

Comment on “Time-reversal symmetry-breaking superconductivity”

Sadhan K. Adhikari

*Instituto de Física Teórica, Universidade Estadual Paulista, 01.405-900 São Paulo, SP, Brazil**
and Instituto de Física, Universidad Nacional Autónoma de México, 01.000 México City, DF, Mexico

(Received 15 July 1999; revised manuscript received 26 September 2000; published 18 May 2001)

It is pointed out that erroneous Bardeen-Cooper-Schrieffer model equations have been used by Haranath Ghosh in his recent treatment of time-reversal symmetry-breaking superconductivity. Consequently, his numerical results are misleading, and his conclusions are not to the point.

DOI: 10.1103/PhysRevB.63.226501

PACS number(s): 74.20.Fg, 74.62.-c, 74.25.Bt

Some recent studies provide increasing evidence that the pairing symmetry of some of the cuprates at low temperatures allow an order parameter in a mixed symmetry state. At higher temperatures, below the critical temperature T_c , the symmetry of the order parameter is of the $d_{x^2-y^2}$ type. At a lower temperature there could be an admixture of a minor component, such as d_{xy} , on the predominant $d_{x^2-y^2}$ symmetry. This general time-reversal symmetry-breaking order parameter has the form $d_{x^2-y^2} + \exp(i\theta)d_{xy}$, where θ is the mixing angle.

Recently, Ghosh¹ presented a theoretical study of superconductivity for this mixed-symmetry case based on the Bardeen-Cooper-Schrieffer (BCS) equation. In this comment we point out that the coupled equations used by him for the two components of the order parameter are erroneous and present a rederivation of the appropriate equations. This comment also applies to latter investigations where Ghosh further used the erroneous equations in subsequent studies of (i) superconductors of mixed order parameter symmetry in a Zeeman magnetic field,² and (ii) pairing symmetry and long-range pair potential in a weak-coupling theory of superconductivity.³

We use the two-dimensional tight-binding model as in Ref. 1. The effective interaction, after including the two appropriate basis functions, is taken as

$$V_{\mathbf{kq}} = -V_1 \eta_{1\mathbf{k}} \eta_{1\mathbf{q}} - V_2 \eta_{2\mathbf{k}} \eta_{2\mathbf{q}}, \quad (1)$$

where $\eta_{1\mathbf{q}} = \cos q_x - \cos q_y$ corresponds to $d_{x^2-y^2}$ symmetry and $\eta_{2\mathbf{q}} = \sin q_x \sin q_y$ corresponds to d_{xy} symmetry. The orthogonal functions $\eta_{1\mathbf{q}}$ and $\eta_{2\mathbf{q}}$ are associated with a one-dimensional irreducible representation of the point group of square lattice C_{4v} (Ref. 4) and can be considered appropriate generalizations of the circular harmonics $\cos(2\phi)$ and $\sin(2\phi)$ incorporating the proper lattice symmetry. The orthogonality condition of these functions is

$$\sum_{\mathbf{q}} \eta_{1\mathbf{q}} \eta_{2\mathbf{q}} = 0. \quad (2)$$

This orthogonality relation is readily verified as under the transformation $q_x \rightarrow -q_x$ (or $q_y \rightarrow -q_y$) $\eta_{2\mathbf{q}}$ changes sign and $\eta_{1\mathbf{q}}$ remains unchanged. Although, the proof could be slightly different, a similar orthogonality relation exists between the basis functions of states on a square lattice, such as, $d_{x^2-y^2}$, s ($\eta = 1$), $s_{x^2+y^2}$ ($\eta_{\mathbf{q}} = \cos q_x + \cos q_y$), and s_{xy} ($\eta_{\mathbf{q}} = \cos q_x \cos q_y$), and the present discussion equally ap-

plies to mixtures involving such orthogonal states. On the continuum the s -wave angular function $\zeta_1(\phi) = 1$, and the d -wave circular harmonics $\zeta_2(\phi) = \cos(2\phi)$ and $\zeta_3(\phi) = \sin(2\phi)$ satisfy the trivial orthogonality relation

$$\int_0^{2\pi} \zeta_i(\phi) \zeta_j(\phi) d\phi = 0, \quad i \neq j. \quad (3)$$

One passes from the lattice to the continuum description by replacing (a) the sum over \mathbf{q} by an integral over ϕ and (b) the functions $\eta_{\mathbf{q}}$ by the circular harmonics $\zeta(\phi)$.

Although Ghosh¹ considered the BCS model at a finite temperature, we consider its zero-temperature version, which is enough for our purpose:

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{q}} V_{\mathbf{kq}} \frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{q}}}, \quad (4)$$

with $E_{\mathbf{q}} = [(\epsilon_{\mathbf{q}} - \mu)^2 + |\Delta_{\mathbf{q}}|^2]^{1/2}$, where $\epsilon_{\mathbf{q}}$ is the single-particle energy and μ is the chemical potential. The order parameter has the following general anisotropic form:

$$\Delta_{\mathbf{q}} \equiv \Delta_1 \eta_{1\mathbf{q}} + C \Delta_2 \eta_{2\mathbf{q}}, \quad (5)$$

where $C \equiv \exp(i\theta) = (a + ib)$ is a complex number of unit modulus $|C|^2 = 1$ and $a \equiv \cos \theta$ and $b \equiv \sin \theta$ are real numbers. If we substitute Eqs. (1) and (5) into the BCS equation (4), for orthogonal functions $\eta_{1\mathbf{q}}$ and $\eta_{2\mathbf{q}}$, one can separate the resultant equation into the following components:

$$\Delta_1 = V_1 \sum_{\mathbf{q}} \frac{\eta_{1\mathbf{q}} [\Delta_1 \eta_{1\mathbf{q}} + (a + ib) \Delta_2 \eta_{2\mathbf{q}}]}{2E_{\mathbf{q}}}, \quad (6)$$

$$(a + ib) \Delta_2 = V_2 \sum_{\mathbf{q}} \frac{\eta_{2\mathbf{q}} [\Delta_1 \eta_{1\mathbf{q}} + (a + ib) \Delta_2 \eta_{2\mathbf{q}}]}{2E_{\mathbf{q}}}. \quad (7)$$

Equations (6) and (7) have a solution for real Δ_1 and Δ_2 , when the complex parameter C is either purely real or purely imaginary.

Equations (6) and (7) can be substantially simplified for a purely imaginary C , e.g., for $C = i$ or $a = 0$ and $b = 1$ ($\theta = \pi/2$). In this case for real components Δ_1 and Δ_2 , the real and imaginary parts of Eqs. (6) and (7) become, respectively,

$$\Delta_1 = V_1 \sum_{\mathbf{q}} \frac{\eta_{1\mathbf{q}}^2 \Delta_1}{2E_{\mathbf{q}}}, \quad (8)$$

$$\Delta_2 = V_2 \sum_{\mathbf{q}} \frac{\eta_{2\mathbf{q}}^2 \Delta_2}{2E_{\mathbf{q}}}. \quad (9)$$

Here we have used the identity

$$\sum_{\mathbf{q}} \frac{\eta_{1\mathbf{q}} \eta_{2\mathbf{q}}}{2E_{\mathbf{q}}} = 0, \quad (10)$$

which holds in this case as $E_{\mathbf{q}} \equiv [(\epsilon_{\mathbf{q}} - \mu)^2 + \Delta_1^2 \eta_{1\mathbf{q}}^2 + \Delta_2^2 \eta_{2\mathbf{q}}^2]^{1/2}$ is invariant under transformation $q_x \rightarrow -q_x$ or under $q_y \rightarrow -q_y$, whereas under either of these transformations $\eta_{2\mathbf{q}}$ changes sign and $\eta_{1\mathbf{q}}$ remains unchanged. Hence using the integration of \mathbf{q} , one can establish identity (10). Equations (8) and (9) have been used in the study of the mixed-symmetry states of types $d_{x^2-y^2} + id_{xy}$ and $d_{x^2-y^2} + is$.⁵

Equations (6) and (7) also lead to a simple form for a purely real C , e.g., for $C=1$ or for $a=1$ and $b=0$ ($\theta=0$). However, in this case $E_{\mathbf{q}} \equiv [(\epsilon_{\mathbf{q}} - \mu)^2 + (\Delta_1 \eta_{1\mathbf{q}} + \Delta_2 \eta_{2\mathbf{q}})^2]^{1/2}$ contains cross terms of the type $\eta_{1\mathbf{q}} \eta_{2\mathbf{q}}$, and is not invariant under the transformation $q_x \rightarrow -q_x$ or under $q_y \rightarrow -q_y$. Consequently, Eq. (10) is not satisfied and coupled angular terms will be present in the BCS equation. In this case for real Δ_1 and Δ_2 , Eqs. (6) and (7) become the following set of coupled equations, respectively,

$$\Delta_1 = V_1 \sum_{\mathbf{q}} \frac{\eta_{1\mathbf{q}} [\Delta_1 \eta_{1\mathbf{q}} + \Delta_2 \eta_{2\mathbf{q}}]}{2E_{\mathbf{q}}}, \quad (11)$$

$$\Delta_2 = V_2 \sum_{\mathbf{q}} \frac{\eta_{2\mathbf{q}} [\Delta_1 \eta_{1\mathbf{q}} + \Delta_2 \eta_{2\mathbf{q}}]}{2E_{\mathbf{q}}}. \quad (12)$$

In the case of a general mixture, e.g., $a \neq 0$ and $b \neq 0$, Eq. (10) is not valid. However, for real Δ_1 and Δ_2 , one can break up Eqs. (6) and (7) into their real and imaginary parts, e.g., into four coupled equations for two unknowns, Δ_1 and Δ_2 . As Eq. (10) does not hold in this general case, the four

coupled equations are consistent only if $\Delta_2=0$, or $\Delta_1=0$, which corresponds to no coupling between the two components. Hence the permissible values for the mixing angle θ are 0, $\pi/2$, π , and $3\pi/2$.

In his study, Ghosh¹ implicitly assumed Eq. (10) to be valid in all the cases discussed above, including (i) the case of a general C with $a \neq 0$ and $b \neq 0$, and (ii) the case with $a=1$ and $b=0$. Consequently, he arrived at the wrong Eqs. (8) and (9) for a general C , which he used in his numerical treatment, specifically for mixing angles $\theta=0$, and $\pi/4$ [see Eq. (9) of Ref. 1, Eq. (6) of Ref. 2, and Eq. (5) of Ref. 3]. For $\theta=0$ he used inappropriate equations and for $\theta=\pi/4$ there should not be any mixing.

It is interesting to recall that using the orthogonality relation (3) on the continuum, Musaelian *et al.*⁶ derived the BCS equations for the mixed-symmetry states $s+d$ and $s+id$. In agreement with the present comment and in contradiction with the investigation by Ghosh¹⁻³ they (a) confirmed the existence of mixed-symmetry states for the mixing angles $\theta=0$ and $\pi/2$ only, and (b) reported the BCS equation for the $s+d$ state, which is structurally quite similar to Eqs. (11) and (12) above. As the study of Musaelian *et al.*⁶ referred to the continuum, in that work the discrete sum over \mathbf{q} was replaced by the integral over ϕ and the functions η replaced by the circular harmonics ζ .

Recently, we used the correct Eqs. (11) and (12) for a description of the $d_{x^2-y^2} + d_{xy}$ symmetry case,⁷ which corresponds to $\theta=0$ above. The qualitative feature of the temperature dependence of the Δ 's in that study is quite distinct from the erroneous results obtained by Ghosh^{1,2} by using the inappropriate equations.

The author thanks Dr. Manuel de Llano, Dr. Mauricio Fortes, and Dr. Miguel Angel Solís for very kind hospitality at the Universidad Nacional Autónoma de México. Partial support from UNAM-DGAPA-PAPIIT and CONACyT (México), and CNPq and FAPESP (Brazil) is gratefully acknowledged.

*Permanent address.

¹H. Ghosh, Phys. Rev. B **59**, 3357 (1999).

²H. Ghosh, Phys. Rev. B **60**, 3538 (1999).

³H. Ghosh, Phys. Rev. B **60**, 6814 (1999).

⁴R. Fehrenbacher and M.R. Norman, Phys. Rev. Lett. **74**, 3884 (1995).

⁵A. Ghosh and S.K. Adhikari, Physica C **309**, 251 (1998); **322**, 37 (1999).

⁶K.A. Musaelian, J. Betouras, A.V. Chubukov, and R. Joynt, Phys. Rev. B **53**, 3598 (1996).

⁷A. Ghosh and S.K. Adhikari, Phys. Rev. B **60**, 10 401 (1999).