Gauge Invariant Formulation of the Bardeen-Cooper-Schrieffer Theory of Superconductivity*

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The Bardeen-Cooper-Schrieffer theory of superconductivity is reformulated in a way which is manifestly gauge invariant. The method used is to pair electrons having equal and opposite angular momentum rather than equal and opposite linear momentum.

THIS short note will describe a reformulation of the Bardeen, Cooper, and Schrieffer (BCS) theory which is gauge invariant. The central idea underlying the reformulation is the use of wave functions of cylindrical symmetry for the free electrons. This type of symmetry was exploited by Dingle[1] in a study of the magnetic properties of small systems of electrons. Besides being gauge invariant this formulation has the advantage that the effect of the magnetic field on the energy gap can be formulated.

We consider a system of electrons whose interactions with one another are described by a two-body potential which is attractive for some regions of momentum space. The system of electrons is large enough so that statistical methods apply, but small enough so that the magnetic field in the system is not substantially altered by the response of the electrons and may thus be taken to be uniform. We now carry through the derivation of BCS[2] or Valatin[3] except that the index $k=(k_x,k_y,k_z)$ which represents the wave number of an electron in a momentum eigenstate must be replaced by $\kappa=(lmn)$, the quantum numbers for the cylindrical wave function of an electron in a uniform magnetic field[4]:

$$\psi_{lmn}(\mathbf{r})=\sin(l\pi z/L)e^{im\varphi}\chi_{nl|m|}(r), \tag{1}$$

where

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{|m|^2}{r^2}+K^2-Q^4r^2\right)\chi=0, \tag{2}$$

$$K^2=\frac{2M}{\hbar^2}\epsilon(\kappa)-\frac{l^2\pi^2}{L^2}-2mQ^2, \tag{3}$$

$$Q^2=|eB/2\hbar|, \tag{4}$$

and $\epsilon(\kappa)$ is the energy of a free electron in the state $\kappa=(lmn)$. The energy $\epsilon(\kappa)$ in the weak field approximation is given by

$$\epsilon(\kappa)=\frac{\hbar^2\pi^2}{2MR^2}\left(\frac{l^2}{\mathfrak{L}^2}+\frac{a(|m|,n)^2}{\pi^2}\right)-m\mu_BB, \tag{5}$$

where

$$\mathfrak{L}=L/R,$$

μ_B is the Bohr magneton, R is the radius of the cylinder in which the electrons are contained, L is its length, and $a(m,n)$ is the nth zero of the Bessel function of order m. The Z axis is chosen parallel to the direction of the magnetic field B.

Instead of pairing electrons with equal and opposite momentum, we pair electrons with equal and opposite angular momentum: $\kappa=l,m,n$ and $-\kappa=l,-m,n$. Then the derivation of BCS or Valatin can be carried through with only minor modifications. The formation of pairs of electrons with opposite values of m has been employed by Rogers[5] in the study of superconductivity in small systems. Anderson[6] has suggested that the appropriate criterion for pairing electrons in the BCS theory is that the two states be time reversal conjugates. This differs from our choice which corresponds to pairing electrons whose wave functions are complex conjugates of each other. These two criteria would coincide if the Hamiltonian were properly time reversal invariant. Our Hamiltonian is not invariant under time reversal because of the presence of the external magnetic field. As a consequence the two electrons making a pair have different magnetic energies. When this difference becomes comparable to the energy gap, the pairs tend to break up and superconductivity is destroyed.

At temperature T the function h_κ, which gives the probability of finding the pair of states $\kappa=l,\pm m,n$ occupied, is given by

$$h_\kappa=\frac{1}{2}\left(1-\frac{(\bar{\epsilon}-\mu)}{[(\bar{\epsilon}-\mu)^2+\epsilon_0^2]^{\frac{1}{2}}}\right), \tag{6}$$

where

$$\bar{\epsilon}(\kappa)=\tfrac{1}{2}[\epsilon(\kappa)+\epsilon(-\kappa)], \tag{7}$$

and μ is the Fermi energy. The (pseudoparticle) exci-

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2 J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
3 J. G. Valatin, Nuovo cimento **7**, 843 (1957).
4 J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, New York, 1932), p. 353.
5 K. T. Rogers, thesis, University of Illinois, 1960 (unpublished).
6 P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).

tation energy is

$$E_\kappa=\epsilon(\kappa)-\bar{\epsilon}(\kappa)+[(\bar{\epsilon}(\kappa)-\mu)^2+\epsilon_0^2]^{\frac{1}{2}}. \tag{8}$$

The expectation value of the pseudoparticle occupation number is, as before,

$$f_\kappa=(1+e^{E_\kappa/kT})^{-1}. \tag{9}$$

The expectation value of the current density

$$\mathbf{J}(\mathbf{r})=-\sum_i \frac{e}{2M}[\delta(\mathbf{r}-\mathbf{r}_i)(\mathbf{p}_i+e\mathbf{A})+(\mathbf{p}_i+e\mathbf{A})\delta(\mathbf{r}-\mathbf{r}_i)] \tag{10}$$

is

$$\begin{aligned}\langle\mathbf{J}(\mathbf{r})\rangle&=-\frac{e}{2M}\sum_\kappa \left\{\frac{\hbar}{i}(\psi_\kappa{}^*\nabla\psi_\kappa-\psi_\kappa\nabla\psi_\kappa{}^*)-2e\mathbf{A}\psi_\kappa{}^*\psi_\kappa\right\}\times[h_\kappa+f_\kappa-h_\kappa(f_\kappa+f_{-\kappa})]\\&=-\frac{e\hbar}{M}\sum_\kappa m|\psi_\kappa|^2[h_\kappa+f_\kappa-h_\kappa(f_\kappa+f_{-\kappa})]\mathbf{u}_\varphi\\&\quad+\frac{e^2A_\varphi}{M}\sum_\kappa |\psi_\kappa|^2[h_\kappa+f_\kappa-h_\kappa(f_\kappa+f_{-\kappa})]\mathbf{u}_\varphi,\end{aligned} \tag{11}$$

where the result is seen to be purely transverse. This quantity is obviously gauge invariant since under a gauge transformation,

$$\mathbf{A}\rightarrow\mathbf{A}+\nabla\Lambda, \tag{12}$$

and

$$\psi_\kappa\rightarrow\psi_\kappa\exp(-ie\Lambda/\hbar). \tag{13}$$

The second term in (11) is the London current while the first term is the Landau diamagnetic current.

The energy gap ϵ_0 is the solution of the following integral equation:

$$\epsilon_0(\kappa)=-\frac{1}{4}\sum_{\kappa'}\frac{V_{-\kappa\kappa-\kappa'\kappa'}\epsilon_0(\kappa')}{[(\bar{\epsilon}(\kappa')-\mu)^2+\epsilon_0(\kappa')^2]^{\frac{1}{2}}}(1-f_{\kappa'}-f_{-\kappa'}), \tag{14}$$

where

$$\begin{aligned}V_{-\kappa\kappa-\kappa'\kappa'}&=\langle-\kappa\kappa|V|-\kappa'\kappa'\rangle-\langle-\kappa\kappa|V|\kappa'-\kappa'\rangle,\\\langle\alpha\beta|V|\gamma\delta\rangle&=\int d\mathbf{r}_1\int d\mathbf{r}_2\psi_\alpha(\mathbf{r}_1)^*\psi_\beta(r_2)^*V(\mathbf{r}_1,\mathbf{r}_2)\times\psi_\gamma(\mathbf{r}_1)\psi_\delta(\mathbf{r}_2),\end{aligned} \tag{15}$$

and $V(\mathbf{r}_1,\mathbf{r}_2)$ is the potential between electron 1 and electron 2.

The sum over κ' in Eq. (14) represents a sum over the quantum numbers $l'm'n'$ and σ'. The sum on l' can be well approximated by a continuous integral. Making a change of variable from l' to $\epsilon(\kappa')$, we find

$$\epsilon_0(q)=-\frac{\mathfrak{L}}{8\mu_0}\sum_{m'n'\sigma'}\int d\epsilon\frac{V_{-qq-q'q'}}{[(\epsilon/\mu_0)-a(m',n')^2/\pi^2]^{\frac{1}{2}}}\times\frac{\epsilon_0(q')}{[(\bar{\epsilon}(q')-\mu)^2+\epsilon_0(q')^2]^{\frac{1}{2}}}(1-f_{q'}-f_{-q'}), \tag{16}$$

where

$$q=(\epsilon,m,n,\sigma),$$
$$\mu_0=(\hbar^2/2M)(\pi^2/R^2).$$

By carrying out an analysis like that of Bardeen and Pines[7] we can show that $V_{-qq-q'q'}$ does become attractive near the Fermi surface just as Bardeen and Pines find using momentum eigenstates instead of cylindrical eigenstates.

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[7] J. Bardeen and D. Pines, Phys. Rev. **99**, 1140 (1955).