Failure of conventional superconductivity theory for optical-phonon mediated d-wave pairing

J P Hague

1 Department of Physics, Loughborough University, Loughborough, LE11 3TU, UK
E-mail: J.P.Hague@lboro.ac.uk

Abstract. A kink in the electronic dispersion associated with the active optical phonon, an anomalous change in the phonon spectrum at the superconducting transition, and strong isotope effects indicate that phonons play an interesting role in the cuprates. This opens the question of how phonon-mediated mechanisms for superconductivity could fit in with the claims of d-wave order parameters. Since the magnitude of the electron-phonon coupling, and the energy of the phonon mode in cuprates are outside the limited region of applicability for BCS theory, more sophisticated schemes need to be developed. I describe an approach that extends the Eliashberg theory through systematic expansion in the vertex function. By examining limiting behaviours of the electron-phonon problem for optical phonon modes, including the mapping to the BCS Hamiltonian, I argue why vertex corrections are essential for examining pairing with angular momentum, even for weak coupling. An extended scheme for the superconducting state leads to the important conclusion that d-wave superconductivity can be mediated by phonons, with the inclusion of Coulomb repulsion stabilising d-pairing.

1. Introduction: Conventional theory of superconductivity

The theory of conventional superconductivity devised by Bardeen, Cooper and Schrieffer remains one of the most elegant pieces of 20th century theoretical physics [1]. A major achievement of superconductivity theory is to explain how the fine balance between inter-electron repulsion and phonon-mediated attraction can lead to bound pairs. As we know today, the initial harmony is achieved using Landau Fermi-liquid theory to recast the problem as weakly interacting quasi-particles. The second part of the balance is the observation that phonon scattering is strongest at the Fermi-surface, thus mapping from a 3D to a 2D problem where bound states are guaranteed. This qualitative picture was put on a firm footing by Morel and Anderson [2].

Surprisingly, it is not widely noted that the BCS theory is only applicable to the very special case of vanishing phonon frequency and electron-phonon coupling. Thus the BCS theory accurately describes the lowest temperature superconductors, but only gives a qualitative agreement for intermediate-$T_C$ superconductors such as lead. For such cases, it is necessary to apply the more sophisticated Eliashberg theory of superconductivity, which takes into account the summation of a subset of terms in the perturbation theory, that (in the language of Feynman diagrams) do not contain any vertex corrections [3]. The small parameter associated with this expansion is the dimensionless electron-phonon coupling $\lambda$. Eliashberg theory fails for $\lambda > 1$, but correctly reproduces the BCS theory in the limit of very small $\lambda$. 
Figure 1. Schematic showing regions of applicability for different schemes of superconductivity theory. Also shown is the low and high phonon frequency behaviour when superconductivity is suppressed. For very low phonon frequencies, electrons move significantly faster than the ions, thus for $T > \omega_0$, the electrons are scattered from a random potential landscape as single particles (ions can’t move to mediate). For $\omega_0 \to \infty$, the model tends to an attractive Hubbard model and all 2nd order diagrams are required to get the correct weak-coupling behaviour. Thus, as $\omega_0$ is increased, Eliashberg theory requires vertex corrections. All second order diagrams are included in extended Eliashberg theory, which is therefore valid at weak coupling for all phonon frequencies. As shown here, the 2nd order term is the leading order for the theory of optical-phonon mediated $d$-wave superconductivity.

A generic model of electron-phonon interactions ($\hbar = 1$) is,

$$H = \sum_{k\sigma} c_k^\dagger c_{k,\sigma} + \sum_{kq} \frac{g_q}{\sqrt{\omega_q}} c_{k-q,\sigma} c_{k,\sigma} (b_q^\dagger + b_q) + \sum_q \omega_q (b_q^\dagger b_q + 1/2)$$

(1)

The special case where $g_q = g_0$ and $\omega_q = \omega_0$ is known as the Holstein model, for which, $\lambda = \frac{g_0^2}{\omega_0^2 W}$ is the dimensionless electron phonon coupling, and $W$ is the half-band width. The momentum independent phonon dispersion approximates an optical phonon, and the momentum independent el-ph coupling a local interaction. A Hubbard style repulsion term (Coulomb pseudo-potential), $H_U = U_C \sum_i n_i^\uparrow n_i^\downarrow$, may be added at the Hartree–Fock level.

A BCS-style Hamiltonian is constructed by noting that there are only certain sets of measurable non-vanishing correlators. As is normally the case, the number operator $\langle c_{k}^\dagger c_{k} \rangle = \delta_{k,q} \langle c_{k_1}^\dagger c_{k_1} \rangle$ is one of the non-vanishing averages. Superconductivity occurs when certain pair correlators are non-vanishing $\langle c_{k}^\dagger c_{p}^\dagger \rangle = \delta_{k,p} \langle c_{k}^\dagger c_{k} \rangle$, since then the scattering of an electron with momentum $k$ is completely correlated with the scattering of the opposite momentum electron (i.e. the total momentum of a pair does not change on scattering). By taking account of these anomalous averages, a Hartree–Fock (BCS) Hamiltonian is derived from the Holstein-Hubbard model by considering only non-retarded diagrams in the perturbation expansion. (N.B. For strong coupling, the Fock diagram is retarded, forming the core of Eliashberg theory):

$$H_{BCS} = (U_C - W\lambda) \sum_{kq\sigma} n_{k\sigma} \langle q\bar{\sigma} \rangle - (U_C - W\lambda) \sum_{kq\sigma} \langle c_{q\bar{\sigma}}^\dagger c_{-q\bar{\sigma}} \rangle c_{k\sigma} c_{-k\bar{\sigma}} + h.c.$$

(2)

The transition temperature for $s$-symmetric pairs in this model has the form $T_C \sim \omega_0 \exp(-1/(\lambda - \mu_C))$, where $\mu_C = U_C/W$. Thus for large $U_C$, there is no superconductivity in the $s$ channel.
2. Failure of the conventional theory for optical phonons

There is currently a heated argument about the order parameter of the cuprate superconductors, especially about whether the pairs have angular momentum. Standard forms for the order parameter in 2D are for example, \( \Delta_0(k_x, k_y) = \Delta_0(\cos(k_x a) - \cos(k_y a)) \), \( \Delta_{x_0}(k_x, k_y) = \Delta_0(\cos^2(k_x a) + \cos^2(k_y a)) \) and \( \Delta_x(k_x, k_y) = \Delta_0 \).

It is instructive to examine the effect of the different ordering types on the BCS Hamiltonian. It is immediately clear that the sum over \( q \) in equation 2 renders the gap for the \( d \)-wave state zero (\( \sum_q \langle c_{q\sigma}^\dagger c_{-q\sigma} \rangle \sim 0 \) for \( d \) and is a constant for \( s \) components). This has been given as an argument against a phonon-mediated mechanism for \( d \)-wave superconductivity. However, BCS theory is an extreme limiting case of the theory of superconductivity determined from the lowest order terms in an expansion in the electron-phonon coupling. Thus, the absence of a stable \( d \)-wave gap in BCS theory means that one needs to examine the next (i.e. 2nd order term) in the expansion in order to study \( d \)-pairing.

First, it is necessary to confirm that the 1st order term really doesn’t contribute to the anomalous self-energy. The lowest order non-retarded expression for the self-energy is,

\[
\Phi(k, i\omega_n) = W\lambda T \sum_{q,s} F(k - q, i\omega_n - i\omega_s) D(q, i\omega_s)
\]  

(3)

The phonon propagator has the form,

\[
D(q, i\omega_s) = \frac{\omega_s^2}{\omega_s^2 + \omega_0^2 - \omega_0^2\Pi(q, i\omega_s)}
\]  

(4)

In the limit that \( \Pi(q, 0) \ll 1 \), (i.e. \( \lambda \rightarrow 0 \)), the phonon propagator is essentially momentum independent (\( \Pi(K) = 2W\lambda T \sum_q |G(Q)|G(K + Q) - F(Q)F^*(K + Q)| + O(\lambda^2) \) with \( K \) and \( Q \) 4-vectors). The anomalous propagator \( F \) has the same symmetry as the order parameter, thus for \( d \)-wave order, \( \sum_k F(k, i\omega_n) = 0 \) (this is also true for \( p, f, g \) etc.) and

\[
\Phi(k, i\omega_n) \approx W\lambda T \sum_s D(i\omega_s) \sum_q F(q, i\omega_n - i\omega_s) = 0
\]  

(5)

This is exact for \( \lambda \rightarrow 0 \) and shows that the true weak-coupling limit is quite different to BCS / Eliashberg. A similar cancellation is present for the Coulomb pseudopotential term,

\[
\Phi_C = U_C \sum_{n,k} F(i\omega_n, k) = 0
\]  

(6)

thus the \( d \)-wave state is unaffected by the Coulomb pseudopotential, whereas \( s \)-wave states are destroyed by the pseudopotential as seen in the expression for \( T^* \) (this is especially clear for small couplings). Thus there is at least a region of the parameter space of the model where the

![Figure 2. Order parameter predicted from the extended Eliashberg theory \( \langle n_s(k) = \langle c_{k\uparrow}^\dagger c_{-k\uparrow} \rangle \rangle \). \( W\lambda = 0.6 \) and \( \omega_0 = 0.392W \), doped to electron density \( n = 1.15 \). The \( d \)-wave symmetry is very clear. What is particularly appealing about the result here is that the symmetry was not imposed on the self-consistent equations, rather that it emerges directly on numerical solution.](image)
only possible superconductivity must have angular momentum. For 2D (by symmetry) this is most likely to be \(d\)-rather than \(p\)-wave, although the argument holds for any states with angular momentum if the symmetry allows (e.g. \(f\)-wave on a triangular lattice). A particular point of interest here is that when the phonon frequency is very large, and an attractive Hubbard model results, the leading (2nd order) terms of both the repulsive and attractive Hubbard models are identical. It was noted some time ago by Kohn and Luttinger that intrinsic pairing with angular momentum is possible in the very dilute limit of repulsive models [4]. For a review of how phonons may enhance intrinsic superconductivity (and a summary of alternative studies of vertex corrections) please see Ref. [5].

3. Phonon-mediated \(d\)-wave superconductivity from an extended Eliashberg theory

In the normal state, the effects of including the vertex corrections to the Migdal-Eliashberg theory are mostly quantitative, as well as strengthening the internal consistency of the theory [6]. However, as I demonstrated in the previous section of this article, the **vertex corrections are the leading order term of the superconducting (anomalous) self-energy**. Full details of including higher order terms can be found in references [6, 7, 8]. The main difficulty with implementation is to carry out the double momentum integrals. These are simplified using the dynamical-cluster approximation (DCA) as a coarse graining procedure. DCA is similar in spirit to the local (dynamical mean-field) approach used when deriving the Eliashberg equation.

The main result from the extended theory is the prediction of \(d\)-wave superconductivity (figure 2). No assumptions were made in advance about the symmetry of the order parameter: the symmetry simply emerges from the self consistency, as a direct result of the phonons. The reason for the \(d\)-wave order is clear if one considers the anti-adiabatic limit [8]. There the leading 2nd order term in the perturbation theory for the anomalous self-energy is identical for both attractive and repulsive cases. So one expects a similar order parameter in both cases.

To summarise, I have shown that significant corrections must be made to the theory of superconductivity when pairing is via optical phonons: in particular vertex corrections must be included, since they contain the leading order terms. In cuprate superconductors, one of the optical phonons has anomalous behaviour around the phase transition, indicating that the optical phonons may have a role in the pairing [9]. Examination of the spectral functions in the normal phase has clearly shown that the kinks measured by ARPES appear in the extended theory [6]. It now remains to be seen whether the anomalous phonon modes are found using the theory presented here. Another major extension of this work is a proper treatment of the Coulomb repulsion beyond the mean-field level. This will form the subject of future articles.

Acknowledgments

I would like to thank EPSRC grant no. EP/C518365/1 for funding at Loughborough University, the MPIPKS guest scientist program and additional hospitality from Leicester University during the course of this research.

References

[1] Bardeen J, Cooper L N and Schrieffer J R 1957 *Phys. Rev. B* 108 1175
[2] Morle P and Anderson P W 1962 *Phys. Rev.* 125 1263
[3] Eliashberg G M 1960 *JETP letters* 11 696
[4] Kohn W and Luttinger J M 1965 *Phys. Rev. Lett.* 15 524–526
[5] Kulic M L 2000 *Physics Reports* 338 1
[6] Hague J P 2003 *J. Phys.: Condens. Matter* 15 2535
[7] Hague J P 2005 *J. Phys.: Condens. Matter* 17 5663
[8] Hague J P 2006 *Phys. Rev. B* 73 060503(R)
[9] Chung J H, Egami T, McQueeney R J, Yethiraj M, Arai M, Yokoo T, Petrov Y, Mook H A, Endoh Y, Tajima S, Frost C and Dogan F 2003 *Phys. Rev. B* 67 014517