ORDER PARAMETER PHASE IN CDWs AND SUPERCONDUCTORS: A COMPARISON

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Abstract. Both the superconducting and charge-density wave (CDW) states have complex order parameters characterized by a magnitude and phase. The special relation of the superconducting phase to the many-body number eigenstates results in the Josephson effect and many other widely studied properties. In this brief review we discuss the role of the nature of the CDW ground state and the role of the CDW phase in an analogous context.

1. INTRODUCTION

Although the BCS superconducting and CDW ground states describe different physical systems, the mathematical apparatus that describes them is extremely similar. Both are coherent quantum ground states, and can be explained as instabilities of the Fermi sea due to electron-phonon interactions. In both cases, theoretical analysis starts from the Frohlich Hamiltonian [1,2]:

$$H = \underbrace{\sum_{k,\sigma} \epsilon_{k,\sigma}\, c^\dagger_{k,\sigma} c_{k,\sigma}}_{\text{electron term}} + \underbrace{\sum_{q} \hbar\omega_q\, b^\dagger_q b_q}_{\text{phonon term}} + \underbrace{\sum_{k,q,\sigma} g_{k,q}\, c^\dagger_{k+q,\sigma} c_{k,\sigma}\, (b^\dagger_{-q} + b_q)}_{\text{electron-phonon interaction}} \tag{1}$$

Where $\epsilon_{k,\sigma}$ is the (renormalized) energy of an electron with momentum k and spin σ, $c^{+}_{k,\sigma}$ and $c_{k,\sigma}$ are electron creation and annihilation operators, $\hbar\omega_q$ is the energy of a phonon of momentum q, b^{+}_{q} and b_q are phonon creation and annihilation operators, and $g_{k,q}$ is the electron-phonon coupling constant. The last term in (1) describes the electron-phonon scattering: a phonon in mode q ($-q$) is annihilated (created) when an electron is scattered from a state with momentum k into a state with momentum $k+q$. The 3D vector spaces of k's and q's are reduced to 1D in the CDW case.

A CDW is a periodic modulation of electron charge at twice the Fermi wavevector, $2k_F$, coupled to a corresponding ion-lattice modulation ("frozen" $2k_F$-phonon). Consequently, the CDW ground state can be expressed in two equivalent representations: one in terms of $2k_F$-phonons, the other electron-hole pairs. Table 1 compares the superconducting (BCS) ground state to the corresponding CDW ground state in these representations [1,2].

Table 1

Superconducting State	**CDW State** (2 equivalent representations)	
Cooper Pairs: Electrons over-screen ions, producing an effective attractive potential and pairing between electrons with opposite spin and momentum. These pairs condense into a macroscopically occupied state: $\mid\psi_S\rangle = \prod_{k=k_1,k_2,\ldots,k_M} (u_k + e^{i\phi_S} v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}) \mid 0\rangle$ u_k, v_k are real and satisfy $u_k + v_k = 1$ ϕ_S = superconducting phase	**$2k_F$-Phonons:** Electron-phonon scattering in 1D produces a macroscopically occupied phonon state with wavevector $2k_F$: $\mid\psi_{cdw,\,ph}\rangle = e^{-\mid\alpha\mid^2} \sum_{n=1,\ldots,\infty} \left(\frac{\alpha^n}{\sqrt{n!}} (b^\dagger_{2k_F})^n + \frac{(\alpha^*)^n}{\sqrt{n!}} (b^\dagger_{-2k_F})^n \right) \mid 0\rangle$ $2\alpha = \Delta_o e^{i\phi_{cdw}}$, Δ_o = one-half of CDW gap ϕ_{cdw} = CDW phase	**Electron-Hole Pairs:** An electron of momentum k is scattered by a $2k_F$-phonon, increasing its momentum by $2k_F$ and leaving behind a hole of momentum $k-2k_F$: $\mid\psi_{cdw,\,e\text{-}h}\rangle = \prod_{k=k_1,k_2,\ldots,k_N} (v_k c^\dagger_k + e^{-i\phi_{cdw}} u_k c^\dagger_{k-2k_F}) \mid 0\rangle$ u_k, v_k are real and satisfy $u_k + v_k = 1$ (continued →)

<table>
<tr><th>Superconducting State</th><th colspan="2">CDW State (2 equivalent representations)</th></tr>
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$|\Psi_S\rangle$ has the following form:

$$|\psi_S\rangle \propto |0\rangle + e^{i\phi_S}\begin{pmatrix}\text{group of}\\ \text{1 Cooper-pair states}\\ \text{each with}\\ Q_{tot}=0\end{pmatrix} + e^{2i\phi_S}\begin{pmatrix}\text{group of}\\ \text{2 Cooper-pair states}\\ \text{each with}\\ Q_{tot}=0\end{pmatrix} + e^{3i\phi_S}\begin{pmatrix}\text{group of}\\ \text{3 Cooper-pair states}\\ \text{each with}\\ Q_{tot}=0\end{pmatrix} + \ldots$$

where Q_{tot} is total momentum.

$|\Psi_S\rangle$ = superposition of states with different Cooper-pair numbers but the same momentum.

⇒ $|\Psi_S\rangle$ has an ill-defined Cooper-pair number but a well defined momentum. ϕ_S connects states with well-defined Cooper-pair numbers in $|\Psi_S\rangle$.

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$|\Psi_{cdw,ph}\rangle$ has the following form:

$$|\psi_{cdw,\,ph}\rangle \propto e^{i\phi_{cdw}}\begin{pmatrix}\text{state with 1}\\ 2k_F\text{-phonon}\\ Q_{tot}=2k_F\end{pmatrix} + e^{-i\phi_{cdw}}\begin{pmatrix}\text{state with 1}\\ -2k_F\text{-phonon}\\ Q_{tot}=-2k_F\end{pmatrix} + e^{2i\phi_{cdw}}\begin{pmatrix}\text{state with 2}\\ 2k_F\text{-phonons}\\ Q_{tot}=4k_F\end{pmatrix} + e^{-2i\phi_{cdw}}\begin{pmatrix}\text{state with 2}\\ -2k_F\text{-phonons}\\ Q_{tot}=-4k_F\end{pmatrix} + e^{3i\phi_{cdw}}\begin{pmatrix}\text{state with 3}\\ 2k_F\text{-phonons}\\ Q_{tot}=6k_F\end{pmatrix} + e^{-3i\phi_{cdw}}\begin{pmatrix}\text{state with 3}\\ -2k_F\text{-phonons}\\ Q_{tot}=-6k_F\end{pmatrix} + \ldots$$

where Q_{tot} is total momentum.

$|\Psi_{cdw,ph}\rangle$ = superposition of states with different numbers of $2k_F$-phonons.

⇒ $|\Psi_{cdw,ph}\rangle$ has an ill-defined phonon number and ill-defined momentum. ϕ_{cdw} connects states with well-defined phonon numbers in $|\Psi_{cdw,ph}\rangle$.

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$|\Psi_{cdw,e\text{-}h}\rangle$ has the following form:

$$|\psi_{cdw,\,e\text{-}h}\rangle \propto |0\rangle + e^{i\phi_{cdw}}\begin{pmatrix}\text{group of}\\ \text{N-electron states}\\ \text{each with}\\ Q_{tot}=-2k_F\end{pmatrix} + e^{2i\phi_{cdw}}\begin{pmatrix}\text{group of}\\ \text{N-electron states}\\ \text{each with}\\ Q_{tot}=-4k_F\end{pmatrix} + e^{3i\phi_{cdw}}\begin{pmatrix}\text{group of}\\ \text{N-electron states}\\ \text{each with}\\ Q_{tot}=-6k_F\end{pmatrix} + \ldots$$

where Q_{tot} is total momentum.

$|\Psi_{cdw,e\text{-}h}\rangle$ = superposition of states with the same number of electrons but different total momentum.

⇒ $|\Psi_{cdw,e\text{-}h}\rangle$ has a well-defined electron number and ill-defined momentum. ϕ_{cdw} connects states with well-defined total momentum in $|\Psi_{cdw,e\text{-}h}\rangle$.

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<tr><td colspan="3">In this sense ϕ_S and ϕ_{cdw} are both true quantum-mechanical phases of their corresponding states. In addition ϕ_{cdw}, unlike ϕ_S, has a more physical meaning: ϕ_{cdw} describes a CDW position relative to the lattice, and appears explicitly in the phenomenological equations of motion.</td></tr>
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Order Parameter: Operator $c_{-k\uparrow}\,c_{k\downarrow}$ destroys a Cooper pair. Since $|\Psi_S\rangle$ is a superposition of states with different number of Cooper pairs,

$$\sum_k \langle c_{-k\downarrow}c_{k\uparrow}\rangle_{|\psi_S\rangle} = e^{i\phi_S}\sum_k u_k v_k \propto \Delta_o e^{i\phi_S}$$

≠ 0 in general

⇒ good order parameter.

Off-Diagonal Long Range Order (ODLRO): The matrix of the order parameter operator has non-vanishing off-diagonal elements when represented in a basis of particle (i.e. electron-, Cooper pair-) number eigenstates.

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Order Parameter: Operator b_{2kF} destroys a $2k_F$-phonon. Since $|\Psi_{cdw,ph}\rangle$ is a superposition of states with different number of $2k_F$-phonons,

$$\sum_k \langle b_{2k_F}\rangle_{|\psi_{cdw,\,ph}\rangle} \propto \Delta_o e^{i\phi_{cdw}}$$

≠ 0 in general

⇒ good order parameter.

ODLRO: The matrix of the order parameter operator has non-vanishing off-diagonal elements when represented in a basis of particle (i.e. $2k_F$-phonon-) number eigenstates.

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Order Parameter: Operator $c_k\, c^{+}_{k\text{-}2kF}$ destroys an electron-hole pair (changes momentum of a state by $2k_F$). Since $|\Psi_{cdw,e\text{-}h}\rangle$ is a superposition of states which differ in momentum by $2k_F$,

$$\sum_k \langle c_k c^{\dagger}_{k-2k_F}\rangle_{|\psi_{cdw,\,e\text{-}h}\rangle} = e^{i\phi_{cdw}}\sum_k u_k v_k \propto \Delta_o e^{i\phi_{cdw}}$$

≠ 0 in general

⇒ good order parameter.

ODLRO: The matrix of the order parameter operator has non-vanishing off-diagonal elements when represented in a basis of momentum eigenstates.

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<tr><td colspan="3">In superconductors, the special role of ϕ_S in connecting states with different number of charged particles in $|\Psi_S\rangle$ and associated ODLRO with respect to electron-number eigenstates leads to the Josephson effect (zero bias electrical current across an SNS junction). The CDW state has no ODLRO with respect to the basis of electron-number eigenstates and zero-bias charge current should not be observed in CDW-N-CDW junctions. An equivalent phenomenon for CDW systems, however, has been predicted: a zero bias momentum current across the junction [3].</td></tr>
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References

[1] Frohlich, H. *Proc. R. Soc. Lond.* **A223** (1954) 296-305; Rice, M. J., and Strassler, S. *Solid State Commun.* **13** (1973) 125-128; Gruner G., *Density Waves in Solids* (Addison-Wesley, New York, 1994) pp.32-35.

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[3] Visscher M. I., Bauer G. E. W., *Phys. Rev. B* **54** (1996) 2798-2805.