Wave function for odd-frequency superconductors

Hari P Dahal\textsuperscript{1}, E Abrahams\textsuperscript{2}, D Mozyrsky\textsuperscript{1}, Y Tanaka\textsuperscript{3} and A V Balatsky\textsuperscript{1,4,5}

\textsuperscript{1} Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
\textsuperscript{2} Serin Physics Laboratory, Rutgers University, PO Box 849, Piscataway, NJ 08855, USA
\textsuperscript{3} Department of Applied Physics, Nagoya University, Chikusa-ku, Nagoya 464-8603, Japan
\textsuperscript{4} Center for Integrated Nanotechnology, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
\textsuperscript{*} E-mail: avb@lanl.gov, http://theory.lanl.gov

New Journal of Physics \textbf{11} (2009) 065005 (15pp)
Received 28 December 2009
Published 22 June 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/6/065005

Abstract. We revisit the question of the nature of odd-frequency superconductors, first proposed by Berezinskii in 1974 (\textit{JETP Lett.} \textbf{20} 287). We start with the notion that the order parameter of odd-frequency superconductors can be thought of as a time derivative of the odd-time pairing operator. This leads to the notion of the composite boson condensate (Abrahams \textit{et al} 1995 \textit{Phys. Rev. B} \textbf{52} 1271; Balatsky and Bonca 1993 \textit{Phys. Rev. B} \textbf{48} 7445). To elucidate the nature of broken symmetry states in odd-frequency superconductors, we consider a wave function that properly captures the coherent condensate of composite charge $2e$ bosons in an odd-frequency superconductor. We consider the Hamiltonian that describes the equal-time composite boson condensation as proposed earlier by Abrahams \textit{et al} (1995 \textit{Phys. Rev. B} \textbf{52} 1271). We propose a Bardeen–Cooper–Schrieffer (BCS)-like wave function that describes a composite condensate comprised of a spin-0 Cooper pair and a spin-1 magnon excitation. We derive the quasi-particle dispersion, the self-consistent equation for the order parameter and the density of states. We show that the coherent wave function approach recovers all the known proprieties of odd-frequency superconductors: the quasi-particle excitations are gapless and the superconducting transition requires a critical coupling.

\textsuperscript{5} Author to whom any correspondence should be addressed.
1. Introduction

The discussion about possible symmetry types of the superconducting order parameter \( \Delta(k, \tau) \) (\( \tau \) denotes imaginary time) has drawn significant research interest. The conventional singlet (triplet) superconductor follows \( P T \Delta(k, \tau) = \Delta(k, \tau) \) ([\( P T \Delta(k, \tau) = -\Delta(k, \tau) \)]) under parity \( P \) and time \( T \) transformations. The singlet (\( P T = 1 \)) and triplet (\( P T = -1 \)) conditions can be satisfied by either taking \( P = T = 1 \) and \( P = -1, T = 1 \) for an even-in-frequency gap, or \( P = T = -1 \) and \( P = 1, T = -1 \) for the odd-frequency pairing.

Although mainstream discussions of superconductivity are for even-frequency pairing, there is a growing interest in understanding the odd-frequency pairing. The discussion of unconventional pairing (\( P = 1, T = -1 \)) was initiated by Berezinskii [1] to explain the superfluid phase of \(^3\)He. Although his proposal of triplet odd-frequency pairing could not explain the superfluid phase of \(^3\)He, it certainly motivated a search for other possibilities of the pairing symmetries. Balatsky and Abrahams [3] later extended the concept of odd-frequency pairing to the singlet superconductor (\( P = T = -1 \)).

Although the realization of the odd-frequency pairing in current systems is still under debate, several reports consider this possibility in a number of systems. Odd-frequency pairing in the Kondo lattice has been investigated to study superconductivity in heavy-fermion compounds [5]. The proximity effects in a superconductor–ferromagnet structure [6], a normal-metal/superconductor junction [7] and diffusive normal-metal/unconventional superconductor interface [8] have been attributed to the odd-frequency pairing. The \( p \)-wave singlet odd-frequency pairing is argued to be a viable pairing in the coexistence region of antiferromagnetism and superconductivity and/or near the quantum critical point in CeCu\(_2\)Si\(_2\).
and CeRhIn$_3$ [9]. In addition, hydrated Na$_x$CoO$_2$ is suggested to support an s-wave triplet odd-frequency gap [10]. Very recently, Kalas et al [11] have argued that the boson–fermion cold atom mixture exhibits s-wave triplet odd-frequency pairing above some critical coupling at which the mixture phase separates.

Motivated by the growing interest and possibilities of odd-frequency pairing, here we address the missing part of the odd-frequency superconductivity discussion: what is the wave function of the odd-frequency superconductors? One might wonder how one can even ask this question given that superconducting correlations of two fermion operators in odd-frequency superconductors do not have an equal-time expectation value? We assume (a pretty safe assumption in fact) that any state, including odd-frequency superconductors, does have a many-body wave function that captures superconducting correlations. Any state of matter has an associated wave function $|\psi\rangle$ that captures the amplitude distribution of the particles forming this state. Hence, we are asking exactly this question about the many-body wave function of the odd-frequency superconductors. Our wave function builds upon a long discussion [2] on the possible order parameter and equal-time composite operators that capture superconducting correlations of odd-frequency superconductors in the equal-time domain.

We propose a Bardeen–Cooper–Schrieffer (BCS)-like pairing wave function for an odd-frequency superconductor, and study its consequences for the energy dispersion, superconducting order parameter, and density of states (DOS). The wave function, which describes a condensate of a spin-0 Cooper pair and a spin-1 magnon excitation, is consistent with the Hamiltonian suggested earlier in [2] to study the odd-frequency superconductivity. We minimize this Hamiltonian with respect to the proposed wave function and derive an expression for the quasi-particle dispersion, a self-consistent gap equation and the DOS. We find that (a) the quasi-particle dispersion is gapless, (b) the gap equation has nonzero solution only for a critical value of the coupling, (c) the DOS is finite even for an energy less than the gap energy, and (d) the DOS is reduced at the gap edge compared with that of the BCS case.

Before introducing the wave function and getting into the details of the minimization of the Hamiltonian, we would like to show that $PT = 1$ can be obtained by taking $P = T = -1$ in $S = 0$ singlet case. Any superconducting order with translational invariance, equilibrium and broken $U(1)$ symmetry would result in an anomalous (Gor’kov) Green’s function

$$\mathcal{F}_{\alpha\beta}(\tau, \mathbf{k}) = \langle T_c c_{\alpha, \mathbf{k}}(\tau)c_{\beta, -\mathbf{k}}(0) \rangle,$$

where $\alpha$ and $\beta$ are spin indices. We assume that the transition occurs only in a well-defined representation. Thus, for $S = 0$ singlet pairing, we may define

$$F(\tau, \mathbf{k}) = \epsilon_{\alpha\beta} \mathcal{F}_{\alpha\beta}(\tau, \mathbf{k}),$$

and for $S = 1$ triplet pairing,

$$\bar{F}(\tau, \mathbf{k}) = (i\sigma \bar{\sigma})_{\alpha\beta} \mathcal{F}_{\alpha\beta}(\tau, \mathbf{k}).$$

We now show the properties of $F(\tau, \mathbf{k})$ under $P$ and $T$ transformations. For $S = 0$ from equation (2),

$$F(\mathbf{k}, \tau) = \epsilon_{\alpha\beta} \left[ \theta_{r} \langle c_{\alpha, \mathbf{k}}(\tau)c_{\beta, -\mathbf{k}}(0) \rangle - \theta_{-r} \langle c_{\beta, -\mathbf{k}}(0)c_{\alpha, \mathbf{k}}(\tau) \rangle \right],$$

where $\theta_{r}$ is the Heaviside theta function.
We apply $PT$ to this $F$:

$$F(-k, -\tau) = \epsilon_{\mu \nu} [\theta_{-\tau} \langle c_{\mu, k}(-\tau)c_{\nu, k}(0) \rangle - \theta_{\tau} \langle c_{\nu, k}(0)c_{\mu, -k}(-\tau) \rangle]$$

$$= \epsilon_{\mu \nu} [\theta_{-\tau} \langle c_{\mu, -k}(0)c_{\nu, k}(\tau) \rangle - \theta_{\tau} \langle c_{\nu, k}(\tau)c_{\mu, -k}(0) \rangle],$$

(5)

where in the last line we have used the fact that $\langle TA(-\tau)B(0) \rangle = \langle TA(0)B(\tau) \rangle$, which agrees with the cyclicity of the trace,

$$\langle A(-\tau)B(0) \rangle = \text{Tr}(e^{-HT} Ae^{HT} B)$$

$$= \text{Tr}(Ae^{HT} B e^{-HT}) = \langle A(0)B(\tau) \rangle.$$  

(6)

Going back to equation (5), we permute $\mu \leftrightarrow \nu$,

$$F(-k, -\tau) = \epsilon_{\mu \nu} [\Theta_{\tau} \langle c_{\mu, k}(\tau)c_{\nu, -k}(0) \rangle - \Theta_{-\tau} \langle c_{\nu, -k}(0)c_{\mu, k}(\tau) \rangle]$$

$$= F(k, \tau).$$  

(7)

All these properties of the Gor’kov function will be reflected in the behavior of the gap function as well. Therefore, the gap function in general is even only under simultaneous transformation: $k \to -k$ ($P$) and $\tau \to -\tau$ ($T$). We recall that $PT = 1$ is not only satisfied by $P = +1, T = +1$ but also by $P = -1$ and $T = -1$. The former describes the BCS s-wave (even-frequency) pairing, whereas the latter describes the odd-frequency pairing.

2. Hamiltonian and wave function

When the idea of the odd-frequency pairing was first formulated for the singlet superconductor, an effective spin-independent interaction mediated by phonons was considered [4]. It was realized that this kind of interaction was unphysical for the singlet pairing [4]. The problem was solved by considering spin-dependent electron–electron interactions. The odd-frequency pairing posed another problem related to the selection of the order parameter. In the BCS case, the order parameter is generated from the expectation value, $F(r, t; r', t' \to t) = \langle \psi(r, t)\psi(r', t) \rangle$. But for the odd-frequency superconductor the equal-time gap vanishes since the gap is odd in frequency. This problem was solved by taking $dF(r, t; r', t' \to t)/dt|_{t \to t'}$ as the equal-time order parameter [2].

A Hamiltonian having a spin-dependent electron–electron interaction was introduced by Abrahams et al [2]. Using the equation of motion they derived an expression for $dF(r, t; r', t' \to t)/dt|_{t \to t'}$. It was shown that the equal-time condensate for the odd-frequency pairing is the expectation value of the product of a pair operator and a spin excitation operator. In what follows, we adopt this approach, but for an odd-frequency s-wave $m = 1$ triplet phase. We rewrite the Hamiltonian from [2] in the following form:

$$H = \sum_{k} \epsilon_{k^\uparrow\downarrow} c_{k^\uparrow}^{\dagger} c_{k^\downarrow}^{\dagger} + \sum_{k} \epsilon_{k^\uparrow\downarrow} c_{k^\downarrow}^{\dagger} c_{k^\uparrow} + \sum_{q} \omega_{q} S_{q}^{+} S_{q}^{-}$$

$$+ \sum_{k,q,p} V_{klqp} c_{k^\uparrow}^{\dagger} c_{l^\downarrow}^{\dagger} S_{q}^{+} c_{p^\downarrow}^{\dagger} c_{p^\uparrow} S_{p}^{-},$$

(8)

where $\epsilon_{k^\uparrow\downarrow}$ refers to the kinetic energy of the $\uparrow \downarrow$ electrons measured from the Fermi energy, $\omega_{q}$ is the magnon kinetic energy, and $V_{klqp}$ is an attractive interaction, which mediates the condensation. $c_{k^\sigma}^{\dagger}$ and $c_{k^\sigma}$ create and annihilate electrons in the state $k \sigma$. $S^{\pm}$ describes magnon...
excitations. Using this Hamiltonian, we propose a BCS-like wave function and study the superconducting state.

The proposed wave function is written as

$$|\psi\rangle = \prod_{kq} \left( u_{kq} + v_{kq} c_{k+\frac{1}{2},q}^\dagger c_{-k+\frac{1}{2},q}^\dagger S_q^+ \right) |0\rangle,$$

where $|0\rangle$ represents the vacuum for both the electrons and the spin bosons. This wave function describes the superposition of the wave functions having two paired electrons with $\mathbf{k} + \frac{q}{2}$ and $-\mathbf{k} + \frac{q}{2}$ momentum and carrying opposite spins and condensed along with spin excitations $(S_q^+)$.

$v_{kq}$ ($u_{kq}$) represent the amplitude of the occupation (or unoccupation) of these electron pairs with the spin excitation.

There are key properties that explain this particular choice of variational function:

1. $|\psi\rangle$ is a coherent state of composite bosons ($c_{k+\frac{1}{2},q}^\dagger c_{-k+\frac{1}{2},q}^\dagger S_q^+$) that carry charge $2e$;
2. This wave function describes a coherent state that has broken $U(1)$ symmetry associated with the superconducting condensate, as can be explicitly verified by using $c_k \rightarrow \exp(i\phi)c_k$;
3. A composite boson that condenses is not a simple Cooper pair [2] but contains two fermions and a spin-1 boson; (iv) the composite boson field has finite expectation value in this state

$$\langle |\psi\rangle c_{k+\frac{1}{2},q}^\dagger c_{-k+\frac{1}{2},q}^\dagger S_q^+ |\psi\rangle = u_{kq} v_{kq}$$

and therefore $|\psi\rangle$ is a mean-field wave function for the composite condensate.

The normalization of the wave function is given by,

$$\langle |\psi\rangle |\psi\rangle = \prod_{kq} (|u_{kq}|^2 + |v_{kq}|^2 (S^+ S_q^+)) = 1,$$

which implies that $|u_{kq}|^2 + |v_{kq}|^2 (S^+ S_q^+) = 1$ for all $k$, $q$.

To make a next step we need to find the expectation value of the Hamiltonian (equation (8)) with respect to the wave function (equation (9)) and minimize it. Then we will proceed to derive the quasi-particle dispersion, DOS and the self-consistent equation for the order parameter.

3. Total energy and its minimization

The calculation of each term in equation (8) is shown in the appendix. Using equations (A.2), (B.2), (C.2) and (D.1), the total energy can be written as

$$E = \sum_{kq} (\epsilon_{k+\frac{1}{2}} + \epsilon_{k-\frac{1}{2}} + \omega_q (S^+ S_q^+)) |v_{kq}|^2 (S^+ S_q^+) + \sum_{klqp} V_{klqp} u_{kq} v_{lq} u_{lp}^* (S^+ S_q^+) (S^+ S_p^+).$$

Following the BCS method, we choose $u_{kq}$, $v_{kq}$ such that they satisfy the normalization condition so that $u_{kq} = \sin \theta_{kq}$ and $v_{kq} = \cos \theta_{kq}/\sqrt{(S^+ S_q^+)q}$. Then the expression for the energy reads

$$E = \sum_{kq} \cos^2 \theta_{kq} (\epsilon_{k+\frac{1}{2}} + \epsilon_{k-\frac{1}{2}} + \omega_q (S^+ S_q^+)) + \frac{1}{4} \sum_{klqp} V_{klqp} \sin 2\theta_{kq} \sin 2\theta_{lp} \sqrt{(S^+ S_q^+)q} \sqrt{(S^+ S_p^+)p}.$$
The minimization of the energy with respect to $\theta_{kq}$ gives
\[
\frac{\partial E}{\partial \theta_{kq}} = -\sin 2\theta_{kq}(\epsilon_{k+\frac{q}{2}} + \epsilon_{k-\frac{q}{2}} + \omega_q(S^-S^+)_q)
+ \sum_{lp} V_{klqp} \cos 2\theta_{kq} \sin 2\theta_{lp} \sqrt{(S^-S^+)_q} \sqrt{(S^-S^+)_p} = 0,
\]
which can be rewritten as
\[
tan 2\theta_{kq} = \frac{\sum_{lp} V_{klqp} \sin 2\theta_{lp} \sqrt{(S^-S^+)_q} \sqrt{(S^-S^+)_p}}{\epsilon_{k+\frac{q}{2}} + \epsilon_{k-\frac{q}{2}} + \omega_q(S^-S^+)_q}.
\]
We proceed by defining the two quantities $\Delta$ and $E$ that will turn out to be the gap parameter and the energy of a composite excitation.
\[
\Delta_{kq} = -\frac{1}{2} \sum_{lp} V_{klqp} \sin 2\theta_{lp} \sqrt{(S^-S^+)_q} \sqrt{(S^-S^+)_p},
\]
\[
E_{kq} = \sqrt{\left(\frac{\epsilon_{k+\frac{q}{2}} + \epsilon_{k-\frac{q}{2}} + \omega_q(S^-S^+)_q}{2}\right)^2 + \Delta_{kq}^2}
= \sqrt{\left(\frac{\epsilon_k + \frac{q^2}{2m} + \omega_q(S^-S^+)_q}{2}\right)^2 + \Delta_{kq}^2}.
\]
Then
\[
\sin 2\theta_{kq} = 2u_{kq} v_{kq} \sqrt{(S^-S^+)_q} = \frac{\Delta_{kq}}{E_{kq}},
\]
and
\[
\cos 2\theta_{kq} = v_{kq}^2 (S^-S^+)_q - u_{kq}^2 = -\frac{\xi_{kq}}{E_{kq}},
\]
where we have introduced the abbreviation
\[
\xi_{kq} = \frac{\epsilon_{k+\frac{q}{2}} + \epsilon_{k-\frac{q}{2}} + \omega_q(S^-S^+)_q}{2}.
\]
Solving the normalization condition and equation (17), we can show that,
\[
u_{kq}^2 = \frac{1}{2} \left(1 + \frac{\xi_{kq}}{E_{kq}}\right),
\]
\[
u_{kq}^2 = \frac{1}{2} \frac{1 - \xi_{kq}}{E_{kq}}.
\]
The BCS limit can be recovered at any stage of this analysis if we assume that spin correlators are factorized and have a peak at $q = 0$. This limit corresponds to the condensation of spin field $(S^-S^+)_q = (S^-)_q(S^+)_q\delta_{q,0}$. In this limit, additional summation over $q$ drops out and we recover the standard BCS logarithm in the self-consistency equation, equation (16a), along with other features of the BCS solution. This limit corresponds to the factorization of a composite boson into a product $\langle \psi | c_{k+\frac{q}{2}}^\dagger c_{k-\frac{q}{2}}^\dagger S^+_q | \psi \rangle \rightarrow \langle \psi | c_{k+\frac{q}{2}}^\dagger c_{k-\frac{q}{2}}^\dagger | \psi \rangle \langle \psi | S^+_q | \psi \rangle \delta_{q,0}$. 

New Journal of Physics 11 (2009) 065005 (http://www.njp.org/)
4. Energy spectrum

Unlike the BCS case, $E_{kq}$ is not a single-particle excitation energy. Therefore, we shall derive an expression for the energy required to excite an electron from the superconducting ground state. The excited state for an up spin is given by,

$$\tilde{\psi}_\uparrow = \prod_{q,k \neq k'} \left( u_{kq} + v_{kq} b^\dagger_{kq} \right) c^\dagger_{k+\frac{1}{2}\uparrow} | 0 \rangle,$$

where we have defined the composite creation operator $b^\dagger_{kq} = c^\dagger_{k+\frac{1}{2}\uparrow} c^\dagger_{-k+\frac{1}{2}\downarrow} s^+$. We calculate the expectation value of the Hamiltonian equation (8) with respect to the excited state wave function equation (20). The details are given in appendix E. The expectation value can be expressed as

$$\langle \tilde{\psi}_\uparrow | H | \tilde{\psi}_\uparrow \rangle = \langle \psi | H | \psi \rangle + \epsilon_{k+\frac{1}{2}\uparrow} + \frac{\Delta^2_{kq}}{E_{kq}} - 2\xi_{kq} E_{kq} \langle S^- S^+ \rangle_q.$$

Using equation (19b), we can rewrite the above equation as,

$$\Delta E_\uparrow = \epsilon_{k+\frac{1}{2}\uparrow} - \xi_{kq} + E_{kq}.$$

where $\Delta E_\uparrow = \langle \tilde{\psi}_\uparrow | H | \tilde{\psi}_\uparrow \rangle - \langle \psi | H | \psi \rangle$ is the excitation energy of the up spin electrons. $\Delta E_\uparrow$ can also be written as $\Delta E_\uparrow = k \cdot q / 2m^* - (\omega_q / 2) \langle S^- S^+ \rangle_q + E_{kq}$. Doing the same for the down spin-excited state $\tilde{\psi}_\downarrow$, we find $\Delta E_\downarrow = -k \cdot q / 2m^* - (\omega_q / 2) \langle S^- S^+ \rangle_q + E_{kq}$.

5. DOS

The DOS as a function of energy, $N(E)$, is defined as

$$N_{\pm}(E) = \sum_{kq} \delta \left[ E - \left( \pm \frac{k \cdot q}{2m^*} - \frac{\omega_q}{2} \langle S^- S^+ \rangle_q + E_{kq} \right) \right],$$

where $\pm$ corresponds to up and down spins, respectively. We numerically calculate the DOS for two cases of the magnon dispersion: (1) $\omega_q = q^2 / 2M$, and (2) $\omega_q = \omega_0$. We set $\langle S^- S^+ \rangle_q = 1.0$, and $M = 10m^*$. The DOS for case 1 is shown in figure 1.

In figure 1(a), we show the DOS as a function of energy and order parameter. We have set a magnon momentum cutoff, $q_c = 0.25k_F$. We see that the DOS can be nonzero for energies less than the superconducting gap parameter. The maximum of the DOS is always at the gap edge, but it is highly reduced at the gap edge compared with the BCS case. For smaller $\Delta$, the DOS can be nonzero at $E = 0$; hence the DOS is gapless. The calculation for a smaller $q_c$ (not shown in the figure) shows that the gap becomes more prominent in the DOS and spectral weight is transferred to the gap edge, similar to the BCS case. Hence $q_c \rightarrow 0$ reproduces the BCS results. In figure 1(b)–(d), we have shown the plane cut of figure 1(a) for different values of $\Delta$. For $\Delta = 0.1$ (figure 1(b)) we see that the DOS is nonzero for $0.05 < E < \Delta$. For $\Delta = 0.04$ (figure 1(c)), we see that the gap is completely closed and the excitations will be gapless. The effect is even bigger for $\Delta = 0.02$.

We also calculated the DOS using case 2: $\omega_q = q^2 / 2M$ for $q_c > k_F$ (the Fermi momentum) for a fixed value of $\Delta = 0.1$. The result is shown in figure 2. In this figure, we can see that the DOS almost closes the gap when $q_c = k_F$. As we increase $q_c$, the gap closes completely. Then
Figure 1. The DOS as a function of energy and superconducting order parameter in an odd-frequency superconductor. The DOS is normalized with respect to the DOS of the normal state. All the energies are normalized with Fermi energy of the system. The result is presented for the magnon momentum cutoff $q_c = 0.25$. In this figure, we show that the DOS is finite even for energy less than the gap energy. The maximum of the DOS is at the gap edge but the DOS is highly reduced compared with the BCS case. For smaller gap energy the DOS is completely gapless. Once the gap is closed the DOS starts to pile up at $E = 0$ for smaller values of $\Delta$.

The quasi-particle excitations become gapless. A still further increase in $q_c$ results in a finite DOS at $E = 0$. For $q_c \geq k_F$ there is no enhancement of the spectral weight at the gap edge.

The calculation of the DOS for $\omega_q = \omega_0$ shows a similar DOS as discussed above for both $q_c = 0.25k_F$ and $q_c \geq k_F$.

6. Superconducting gap versus coupling constant

The self-consistent gap equation (equation 16(a)) can be written as

$$\Delta_{kq} = \frac{V}{2} \sum_{lp} \frac{\Delta_{lp}}{E_{lp}} \sqrt{\langle S^+ S^0 \rangle_q \sqrt{\langle S^+ S^0 \rangle_p}},$$

(24)
Figure 2. The DOS at fixed \( \Delta = 0.1 \) as a function of energy for the magnon momentum cutoff \( q_c \geq k_F \). The values of \( q_c \) are 0.9, 1.1, 1.4, 1.7 times \( k_F \). As we increase \( q_c \) the gap in the DOS gradually closes up. For bigger \( q_c \) the DOS piles up at \( E = 0 \).

where we have taken

\[
V_{kpq} = \begin{cases} 
-V : & |\epsilon_k| \leq 0.2\mu, \\
0 : & |\epsilon_k| > 0.2\mu.
\end{cases}
\]  

(25)

Then \( \Delta_kq = \Delta_q \), and \( \Delta_lp = \Delta_p \). The use of a more complicated interaction potential with a momentum dependence would bring additional calculational complications, which would not change the nature of the results.

We substitute \( \Delta_q \) by \( \Delta(S^-S^+)q \), denote \( p^2/8m^* + (\omega_p/2)(S^-S^+)q \) by \( f(p) \), and first perform the energy integral in equation (24) as follows:

\[
1 = \frac{V}{2} \sum_{l,p} \frac{(S^-S^+)p}{\sqrt{(\epsilon_l + f(p))^2 + \Delta^2}}
\]

\[
= g \int p^2 dp \int_0^{\hbar\omega_c} \frac{(S^-S^+)p d\epsilon}{\sqrt{(\epsilon + f(p))^2 + \Delta^2}}
\]

(26)

\[
= g \int p^2 dp (S^-S^+)p \log \left[ \frac{\epsilon_c(p) + \sqrt{\Delta^2 + \epsilon_c(p)^2}}{f(p) + \sqrt{\Delta^2 + f(p)^2}} \right],
\]

where \( N(0) \) is the DOS in the normal state at the Fermi energy, \( g \) is the dimensionless coupling \( N(0)V/2\pi^2 \), \( \epsilon_c(p) = \hbar\omega_c + f(p) \) and \( \hbar\omega_c = 0.2\mu \). If we assume the spin correlator to have a sharp peak \( \delta_{q,0} \) we recover the BCS self-consistency equation from this equation.

In the BCS case, the gap equation is \( 1 = N(0)V \log[(\hbar\omega_c + \sqrt{\Delta^2 + \hbar\omega_c^2})/\Delta] \). There is a solution for \( \Delta \) for an arbitrary small value of \( N(0)V \) due to the logarithmic divergence of the integral. In our case, in the presence of the magnon, the denominator will have some nonzero
Figure 3. The order parameter is numerically calculated for $\omega_q = q^2/2M$. The magnon momentum cutoff is given by $q_c = Bk_F$, where $B = 0.12, 0.1, 0.08, 0.06$, top to bottom. The order parameter is nonzero only for a critical value of the coupling $g = N(0)V/2\pi^2$. For a given value of $N(0)V$ the larger $\Delta$ corresponds to the larger magnon momentum cutoff.

value because of the nonzero magnon energy. Then the right-hand side can be made equal to 1 only for some critical value of $g$, as can be seen in the numerical evaluation discussed below.

6.1. Case 1, $\omega_p = p^2/2M$

We solve equation (26) numerically for $\Delta$ as a function of the coupling strength $g$. We set $m^*/M = 0.1$ and $\langle S^-S^+ \rangle_p = 1.0$. We note here that a more general treatment of $\langle S^-S^+ \rangle_p$ will effect the result only quantitatively. The cutoff for the magnon momentum is given by $q_c = Bk_F$, where $B$ varies between 0.12 and 0.06 in equal steps of 0.02. The result is shown in figure 3. In this figure, we can see that a nonzero order parameter requires a critical coupling.

6.2. Case 2, $\omega_p = \omega_0$

The gap equation is again given by equation (26) but now

$$f(p) = p^2/8m^* - \omega_0\langle S^-S^+ \rangle_p/2.$$ (27)

We solve equation (26) numerically for $\Delta$ as a function of the coupling strength $g$. We fix the cutoff for the magnon momentum to be $0.1k_F$. The results for various $\omega_0 = C\mu$ where $C = 0, 0.02, 0.04, 0.06, 0.08$ are shown in figure 4. Again, the superconducting transition requires a critical coupling.

7. Meissner effect

The Meissner effect is one of the defining properties of a superconductor. The Meissner effect has been derived for the composite odd-frequency superconductor by Abrahams et al [2]. Here, we summarize the derivation given in that reference.
Figure 4. The order parameter is calculated for $\omega_q = \omega_0$. The magnon momentum cutoff is $q_c = 0.1k_F$. The result is shown for $\omega_0 = C \mu$ where $C = 0, 0.02, 0.04, 0.06, 0.8$, top to bottom. The order parameter is nonzero only for coupling exceeding a critical value. For a given value of $N(0)V$ the bigger $\Delta$ corresponds to the smaller value of $\omega_0$.

A superconductor shows the Meissner effect when the paramagnetic electrodynamic response is less than the diamagnetic response. The dc response is given by

$$j_i(q) = -Q_{ij}(q)A_j(q),$$

where $A(q)$ is the Fourier transform of vector potential $A(r)$, $N$ is the electron density, and $m$ is their mass. $Q_{ij}(q)$ is given by

$$Q_{ij}(q) = \delta_{ij} \frac{ne^2}{m} + Q_{ij}^p(q),$$

where $A(q)$ is the Fourier transform of vector potential $A(r)$, $N$ is the electron density, and $m$ is their mass. $Q_{ij}^p(q)$ is given by

$$Q_{ij}^p(q) = -\frac{e^2}{4m} \sum_{\gamma} \sum_{kk'} \langle 0 | c_\gamma^\dagger(k,0) c_\gamma(k+q/2,\omega) c_\delta^\dagger(k'-q/2,0) c_\delta(k',0) | 0 \rangle,$$  

where $k_\pm = k \pm q/2$. $Q^p$ can be evaluated near the critical temperature $T_c$ by perturbation in the order parameter $\Delta$. The relevant Feynman diagrams of the current–current correlation function for the Meissner effect are used. The analytical expression for $q \to 0$ is

$$Q_{ij}^p(q) - Q_{ij}^n(q) = \frac{e^2 T^2 \Delta^2}{m^2} \sum_{\omega \omega'} \sum_{kk'} k_i k_j' [G^2(k,\omega)G^2(k',\omega') - 2G^3(k,\omega)G(k',\omega')] D(k+k',\omega+\omega'),$$

where, $G(k,\omega)$ and $D(k,\omega)$ are the electron and magnon propagators. The condition for the Meissner effect is given by $Q^p - Q^n > 0$, which signifies the positive superfluid density in the superconductor.

Situations with several models of the magnon propagators are discussed. If the magnon propagator is momentum independent, there is no contribution to $Q_{ij}(q)$ since the momentum
summands are odd functions. So a momentum-dependent magnon propagator is used to discuss the Meissner effect. In the case of a static, spatially uniform magnon propagator having factorized form given by $D(q, \nu) = -\delta_q \delta_{\nu}$, the Meissner effect is found ($Q^p - Q^n > 0$). For spread-out $\delta$-functions, the sign of $Q^p - Q^n$ does not change, thus a positive superfluid density arises with a value between zero and the BCS value. Thus, it is shown that the composite odd-frequency superconductors exhibit the Meissner effect.

8. Conclusion

In this paper, we propose a BCS-like wave function for s-wave triplet odd-frequency superconductors. Our alternative approach to odd-frequency superconductivity is based on the earlier discussion on composite bosons [2]. We present the wave function for the odd-frequency superconductor $|\psi\rangle = \prod_{kq}(u_{kq} + v_{kq}c^\dagger_{k+\frac{\pi}{2} \uparrow\downarrow} S^z_{q})|0\rangle$, equation (9), that explicitly contains only the equal-time operators and hence does not involve the frequency or time domain. The wave function describes a condensate of a Cooper pair of spin $S = 0$ and a magnon of spin $S = 1$. $|\psi\rangle$ describes a coherent state that has nonzero expectation value for the composite boson operator, it captures the charge $2e$ condensate that breaks gauge symmetry and corresponds to the superconducting state. Naturally, since this $|\psi\rangle$ describes the odd-frequency superconductor, spatial parity $P$ of this condensate is reversed compared with the even frequency pairing operators that correspond to a BCS condensate. Specifically, for the case we considered of a spin triple $S = 1$ odd-frequency condensate the spatial parity of the composite boson $\langle c^\dagger_\uparrow(\mathbf{r})c^\dagger_\downarrow(\mathbf{r})S^z(\mathbf{r})\rangle$ is $P = +1$ and hence this order parameter does possess all the quantum numbers inherent to the odd frequency $S = 1$ superconductor.

We present a simplified model that captures the important features of the strong coupling theory developed for the odd-frequency superconductors and our results agree with the predictions of earlier studies: (i) we show that the superconductivity requires a critical coupling. It was argued earlier [1, 3] that a critical coupling is necessary in order to get the superconducting transition in an odd-frequency superconductor, which we have also shown in this work. (ii) We also derive the dispersion relation for the quasiparticles. We determine the DOS of the excitations. The DOS is very different from that of the BCS case. The gapless nature of quasi-particle excitations we find is also in agreement with earlier predictions. The calculation of the DOS shows that it is always higher at the gap edge but its magnitude is highly reduced compared with the BCS case. For a range of parameters, unlike the BCS case, the DOS is finite for energies less than the gap energy and at $E = 0$ it can be nonzero, hence the odd-frequency superconductor is gapless. We also argue how the BCS result is recovered by taking the magnon operator to condense and momentum cutoff $q_c = 0$.

The present discussion could be useful for the equal-time formulation of the odd-frequency superconducting state and physical observables related to condensates. It also could be useful in elucidating the nature of condensates in odd-frequency superconductors.

Acknowledgments

Work at Los Alamos was supported by US DOE through LDRD and BES. We also acknowledge the hospitality of KITP at UC Santa Barbara.

New Journal of Physics 11 (2009) 065005 (http://www.njp.org/)
Appendix A. Kinetic energy of up-spin electrons

It is convenient to rewrite $\sum_k \epsilon_k \epsilon_k^\dagger \epsilon_k^\dagger$ as

$$\left( \frac{1}{N} \sum_q \right) \sum_k \epsilon_k \epsilon_k^\dagger \epsilon_k^\dagger = \frac{1}{N} \sum_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger .$$  \hspace{1cm} (A.1)

This is a trivial identity since we can shift $k \rightarrow k + \frac{q}{2}$ and get the same result.

We denote the $(\text{mn})$ component of the wave function as, $|\psi_{\text{mn}}\rangle = (\mu_{\text{mn}} + v_{\text{mn}}c_{\text{m+\frac{q}{2}}\dagger}^\dagger c_{\text{m-\frac{q}{2}}\dagger}^\dagger \times S_{\text{n}}^\dagger)|0\rangle$. The expectation value of the kinetic energy of the up spin electrons $KE_\uparrow = \frac{1}{N} \sum_{\text{kq}} \langle \psi_{\text{mn}}^\ast | \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger | \psi_{\text{mn}} \rangle$ is given by

$$KE_\uparrow = \frac{1}{N} \sum_{\text{kq}} \langle \psi_{\text{kq}}^\ast | \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger | \psi_{\text{kq}} \rangle = \frac{1}{N} \sum_{\text{kq}} \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger v_{\text{kq}}^2 \langle S^- S^+ \rangle_q .$$  \hspace{1cm} (A.2)

Here we use the normalization condition that $\langle \psi_{\text{m\neq k,q}}^\ast | \psi_{\text{m\neq k,q}} \rangle = \delta_{\text{mn}}\delta_{\text{qq}}$.

Then the kinetic energy of the up-spin electrons is $KE_\uparrow = \sum_{\text{kq}} \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger v_{\text{kq}}^2 \langle S^- S^+ \rangle_q$.

Appendix B. Kinetic energy of down-spin electrons

Using the same argument as discussed in appendix A, we rewrite $\sum_k \epsilon_k \epsilon_k^\dagger \epsilon_k^\dagger$ as

$$\left( \frac{1}{N} \sum_q \right) \sum_k \epsilon_k \epsilon_k^\dagger \epsilon_k^\dagger = \frac{1}{N} \sum_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger .$$  \hspace{1cm} (B.1)

Then the expectation value of the kinetic energy of the down-spin electrons $KE_\downarrow = \frac{1}{N} \sum_{\text{kq}} \langle \psi_{\text{kq}}^\ast | \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger | \psi_{\text{kq}} \rangle$ is given by

$$KE_\downarrow = \frac{1}{N} \sum_{\text{kq}} \langle \psi_{\text{kq}}^\ast | \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger \epsilon_{\text{kq}}^\dagger | \psi_{\text{kq}} \rangle = \frac{1}{N} \sum_{\text{kq}} \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger v_{\text{kq}}^2 \langle S^- S^+ \rangle_q .$$  \hspace{1cm} (B.2)

Then the kinetic energy of the down-spin electrons is $KE_\downarrow = \sum_{\text{kq}} \epsilon_{\text{kq}} \epsilon_{\text{kq}}^\dagger v_{\text{kq}}^2 \langle S^- S^+ \rangle_q$.

Appendix C. Magnon energy

The expectation value of the magnon kinetic energy $KE_m = \sum_q \langle \psi_{\text{q}}^\ast \omega_q S_q^+ S_q^- | \psi \rangle$ can be rewritten as

$$KE_m = \left( \frac{1}{N} \sum_k \right) \sum_q \langle \psi_{\text{kq}}^\ast | \omega_q S_q^+ S_q^- | \psi_{\text{kq}} \rangle .$$  \hspace{1cm} (C.1)
which gives

\[ KE_m = \frac{1}{N} \sum_{kq} \omega_q |v_{kq}|^2 \langle S^- S^+ S^+ S^- \rangle_q. \]  

(C.2)

Appendix D. Interaction energy

In the calculation of the expectation value of the interaction energy, \( E_I \), it is easy to see that the product of only two states, \( kq \) and \( lp \) give nonzero contribution to the interaction term. All the other states are normalized to unity. Then

\[ E_I = \frac{1}{N} \sum_{klpq} \langle \psi^* | V_{klpq} b^*_k b^*_l | \psi \rangle \]

\[ = \frac{1}{N} \sum_{klpq} V_{klpq} \langle \psi^*_{kq} \psi^*_{lp} | b^*_k b^*_l | \psi_{lp} \psi_{kq} \rangle \]

\[ = \frac{1}{N} \sum_{klpq} V_{klpq} \epsilon_{kq} \epsilon_{lq} |v_{kq}|^2 \langle S^- S^+ \rangle_q \langle S^- S^+ \rangle_p. \]  

(D.1)

where \( b^*_k q = c^+_k \uparrow c^+_k \downarrow S^+_q \).

Appendix E. Energy of excited states

The wave function of an excited state is

\[ \tilde{\psi} = \prod_{q,k \neq k'} \left( u_{kq} + v_{kq} b^*_k \right) c^+_k |0\rangle. \]  

(E.1)

Using the procedure of appendix A, we calculate the kinetic energy of the up-spin electrons (\( \tilde{KE}_+ \)) with respect to the excited state wave function:

\[ \tilde{KE}_+ = \frac{1}{N} \sum_{kq} \epsilon_{k+\frac{3}{2}} |v_{kq}|^2 \langle S^- S^+ \rangle_q + \epsilon_{k+\frac{3}{2}}, \]  

(E.2)

where the restriction on \( k \) in the summation is inherited from the restriction imposed on the excited state wave function. \( \epsilon_{k+\frac{3}{2}} \) is due to the creation operator \( c^+_k \downarrow \), which creates an up-spin electron having unit probability of occupation in the state of momentum \( k' + \frac{3}{2} \). We rewrite equation (E.2) in the following form:

\[ \tilde{KE}_+ = \frac{1}{N} \sum_{kq} \epsilon_{k+\frac{3}{2}} |v_{kq}|^2 \langle S^- S^+ \rangle_q + \epsilon_{k+\frac{3}{2}} - \epsilon_{k+\frac{3}{2}} |v_{kq}|^2. \]  

(E.3)

Proceeding similarly, we show that the kinetic energy of the down-spin electrons can be written as

\[ \tilde{KE}_- = \frac{1}{N} \sum_{kq} \epsilon_{k-\frac{3}{2}} |v_{kq}|^2 \langle S^- S^+ \rangle_q - \epsilon_{k-\frac{3}{2}} |v_{kq}|^2. \]  

(E.4)
The kinetic energy of the magnon takes the following form:

$$\tilde{KE}_m = \frac{1}{N} \sum_{kq} \omega_q |v_{kq}|^2 (\langle S^- S^+ \rangle_q - \langle S^- S^+ \rangle_q)^2.$$  \hspace{1cm} (E.5)

The interaction energy can be written as

$$\tilde{E}_I = \frac{1}{N} \sum_{klqp} V_{klqp} v_{kq} u_{kq}^* v_{lp} u_{lp}^* \langle S^- S^+ \rangle_q \langle S^- S^+ \rangle_p - 2 \sum_{lp} V_{k’lqp} v_{kq} u_{kq}^* v_{lp} u_{lp}^* \langle S^- S^+ \rangle_q \langle S^- S^+ \rangle_p.$$  \hspace{1cm} (E.6)

From equation (16a), we can show that

$$\Delta_{k’q} = - \sum_{lp} V_{k’lqp} v_{kq} u_{kq}^* v_{lp} u_{lp}^* \langle S^- S^+ \rangle_q \langle S^- S^+ \rangle_p.$$  \hspace{1cm} (E.7)

We use this relation in the right-hand side of equation (E.6). The second term now gives

$$+ 2v_{kq}^* u_{kq} \sqrt{\langle S^- S^+ \rangle_q} \Delta_{k’q},$$

which, using equation (17a) gives

$$\frac{\Delta_{k’q}^2}{E_{k’q}}.$$  \hspace{1cm} (E.8)

Combining equations (E.3)–(E.5) and (E.8), we get the result that we will use in the DOS calculation

$$\langle \tilde{\psi} | \hat{H} | \tilde{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle = \epsilon_{k’} \frac{\Delta_{k’q}^2}{E_{k’q}} - (\epsilon_{k’} \frac{\Delta_{k’q}^2}{E_{k’q}} + \epsilon_{k’} + \omega_q \langle S^- S^+ \rangle_q |v_{kq}|^2 \langle S^- S^+ \rangle_q.$$  \hspace{1cm} (E.9)

References

[1] Berezinskii V L 1974 \textit{JETP Lett.} 20 287
[2] Abrahams E, Balatsky A, Scalapino D J and Schrieffer J R 1995 \textit{Phys. Rev. B} 52 1271
[3] Balatsky A V and Bonca J 1993 \textit{Phys. Rev. B} 48 7445
[4] Balatsky A and Abrahams E 1992 \textit{Phys. Rev. B} 45 13125
[5] Balatsky A and Abrahams E 1992 \textit{Phys. Rev. B} 45 13125
[6] Abrahams E, Balatsky A, Schrieffer J R and Allen P B 1993 \textit{Phys. Rev. B} 47 513
[7] Coleman P, Miranda E and Tsvelik A 1994 \textit{Phys. Rev. B} 49 8955
[8] Bergeret F S, Volkov A F and Efetov K B 2001 \textit{Phys. Rev. Lett.} 86 4096
[9] Tanaka Y, Tanuma Y and Golubov A A 2007 \textit{Phys. Rev. B} 76 054522
[10] Tanaka Y and Golubov A A 2007 \textit{Phys. Rev. Lett.} 98 037003
[11] Fuseya Y, Kohno H and Miyake K 2003 \textit{J. Phys. Soc. Japan} 72 2914
[12] Johannes M D, Mazin I I, Singh D J and Papaconstantopoulos D A 2004 \textit{Phys. Rev. Lett.} 93 097005
[13] Kalas R M, Balatsky A V and Mozyrsky D 2008 \textit{Phys. Rev. B} 78 184513