integral $\int(I^2/H_k{}^3)g(\epsilon)d\epsilon$ is over a shell of order of thickness I about the Fermi surface, and that $H_k\simeq I$; hence $\Sigma(I^2/H_k{}^3)\approx g(\epsilon_F)$.

[16] P. C. Hohenberg and P. C. Martin, Phys. Rev. Letters 12, 69 (1964).

$\mathbf{R}$, and study the variation of the quantity $\partial F/\partial \mathbf{R}$ due to small independent changes in $\mathbf{R}$ and $\mathbf{H}$.

$$\delta\left(\frac{\partial F}{\partial R_x}\right)=\frac{\partial^2 F}{\partial R_x \partial \mathbf{R}}\cdot\delta\mathbf{R}+\frac{\partial^2 F}{\partial R_x\partial \mathbf{H}}\cdot\delta\mathbf{H}.$$

Taking now $\delta\mathbf{R}$ along the curve $\partial F/\partial\mathbf{R}=0$, the left-hand side is zero. Along the curve we have $(\partial F/\partial H_u)_{\mathbf{R}}=-R_u$, therefore, $0=(\partial^2F/\partial R_x\partial\mathbf{R})\cdot\delta\mathbf{R}+\delta H_x$. If we consider $\delta\mathbf{R}$ as independent, and $\delta\mathbf{H}$ along the equilibrium curve, then, taking for example $\delta\mathbf{R}=\delta R_x$, we have

$$\frac{\partial^2 F}{\partial R_x^2}=\frac{dH_x}{dR_x}=(\chi_{xx})^{-1}. \tag{A.1}$$

The following symmetry argument will now give $\chi_{xx}\rightarrow\infty$. Imagine the symmetry artificially broken in the z direction in the absence of field. Since all directions are equivalent, the system may be rotated with no change in F. Thus a small rotation about the y axis, which produces a small increment δR_x, gives

$$\delta F=0=(\partial F/\partial R_x)\delta R_x+\tfrac{1}{2}(\partial^2F/\partial R_x^2)(\delta R_x)^2.$$

Since δR_x is arbitrary, $\partial^2F/\partial R_x^2=0$, and from (A.1), $\chi_{xx}\rightarrow\infty$. ($\partial F/\partial R_x=0$ in any case by the variation principle.) Since $\chi_{xx}=\beta\langle(S_0^x)^2\rangle$, this gives $\langle(S_0^x)^2\rangle\rightarrow\infty$, where $\langle(S_0^x)^2\rangle=[\mathrm{Tr}e^{-\beta H}(S_0^x)^2]/\mathrm{Tr}e^{-\beta H}$. At $T=0$, $\langle 0|(S_0^x)^2|0\rangle$ is finite, but $\beta\rightarrow\infty$.

[17] Y. Nambu, Phys. Rev. **117**, 648 (1960).
[18] P. Nozières and J. M. Luttinger, Phys. Rev. **127**, 1423 (1962).

PHYSICAL REVIEW VOLUME 147, NUMBER 1 8 JULY 1966

Potential of Average Force in a Plasma*

O. Theimer†
Institut für Plasmaphysik, Garching bei München, Germany

AND

P. Kepple
Department of Physics, New Mexico State University, University Park, New Mexico
(Received 7 February 1966)

The potential of average force $W_{1,2}^{qq'}$ experienced by a charge q' at a distance $|\mathbf{r}_1-\mathbf{r}_2|$ from a charge q is calculated from the Bogoliubov-Born-Green-Kirkwood-Yvon equations of classical statistical mechanics without linearization or equivalent approximations. Diverging integrals are eliminated by the condition that bound-particle states with negative internal energy, e.g., atoms, be excluded from the partition function. The 3-particle distribution functions required for calculating $W_{1,2}^{qq'}$ are obtained as solutions of a nonlinearized Poisson-Boltzmann equation for the average potential in the neighborhood of two charges fixed at $\mathbf{r}_1$ and $\mathbf{r}_2$. For this latter calculation the difference between average potential and potential of average force is neglected. With the help of $W_{1,2}^{qq'}$ the average thermal energy of the plasma is computed and compared with the result of the linearized Debye-Hückel theory. Numerical corrections to the latter theory are presented and it is shown that linearization is a far more significant source of errors than identification of average potential with potential of average force.

I. INTRODUCTION

ONE of the standard methods for calculating the thermodynamic functions of a plasma is the solution of the Poisson-Boltzmann equations. For a plasma consisting of electrons and one species of monovalent ions they have the form[1,2]

$$\nabla^2\phi_{1,2}^{+}=-4\pi e[n_{1,2}^{++}-n_{1,2}^{+-}+\delta(\mathbf{r}_{12})], \tag{1}$$

$$n_{1,2}^{++}=n\exp[-W_{1,2}^{++}/kT], \tag{2}$$

$$n_{1,2}^{+-}=n\exp[-W_{1,2}^{+-}/kT]. \tag{3}$$

Throughout this paper the notation is such that subscripts $i=1, 2, 3, \cdots$ indicate specified particle positions $\mathbf{r}_i$, and superscripts $q=+, -$ the charge qe of specified particles. Thus, $\phi_{1,2}^{+}$, $n_{1,2}^{++}$, $n_{1,2}^{+-}$ are, respectively, the ensemble averages of the potential, the ion density, and the electron density at $\mathbf{r}_2$ if an ion is fixed at $\mathbf{r}_1$; $W_{1,2}^{++}$ and $W_{1,2}^{+-}$ are the potentials of the average force experienced by the particles at $\mathbf{r}_2$; and n, T, k are, respectively, the average electron density, the temperature, and the Boltzmann constant. In a macroscopically homogeneous, isotropic plasma the quantities with subscript ij depend only on the distance

$$r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|, \tag{4}$$

* Work supported by the U. S. Air Force Office of Scientific Research.
† On leave of absence from New Mexico State University, Research Center, University Park, New Mexico.
[1] A. Münster, *Statistische Thermodynamik* (Springer Verlag, Berlin, 1956), Chaps. VIII and XXI.
[2] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), Chap. VII.