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INSTABILITIES OF ELECTRON SYSTEMS WITH NESTING FERMI SURFACES

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A double Nambu formalism is developed which can deal in a straightforward manner with all possible instabilities of a single band with nesting Fermi surfaces. Besides the usual density waves and superconductivity, also strong coupling phenomena are considered, such as ferromagnetism, Martensitic instability, and the somewhat bizarre state of localized Cooper pairs. The system is solved in the mean field approximation which is valid when the Fermi surfaces are not too flat.

THE VARIOUS INSTABILITIES of an electron system with nesting Fermi surfaces (FS) have been investigated by many authors. In particular the one dimensional system, which correspond to parallel flat FS has been recently investigated.

It is advantageous to present a method which can deal with all the instabilities on the same footing and represent them in a straightforward manner. This is accomplished by using a double Nambu representation in the BCS space[1] and in the Peierls space.[2] The various elements in the 4 x 4 matrix of the Green's function represent the possible instabilities.

I solve the system in the mean field (MF) approximation which is valid when the system is not too one dimensional. In particular I have in mind a linear chain system with an interchain coupling η, leading to an electron dispersion of the form

$$\epsilon_{\mathbf{p}} = \epsilon(p_Z) - \eta T_F (\cos ap_x + \cos ap_Y). \qquad (1)$$

Due to electron–hole symmetry $\epsilon(p_F + \delta p_F) = -\epsilon(p_F - \delta p_F)$ (ϵ_p is measured from the Fermi level) the condition for nesting FS is obtained

$$\epsilon_{\mathbf{p}+\mathbf{Q}/2} = -\epsilon_{\mathbf{p}-\mathbf{Q}/2} \qquad (2)$$

with $\mathbf{Q} = (\pi/a, \pi/a, 2p_F)$. I use $|p_z| < p_F$ so that the phase space consists of $-2p_F < p_Z < 2p_F$. The condition (2) is independent of η, so that density wave instabilities are possible for large η where the MF is valid.[3]

In what follows one dimensional notation will be used and $Q = 2p_F$, however interchain coupling is readily introduced by (1). The condition (2) will be the only restriction on the electron dispersion.

The Hamiltonian of the system is

$$\begin{aligned} H = \sum_{p,\sigma} \epsilon_{p+Q/2}(C^+_{p+Q/2\sigma}C_{p+Q/2\sigma} - C^+_{p-Q/2\sigma}C_{p-Q/2\sigma}) \\ + \tfrac{1}{2}g_1 \Big\{ \sum C^+_{p_1+Q/2\sigma}C_{p_4-Q/2\sigma}C^+_{p_2-Q/2\sigma'}C_{p_3+Q/2\sigma'} \\ + \text{H.C.}\Big\} \\ + \tfrac{1}{2}g_2 \Big\{ \sum C^+_{p_1+Q/2\sigma}C_{p_4+Q/2\sigma}C^+_{p_2-Q/2\sigma'}C_{p_3-Q/2\sigma'} \\ + \text{H.C.}\Big\} \\ + \tfrac{1}{2}g_3 \Big\{ \sum C^+_{p_1+Q/2\sigma}C_{p_4-Q/2\sigma}C^+_{p_2+Q/2\sigma'}C_{p_3-Q/2\sigma'} \\ + \text{H.C.}\Big\} \\ + \tfrac{1}{2}g_4 \Big\{ \sum C^+_{p_1+Q/2\sigma}C_{p_4+Q/2\sigma}C^+_{p_2+Q/2\sigma'}C_{p_3+Q/2\sigma'} \\ + (Q/2 \to -Q/2)\Big\} . \end{aligned} \qquad (3)$$

Summations include spins ($\sigma, \sigma' = \uparrow$ or $\downarrow$) and are restricted by $|p_i| < Q/2$ and $p_1 + p_2 = p_3 + p_4$. The couplings g_2, g_4 represent small momentum transfer scattering, g_1 describes the large momentum ($\sim Q$) transfer, while g_3 is due to umklapp processes.[4]

In the usual Nambu formalism of superconductivity[1] the vector field $\tilde{\psi}^+_p = (C^+_{p\uparrow}, C_{-p\downarrow})$ is introduced. In order to account for the special correlation between the two sides of the FS, the Nambu formalism in the Peierls phase is superimposed,

$$\begin{aligned} \psi^+_p = (\tilde{\psi}^+_{p+Q/2}, \tilde{\psi}^+_{p-Q/2}) = \\ (C^+_{p+Q/2\uparrow}, C_{-p-Q/2\downarrow}, C^+_{p-Q/2\uparrow}, C_{-p+Q/2\downarrow}) \end{aligned} \qquad (4)$$

and ψ_p is the hermitian conjugated column vector.

The 4 x 4 space is a direct product of the superconducting 2 x 2 space with σ_i as the Pauli matrices, and the Peierls 2 x 2 space with τ_i as the Pauli matrices, and products appear in this order.

The Hamiltonian can now be transformed into the following form

Table 1. Notation and possible types of phases. The coefficients of the listed matrices in the expansion of Σ *[Equation (6)] are the order parameters of the corresponding phases. Direct and Exchange refer to the two contributions in Fig. 1. The equation of state is within the mean field approximation assuming* $g_2 = g_4$

Notation	Type of phase	Matrix	Direct	Exchange	Equation of state
S	Superconductivity–singlet	$\sigma_1 1, \sigma_2 1$		$-g_1 - g_2$	$1 = (-g_1 - g_2)F_1(\Delta_S)$
T	Superconductivity–triplet	$\sigma_1\tau_3, \sigma_2\tau_3$		$g_1 - g_2$	$1 = (g_1 - g_2)F_1(\Delta_T)$
P	Peierls–CDW	$\sigma_3\tau_1$ or $\sigma_3\tau_2$	$-2g_1 \pm 2g_3$	$g_2 \pm g_3$	$1 = (-2g_1 + g_2 + \lvert g_3\rvert)F_1(\Delta_p)$
AF	Antiferromagnetism–SDW	$1\tau_1$ or $1\tau_2$		$g_2 \pm g_3$	$1 = (g_2 + \lvert g_3\rvert)F_1(\Delta_{AF})$
F	Ferromagnetism	11		$g_1 + g_4$	$1 = (g_1 + g_2)F_2(\Delta_F)$
M	Interband electron shift	$\sigma_3 1$	$-2g_2 - 2g_4$	$g_1 + g_4$	$1 = (-3g_2 + g_1)F_2(\Delta_M)$
L	Localized Cooper pairs	$\sigma_1\tau_1, \sigma_2\tau_1$ or $\sigma_1\tau_2, \sigma_2\tau_2$		$-g_4 \pm g_3$	$1 = (-g_2 + \lvert g_3\rvert)F_2(\Delta_L)$

$$
\begin{aligned}
H = {} & \sum \epsilon_{p+Q/2}\psi_p^+\sigma_3\tau_3\psi_p \\
& + \tfrac{1}{4}(g_1 + g_3)\sum \psi_{p_1}^+\sigma_3\tau_1\psi_{p_4}\psi_{p_2}^+\sigma_3\tau_1\psi_{p_3} \\
& + \tfrac{1}{4}(g_1 - g_3)\sum \psi_{p_1}^+\sigma_3\tau_2\psi_{p_4}\psi_{p_2}^+\sigma_3\tau_2\psi_{p_3} \\
& + \tfrac{1}{4}(g_2 + g_4)\sum \psi_{p_1}^+\sigma_3 1\ \psi_{p_4}\psi_{p_2}^+\sigma_3 1\ \psi_{p_3} \\
& + \tfrac{1}{4}(g_4 - g_2)\sum \psi_{p_1}^+\ 1\tau_3\psi_{p_4}\psi_{p_2}^+\ 1\tau_3\psi_{p_3}. \qquad (5)
\end{aligned}
$$

The Green's function in the Matzubara formalism $[\omega_n = \pi T(2n+1)]$ is a 4×4 matrix.

$$G^{-1}(i\omega_n, p) = i\omega_n 11 - \epsilon_{p+Q/2}\sigma_3\tau_3 - \Sigma(i\omega_n, p) \qquad (6)$$

where Σ can be expanded in the 16 basic matrices. The various instabilities of the system correspond to different coefficients Δ_i of this expansion, as shown in Table 1.

The charge density wave (CDW) and the spin density wave (SDW) correspond to the singlet and triplet electron–hole pairs, while the superconducting phases correspond to singlet and triplet electron–electron pairs. Diagonalizing the relevant Green's functions gives the excitation spectrum $\pm\sqrt{\epsilon^2 + \Delta^2}$ which has a gap, and thus denoted as type I instabilities. All the following phases do not have a gap in the quasi particle spectrum, but lead to a relative shift of the Fermi level between various states and are denoted as type II instabilities. The coefficient of $\sigma_3\tau_3$ represents normal metal renormalization and should not describe any instability. The 11 matrix represents a relative shift of energies between the $\uparrow$ and $\downarrow$ spins and corresponds to Ferromagnetism. The $1\tau_3$ represents an energy shift between the $p > 0$ and $p < 0$ states which implies shift of electrons to the $p > 0$ or $p < 0$ states. Since the interactions depend only on the momentum transfer, the potential energy would not change, while the kinetic energy increases and this phase cannot be stable. (In the present formalism a difference among the couplings in (3) implies that the interaction depend also on the signs of the various momenta. This may lead to a spurious solution only in this case where time reversal is violated.)

The coefficient of $\sigma_3 1$ represents a shift in the energy of the whole band. Thus if another band is available an interband shift of electrons is possible. This is essentially the Labe–Friedel–Barisic model[5] explaining the martensitic transformation in the A15 compounds. These compounds have three orthogonal families of linear chains,[6] so that electron transfer from one chain to the others, will induce a cubic to tetragonal transformation.

Let us next examine the rather unusual phase represented by $\sigma_1\tau_1$, which I label as L,

$$G^{-1}(i\omega_n, p) = i\omega_n 11 - \epsilon_{p+Q/2}\sigma_3\tau_3 - \Delta_L\sigma_1\tau_1.$$

The diagonalizing matrix is $U = (11 + i\sigma_1\tau_2)/\sqrt{2}$,

$$UG^{-1}(i\omega_n, p)U^{-1} = i\omega_n 11 - \epsilon_{p+Q/2}\sigma_3\tau_3 - \Delta_L 1\tau_3.$$

Thus the phase is of the type II-shift in the relative energies. The product $U\psi_p$ gives the eigenstates $(C_{p+Q/2\uparrow} \pm C_{-p+Q/2\downarrow}^+)/\sqrt{2}$ with energies $\epsilon_{p+Q/2} \pm \Delta_L$. This is similar to the BCS type eigenstates, except that the combination has always equal weights for an electron and a hole. Thus all the momentum space $-Q < p < Q$ is uniform – half filled and half empty which means localized electron pairs. These pairs have momentum $\pm Q$ so that this phase is a superposition of a CDW and Cooper pair correlation. This phase has been noted within the Hubbard model,[7] but it is not clear whether it is superconducting.

Replacing σ_1 by σ_2 or τ_1 by τ_2 changes the phase of the wave function and so does not change the nature of the instability. Thus the classification of Table 1 is completed.

The next step is to obtain the various equations of state in the MF approximation, as illustrated in Fig. 1. One should sum the various matrices Γ_i in (5). The direct term gives

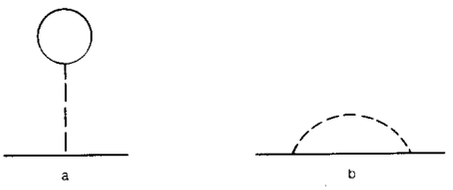

Fig. 1. Mean field diagrams for calculating Σ in equation (6). (a) Direct term. (b) Exchange term.

$$\Sigma \sim \Gamma_i T \sum_{\omega_n} \int \frac{d^3p}{(2\pi)^3} \mathrm{Tr}\,[G(i\omega_n, p)\Gamma_i] + \ldots$$

while the exchange term has an opposite sign and no trace. Equating the coefficients of the various matrices leads to the equations of state in Table 1. The functions $F_1(\Delta), F_2(\Delta)$ characterize the instabilities of type I and II respectively:

$$F_1(\Delta) = \int d\epsilon N(\epsilon) \frac{\tanh(\sqrt{\epsilon^2 + \Delta^2}/2T)}{\sqrt{\epsilon^2 + \Delta^2}} \qquad (7)$$

$$F_2(\Delta) = \int d\epsilon N(\epsilon) \frac{n(\epsilon - \Delta) - n(\epsilon + \Delta)}{2\Delta}.$$

$N(0)$ is the free electron density of states for both spins and $n(\epsilon) = [e^{\epsilon/T} + 1]^{-1}$. An essential difference between the two types of instabilities is that $F_1(\Delta)$ diverges as $\Delta, T \to 0$ while $F_2(\Delta)$ stays finite. Thus type I instabilities exist for any coupling, while type II require rather large couplings. A necessary condition for a solution to $1 = g_{\mathrm{eff}} F_2(\Delta)$ is

$$g_{\mathrm{eff}} N(0) > 4. \qquad (8)$$

The Umklapp coupling g_3 has an interesting effect. The replacement $\tau_1 \longleftrightarrow \tau_2$ changes the sign of g_3 so that the possibility with $|g_3|$ dominates, and the phase of the density wave is determined. Now $g_3 \neq 0$ means that Q is commensurate with the lattice spacing so that commensurability leads to pinning of the density wave, which is a well known effect.[8]

Finally, the phase diagram of Fig. 2 is obtained. Since usually interactions depend only on the momentum transfer I assume $g_2 = g_4$. The type I phases exclude each other (except on the coexistence lines $g_1 = 2g_2 + |g_3|$ and $g_1 = 0$) since they obey the same equation $1 = g_{\mathrm{eff}} F_1(\Delta)$ with different couplings. The comparison between type I and II phases depends sensitively on the form of $N(\epsilon)$, especially through $F_2(\Delta)$. Thus the dashed lines in Fig. 2 describe the necessary condition equation (8) and type II phases may occur beyond these lines. The dashed lines do not limit the type I phases and the two types may coexist. Thus in the A15 compounds somewhat below the Martensitic transition superconductivity appears. Also one should note that the M phase is not always feasible.

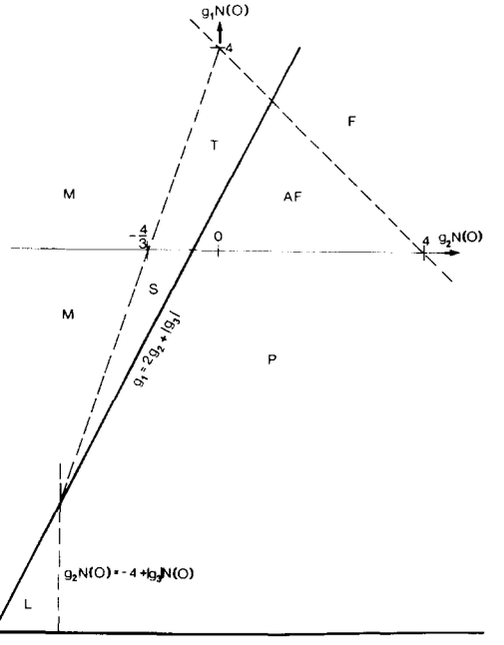

Fig. 2. Phase diagram using notations and equations of state from Table 1. Full lines are phase boundaries, while dashed lines limit the phases further from the origin according to equation (8). ($|g_3|N(0) = 1$ is assumed arbitrarily).

It is quite surprising how close are the results for type I phases with those obtained using more sophisticated methods for the strictly one dimensional problem. Figure 2 is consistent with exact results for the Tomonaga model[9] ($g_1 = g_3 = 0$), for the Luther and Emery case[10] (on the line $\frac{1}{4}g_1 N(0) = -3/5$) and the Hubbard model solutions[11] ($g_1 = g_2 = g_3 = g_4$). Figure 2 (for type I phases) is also very similar to results obtained using renormalization group techniques.[12–14] The only difference is the possible coexistence of two phases in various regions of Fig. 2. However these works[12–14] also differ between themselves in this respect.

A possibly important correction to MF is due to screening effects. This was recently studied, including phonon retardation effects for the P–S coexistence line. It turns out that this line crosses $g_2 = 0$ at some $g_1 < 0$ (for $g_3 = 0$). This is due to the fact that the contribution of g_1 to the P phase comes from the direct term while the S phase is driven by the exchange term. Now only the exchange term needs screening since by iterating the direct term it is seen that screening is already included. Thus screening would enhance only the g_1 term of the S phase, leading to superconductivity for small couplings $g_1 < 0$, even for $g_2 = 0$.

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