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Particle-Hole Inversion in the Fermi Surface: A Symmetry Operation for Collective Excitations

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The operation of transposing particles (or holes) on one side of a Fermi surface into holes (or particles) on the other side is shown to be a symmetry operation of the Bardeen, Cooper, and Schrieffer reduced Hamiltonian, and an approximate symmetry operation of the full two-particle scalar interaction Hamiltonian, insofar as particle-conserving collective excitations are concerned. Calling this operation f inversion, and the conserved quantity associated with it f parity, the zero-rest-energy collective excitations in a Fermi gas with weak attractive interactions prove to have f parity $=-1$.

INTRODUCTION

In the absence of an external potential, the ground state of a system of noninteracting fermions is characterized by the facts that all single-particle number operators $c_k^\dagger c_k$ have expectations $\langle c_k^\dagger c_k\rangle$ that are either 1 or 0, and that no unoccupied state has lower energy than an occupied state. (The subscript k denotes both spin projection σ_z and wave-vector components k_x, k_y, k_z.) For each spin projection, a spherical Fermi surface separates the region in wave-vector space where $\langle c_k^\dagger c_k\rangle=1$ from that where $\langle c_k^\dagger c_k\rangle=0$. When an interaction is introduced, the Fermi surfaces lose some of their sharpness, but may be defined still to exist at the locus where $\langle c_k^\dagger c_k\rangle=\frac{1}{2}$. Figure 1 shows the sort of variation of $\langle c_k^\dagger c_k\rangle$ with $|\mathbf{k}|=|(k_x,k_y,k_z)|$ that is found in the presence of weak interaction.

When the interaction is weak, $\langle c_k^\dagger c_k\rangle$ differs sensibly from 1 or 0 only within a thin shell of wave-vector space containing the Fermi surface. Within this shell the density of states is nearly constant, and the substitution of particles (or holes) on one side of a Fermi surface for holes (or particles) on the other side suggests itself as a symmetry operation.

IDEALIZED MODEL

Consider first an idealized model, consisting of the following:

(1) A gas of n fermions.

(2) Wave vector space restricted to a rectangular box with sides parallel to the k_x, k_y, k_z axes, containing $2n$ states with uniform density. The ranges of k_x and k_y are $\pm\delta$ and the range of k_z is $k_f\pm\Delta$ with $k_f>0$.

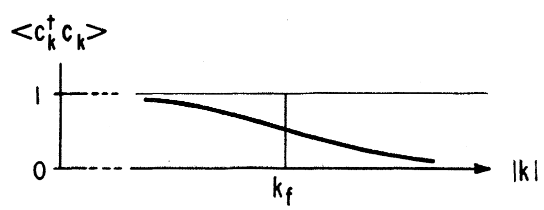

FIG. 1. Variation of $\langle c_k^\dagger c_k\rangle$ with $|\mathbf{k}|$ in the neighborhood of a Fermi surface.

(3) A Hamiltonian operator

$$T=\sum_k(\mu+\epsilon_k)c_k^\dagger c_k,$$

where μ is a constant and $\epsilon_k\sim k_z-k_f$.

The Fermi surface then corresponds to $k_z=k_f$. Let the empty box in wave vector space be represented by the state vector $|0\rangle$. Then the ground state of the system is

$$|G\rangle=\Pi(k\text{ with }k_z<k_f)c_k^\dagger|0\rangle.$$

The proposed symmetry operation is accomplished by the unitary canonical transformation f,

$$fc_k^\dagger f^{-1}=c_{\alpha k},$$
$$fc_kf^{-1}=c_{\alpha k}^\dagger,$$
$$f|0\rangle=\Pi_k c_k^\dagger|0\rangle,$$

where the operator α transforms k to αk, its mirror image across the Fermi surface,

$$\alpha(\sigma_z,k_x,k_y,k_z)=(\sigma_z,k_x,k_y,2k_f-k_z),$$
$$\alpha^2=1.$$

The transformed ground state and Hamiltonian operator are

$$f|G\rangle=|G\rangle,$$
$$fTf^{-1}=T+\mu\sum_k(1-2c_k^\dagger c_k)$$
$$=T+2\mu(n-N),$$

where $N=\sum_k c_k^\dagger c_k$ is the particle-number operator. Multiplying the second of these equations on the right by f, one has

$$fT-Tf=2\mu(n-N)f.$$

Hence f and T commute whenever they act upon a state containing n fermions, for which

$$(n-N)f|n\text{ fermions}\rangle=0.$$

It follows that f is a constant of the motion for the n-fermion system under consideration. The symmetry operation f will be called f inversion, short for particle-hole inversion in the Fermi surface, and the associated conserved quantity will be called f parity.

Any simultaneous eigenstate of N and T can be written in the form $\Lambda|G\rangle$ where Λ is the appropriate

operator and $|G\rangle$ is the n-fermion ground state,

$$N\Lambda|G\rangle=(n+\lambda)\Lambda|G\rangle,$$
$$T\Lambda|G\rangle=(E_\lambda+\mu\lambda)\Lambda|G\rangle.$$

The operator $f\Lambda f^{-1}$ then generates another simultaneous eigenstate of N and T with the properties

$$Nf\Lambda f^{-1}|G\rangle=(n-\lambda)f\Lambda f^{-1}|G\rangle,$$
$$Tf\Lambda f^{-1}|G\rangle=(E_\lambda-\mu\lambda)f\Lambda f^{-1}|G\rangle.$$

[The second of these equations results from transforming the equation $T\Lambda|G\rangle=(E_\lambda+\mu\lambda)\Lambda|G\rangle$, the left-hand term giving

$$\begin{aligned} fT\Lambda|G\rangle &= fTf^{-1}f\Lambda f^{-1}f|G\rangle \\ &= [T+2\mu(n-N)]f\Lambda f^{-1}|G\rangle \\ &= (T+2\mu\lambda)f\Lambda f^{-1}|G\rangle \end{aligned}$$

and the right-hand term giving $(E_\lambda+\mu\lambda)f\Lambda f^{-1}|G\rangle$.]

If the operator Λ conserves particles, $\lambda=0$ and the states $\Lambda|G\rangle$ and $f\Lambda f^{-1}|G\rangle$ are degenerate. The linear combinations

$$|\Lambda+\rangle=(\Lambda+f\Lambda f^{-1})|G\rangle,$$
$$|\Lambda-\rangle=(\Lambda-f\Lambda f^{-1})|G\rangle,$$

then are eigenstates of N and T with, respectively, even and odd f parity,

$$f|\Lambda+\rangle=+|\Lambda+\rangle,$$
$$f|\Lambda-\rangle=-|\Lambda-\rangle.$$

GENERALIZATION

The idealized model can be generalized in steps.

(1) Let the definition of f inversion be changed, from inversion along a line perpendicular to the Fermi surface to inversion along a line parallel to an auxiliary vector $\boldsymbol{\alpha}$. The line joining αk to k then is parallel to $\boldsymbol{\alpha}$ and is bisected by the Fermi surface, as sketched in Fig. 2, and the sides of the box in wave-vector space are taken parallel and perpendicular to $\boldsymbol{\alpha}$. The new definition of f inversion does not affect the results obtained with the idealized model.

(2) Enlarge the volume of wave vector space under consideration, by completely enclosing a spherical Fermi surface in a large number of contiguous boxes with sides parallel to $\boldsymbol{\alpha}$. The allowed volume of wave-vector space then is increased to a thin shell bisected (in the direction of $\boldsymbol{\alpha}$) by the Fermi surface. Again the results obtained with the idealized model are unaffected.

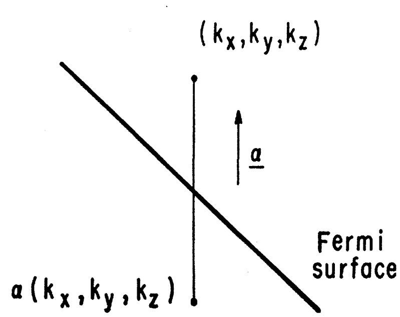

FIG. 2. Transformation of (k_x,k_y,k_z) by the operator α.

(3) Add to the Hamiltonian an interaction term of the form

$$V_s=\tfrac{1}{2}\sum_{kl}V(k-l)c_k^\dagger c_{-k}^\dagger c_{-l}c_l,$$

where $V(k-l)=0$ unless k and l have equal spin projections, and let the shell of wave-vector space be constructed so that it contains both $\pm k$. The transformed interaction is

$$fV_sf^{-1}=\tfrac{1}{2}\sum_{kl}V(\alpha k-\alpha l)c_k^\dagger c_{-k}^\dagger c_{-l}c_l.$$

Because wave-vector space is restricted to a thin shell, it follows that

$$\alpha k-\alpha l\approx k-l,$$
$$fV_sf^{-1}\approx V_s,$$

so that f commutes with V_s to good approximation. The Hamiltonian

$$H_r=T+V_s,$$

with which f commutes to good approximation, is the reduced Hamiltonian used by Bardeen, Cooper, and Schrieffer[1] in their theory of superconductivity.

(4) Finally extend wave-vector space without limit, and enlarge the Hamiltonian operator H to include the full scalar two-body interaction

$$V=\tfrac{1}{2}\sum_{kls}V(s)c_{k+s}^\dagger c_{l-s}^\dagger c_lc_k,$$

where s stands for wave-vector components only. The operation of f inversion is not defined for points in wave-vector space far from the Fermi surface; and even where it can be defined, it no longer commutes with all of H. Hence f parity survives only approximately, to the extent that the parts of the Hamiltonian with which f does not commute are small, and to the extent that wave vector space far from the Fermi surface can be ignored.

APPLICATION TO SUPERCONDUCTORS

Blatt[2] has shown that the Bardeen, Cooper, and Schrieffer superconducting ground state,

$$|\mathrm{BCS}\rangle=\Pi_s[(1-h_s)^{\frac{1}{2}}+h_s^{\frac{1}{2}}c_{\uparrow s}^\dagger c_{\downarrow -s}^\dagger]|0\rangle,$$

can be written

$$|\mathrm{BCS}\rangle=\Pi_s(1-h_s)^{\frac{1}{2}}[1+W^\dagger+(W^\dagger)^2/2!+(W^\dagger)^3/3!+\cdots]|0\rangle,$$

where $W^\dagger$ is the pair creation operator,

$$W^\dagger=\sum_s h_s^{\frac{1}{2}}(1-h_s)^{-\frac{1}{2}}c_{\uparrow s}^\dagger c_{\downarrow -s}^\dagger.$$

The un-normalized portion of $|\mathrm{BCS}\rangle$ with exactly n pairs is

$$|nu\rangle=\Pi_s(1-h_s)^{\frac{1}{2}}(n!)^{-1}(W^\dagger)^n|0\rangle,$$

with all n pairs in the same state. Its length $\langle nu|nu\rangle$ is a maximum in the neighborhood of $n=\langle\mathrm{BCS}|(N/2)|\mathrm{BCS}\rangle=n_0$, so that for $n\approx n_0$ the normalized n-pair

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[2] J. M. Blatt, Progr. Theoret. Phys. (Kyoto) **23**, 447 (1960).

ground state $|n\rangle$ is

$$|n\rangle=(1+\text{terms of order } n_0^{-1})\langle n_0u|n_0u\rangle^{-\frac{1}{2}}|nu\rangle \approx \langle n_0u|n_0u\rangle^{-\frac{1}{2}}|nu\rangle.$$

Further (still for $n\approx n_0$), $n!\approx n_0!(n_0)^{n-n_0}$ so that

$$|n\rangle\approx A(n_0^{-1}W^\dagger)^n|0\rangle,$$

where A is a constant.

In other words, for $n\approx n_0$, the operator

$$B^{(+)}=n_0^{-1}W^\dagger=n_0^{-1}\sum_s h_s^{\frac{1}{2}}(1-h_s)^{-\frac{1}{2}}c_{\uparrow s}{}^\dagger c_{\downarrow -s}{}^\dagger$$

has the simple property of adding one pair to the Bardeen, Cooper, Schrieffer n-pair ground state,

$$B^{(+)}|n\rangle\approx|n+1\rangle.$$

It will be shown that the operator

$$B^{(-)}=-fB^{(+)}f^{-1} = n_0^{-1}\sum_s(1-h_s)^{\frac{1}{2}}h_s^{-\frac{1}{2}}c_{\downarrow -s}c_{\uparrow s}$$

subtracts one pair,

$$B^{(-)}|n\rangle\approx|n-1\rangle.$$

The commutator $[H,A]$ can be linearized with respect to the Bardeen, Cooper, Schrieffer n-pair states $|n\rangle$ with $n\approx n_0$, according to the following prescription proposed by Anderson[3]:

(1) Retain all of $[T,A]$.

(2) Discard all of $[V,A]$ save terms that contain a factor

$$c_k{}^\dagger c_k,\quad c_{\uparrow s}{}^\dagger c_{\downarrow -s}{}^\dagger,\quad \text{or}\quad c_{\downarrow -s}c_{\uparrow s}.$$

(3) Contract the remaining terms in $[V,A]$ by making the substitutions

$$c_k{}^\dagger c_k\to\langle n|c_k{}^\dagger c_k|n\rangle=h_k,$$
$$c_{\uparrow s}{}^\dagger c_{\downarrow -s}{}^\dagger\to\langle n+1|c_{\uparrow s}{}^\dagger c_{\downarrow -s}{}^\dagger|n\rangle B^{(+)}=[h_s(1-h_s)]^{\frac{1}{2}}B^{(+)},$$
$$c_{\downarrow -s}c_{\uparrow s}\to\langle n-1|c_{\downarrow -s}c_{\uparrow s}|n\rangle B^{(-)}=[h_s(1-h_s)]^{\frac{1}{2}}B^{(-)},$$

which leave unaltered all matrix elements between pairs of states $|n\rangle$ with $n\approx n_0$.

The final substitutions for $c_{\uparrow s}{}^\dagger c_{\downarrow -s}{}^\dagger$ and $c_{\downarrow -s}c_{\uparrow s}$ contain ground pair operator factors $B^{(+)}$ and $B^{(-)}$ that are not written down in Anderson's treatment, although their presence is implied in his work. Their explicit introduction makes it clear that Anderson's linearization procedure is appropriate for a Fermi gas containing a fixed number of particles.

The linearization prescription can be applied to $[H,B^{(+)}]$ without making use of $B^{(-)}$. Noting that for the Hamiltonian

$$H=\sum_k T_k c_k{}^\dagger c_k+\tfrac{1}{2}\sum_{kls}V(s)c_{k+s}{}^\dagger c_{l-s}{}^\dagger c_l c_k,$$

the Bardeen, Cooper, Schrieffer analysis gives

$$\mu+\epsilon_s=T_s+\sum_k V(0)h_k-\sum_t V(t)h_{s+t},$$
$$\epsilon_{0s}=-\sum_t V(t)[h_{s+t}(1-h_{s+t})]^{\frac{1}{2}},$$
$$h_s=\tfrac{1}{2}[1-\epsilon_s(\epsilon_s^2+\epsilon_{0s}^2)^{-\frac{1}{2}}],$$

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

it follows that

$$[H,B^{(+)}]_{\text{lin}}=2\mu B^{(+)}.$$

Applying both sides of this equation to the n-pair ground state $|n\rangle$ with energy E_{0n}, one has

$$HB^{(+)}|n\rangle=(E_{0n}+2\mu)B^{(+)}|n\rangle,$$

within the linearization approximation.

Hence the operator $B^{(+)}$ generates a simultaneous eigenstate of H and N within the linearization approximation, and another such operator can be produced from it by f inversion. Noting that $h_{\alpha s}=1-h_s$, this operator is

$$B^{(-)}=-fB^{(+)}f^{-1},$$

and it satisfies the linearized equation

$$[H,B^{(-)}]_{\text{lin}}=-2\mu B^{(-)}.$$

Since $B^{(-)}$ decreases the particle number by two and decreases the energy by the chemical potential of a pair of particles, it is clear that $B^{(-)}$ removes one pair from an n-pair ground state as anticipated. The operator products $B^{(+)}B^{(-)}$ and $B^{(-)}B^{(+)}$ may therefore be replaced by unity when they act upon states near the ground state.

The density wave operator,

$$\rho_q=\sum_s(c_{\uparrow s+q}{}^\dagger c_{\uparrow s}+c_{\downarrow s+q}{}^\dagger c_{\downarrow s}),$$

generates states with odd f parity, since (taking the reference vector $\boldsymbol{\alpha}=q$ so that momentum is conserved)

$$\begin{aligned}f\rho_q f^{-1}&=\sum_s(c_{\uparrow\alpha(s+q)}c_{\uparrow\alpha s}{}^\dagger+c_{\downarrow\alpha(s+q)}c_{\downarrow\alpha s}{}^\dagger)\\&=\sum_s(c_{\uparrow\alpha s-q}c_{\uparrow\alpha s}{}^\dagger+c_{\downarrow\alpha s-q}c_{\downarrow\alpha s}{}^\dagger)\\&=\sum_s(c_{\uparrow s-q}c_{\uparrow s}{}^\dagger+c_{\downarrow s-q}c_{\downarrow s}{}^\dagger)\\&=-\rho_q.\end{aligned}$$

Anderson has shown that a modification of this operator, of the form

$$A_q=\sum_s a_s(c_{\uparrow s+q}{}^\dagger c_{\uparrow s}+c_{\downarrow s+q}{}^\dagger c_{\downarrow s}) +\sum_s b_s(B^{(-)}c_{\uparrow s+q}{}^\dagger c_{\downarrow -s}{}^\dagger+B^{(+)}c_{\downarrow -s}c_{\uparrow s-q}),$$

generates zero-rest-energy spin singlet collective excitations in a neutral Fermi gas with weak attractive interactions. It satisfies the linearized equation of motion

$$[H,A_q]_{\text{lin}}=\hbar c|q|A_q,$$

where c is the velocity of sound, and has odd f parity,

$$fA_qf^{-1}=-A_q.$$

Collective excitations with even f-parity prove to have rest energies comparable with the energy gap ϵ_0.

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