PART V

THEORETICAL PHYSICS

NON-LINEARITY AND COHERENCE IN MODELS OF SUPERCONDUCTIVITY

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Theoretical investigations of standard low-temperature superconductivity frequently proceed in one of two main ways. The first begins with the well-known BCS Hamiltonian which may be written as

$$H^{BCS} = \sum_{\underline{k}\sigma} \omega_{\underline{k}}\, a^{\dagger}_{\underline{k}\sigma} a_{\underline{k}\sigma} + \sum_{\substack{\underline{k},\underline{\ell},\underline{m} \\ \sigma,\sigma'}} \Delta_{\underline{k}\,\underline{\ell}\,\underline{m}}\, a^{\dagger}_{\underline{k}\sigma} a^{\dagger}_{\underline{k}\sigma'} a_{\underline{m}\sigma'} a_{\underline{k}+\underline{\ell}-\underline{m}\sigma} \ . \tag{1}$$

In equation (1) the one-body part of the Hamiltonian is assumed diagonal in the plane-wave basis, each vector being labelled by a wave-vector $\underline{k}$, $\underline{\ell}$ or $\underline{m}$. The two-body term is assumed to be attractive in nature, the vectors on annihilators and creators being arranged to conserve linear momentum. The labels σ and σ' denote the components of spin, the total spin on each particle being $S = 1/2$. One standard approach is to use Bogoliubov-Valatin transformations [1] to diagonalise H^{BCS}, so that the effective one-body term exhibits explicitly a gap representing the minimum energy required to create an excitation in the system. Both this transformation and subsequent approximations are guided by the knowledge, obtained originally variationally [2], that in the ground state electrons are formed into Cooper pairs with their wavevectors and spin components equal and opposite.

The second approach is to take a Landau-Ginzburg (LG) view and write down a free energy density expansion [3] in the form

$$G_S(\underline{r}) = G_N(\underline{r}) + A(T)\,|\psi(\underline{r})|^2 + \frac{1}{2} C|\psi(\underline{r})|^4 + \frac{\hbar^2}{2m^*}|\nabla\psi(\underline{r})|^2 \ , \tag{2}$$

where $A(T) = \overline{a}\ (T-T_c)$, $\overline{a}$ being a constant and $T-T_c$ denoting the temperature difference from the critical temperature $T=T_c$. Here, $\psi(\underline{r})$ is the order parameter and $|\psi(\underline{r})|^2$ measures the density of superconducting electron pairs and hence the local degree of superconductivity. $G_N(\underline{r})$ is the free energy density of the normal state, m* is an effective mass and C a parameter which is assumed to be such that C>0. At this stage, despite the work of Gor'kov [4], this route is usually considered to be phenomenological but at the time this was put forward it constituted a break through in the understanding of critical phenomena [5]. Thus, the first approach uses a number of approximations to incorporate Cooper pairs and an energy gap and the second appears to be phenomenological. However, the present authors [6] have recently developed a novel approach, initially without spin components, using the Hamiltonian

$$H_{TD} = \sum_{\underline{k},\underline{\ell}} \omega_{\underline{k},\underline{\ell}}\, q_{\underline{k}}^{\dagger} q_{\underline{\ell}} + \sum_{\underline{k},\underline{\ell},\underline{m}} \Delta_{\underline{k},\underline{\ell},\underline{m}}\, q_{\underline{k}}^{\dagger} q_{\underline{\ell}}^{\dagger} q_{\underline{m}} q_{\underline{k}+\underline{\ell}-\underline{m}} \ . \tag{3}$$

The idea was to first write down Heisenberg's equations of motion for the annihilators and creators in equation (3). One notices immediately that these rate equations have the same form whether the q_η or $(q_\eta^{\dagger})$'s describe Bosons or Fermions. The next step is to define a quantum field by

$$\psi(\underline{r}) = \Omega^{-1/2} \sum_{\underline{k}} e^{-i\underline{k}\cdot\underline{r}}\, q_{\underline{k}} \quad , \tag{4}$$

and to rewrite the equations of motion in terms of this field alone. This latter part of the procedure is not easy because the parameters or matrix elements in (3) are functions of the subscripted wave-vectors. However, if these elements are expanded as a series about some suitable point in $\underline{k}$-space then clearly the equations of motion may be written in terms of ψ, ψ^* and their gradients. In general, there will be an infinite number of terms as a consequence of this procedure. If the point in $\underline{k}$-space is chosen as a critical point of the system, then it is well known [7] that close to this point the order parameter ψ will be predominantly classical, corrections being very small and of order $\hbar$. It is then only necessary to perform the expansion in $\underline{k}$-space up to second order because Renormalisation Group Theory tells us that we only need to include terms up to ψ^n in the Hamiltonian, in N-dimensional space time [8], where $n = 2N/(N-2) = 4$ – or terms in ψ^3 or its equivalent in the equations of motion. Thus, the form of the second order equations is virtually exact and higher order terms merely redress those in lower orders. This general equation of motion takes the highly non-linear form [6]

$$i\hbar\partial_t\psi = \lambda_o\psi + i\underline{\lambda}_1\cdot(\nabla\psi) - \frac{1}{2}\sum_{i,j}(\underline{\lambda}_2)_{ij}\,\partial^2_{x_i x_j}\psi + v_2\psi^{\dagger}\psi\psi$$

$$+\ \Omega\,[i\,(\nabla_{\underline{n}}f)_o\cdot\psi^{\dagger}\psi\nabla\psi + i\,(\nabla_{\underline{m}}f)_o\cdot\psi^{\dagger}(\nabla\psi)\psi - i\,(\nabla_{\underline{k}}f)_o\cdot(\nabla\psi^{\dagger})\psi\psi]$$

$$+\frac{\Omega}{2!}\sum_{i,j}(\partial^2_{m_i m_j}f)_o\,\{\psi^\dagger\,[-\partial^2_{x_i x_j}\psi - 2i\,(\partial_{x_i}\psi)\,m_j^o + \psi m_i^o m_j^o]\,\psi$$

$$+\psi^\dagger\psi\,[-\partial^2_{x_i x_j}\psi - 2i\,(\partial_{x_i}\psi)\,\eta_j^o + \eta_i^o\eta_j^o\psi] + 2\psi^\dagger[(i\partial_{x_i}\psi - m_i^o\psi)\,(i\partial_{x_j}\psi - \eta_j^o\psi)]\}. \quad (5)$$

What is perhaps so surprising is that, if H_{TD} is itself written in terms of the field ψ a standard Landau-Ginzburg form is retrieved. Furthermore, terms in $\psi(\nabla\psi^\dagger)$, $(\nabla^2\psi^\dagger)\psi$, $(\nabla^2\psi^\dagger)\psi^\dagger\psi\psi$ and $(\nabla\psi^\dagger)(\nabla\psi^\dagger)\psi\psi$, which were actually considered and investigated by Landau, also appear! The equations of motion for ψ turn out to be the Euler-Lagrange equations obtained by finding the extrema, relative to ψ^*, of the Hamiltonian functional, equation (3) being considered as a Hamiltonian density when written in terms of the classical field.

What, therefore, is so significant is that in the first approach above it is not necessary to make approximations; we can retain the full generality of the second quantised form and the second approach is not phenomenological at all but a work of true genius.

So far this new approach has not incorporated spin at all. At this stage this will be omitted and to focus attention on standard low temperature superconductors we put

$$\omega_{\underline{k},\underline{\ell}} = (\frac{\hbar^2 k^2}{2m^*} - E_F)\,\delta_{\underline{k},\underline{\ell}} \quad , \quad (5a)$$

and assume

$$\Delta_{\underline{k},\underline{\ell},\underline{m}} = -V_o\,\delta_E \quad , \quad (5b)$$

as is customarily done in BCS-type theories. In equation (5) E_F is the Fermi energy, V_o is a constant energy and the symbol δ_E is zero unless the kinetic energies are within $\hbar\omega_D$ (where ω_D is the Debye angular frequency). Using standard methods in quantum field theory [7], near the critical point we describe the field ψ by

$$\psi = \phi + \Lambda \quad ,$$

where ϕ is a large classical envelope and Λ is the smaller quantum component and, as a first approximation in the equations of motion, drop the quantum component Λ. In zeroth order the equations of motion reduce to

$$i\hbar\partial_t\phi = -E_F\,\phi + \frac{\hbar^2}{2m^*}\nabla^2\phi - 2\Omega V_o\phi^*\phi\phi \quad , \quad (6)$$

which is a non-linear Schrödinger equation in three-dimensional space. This equation is integrable in 1+1 dimensions, as is well known, and among its solutions are stable solitons. It has also been studied in depth using the Symmetry Reduction method [8]. Analytical results appear to be only found when the level surfaces of the symmetry variable ξ correspond to planar, cylindrical and spherical manifolds. Asymptotic behaviour for some of these geometries corresponds to solutions of the quasi-linear equation and for this reason we confine our attention to these. Writing the classical field ϕ as

$$\phi = \exp(+i\frac{Et}{\hbar}) \exp(i\chi)\, \eta \quad , \tag{7}$$

substituting into (6), and separating real and imaginary parts results in

$$A\eta + C\eta^3 - \frac{\hbar^2}{2m^*} \nabla^2\eta + \frac{\hbar^2}{2m^*\eta^3} C_1^3 = 0 \tag{8}$$

where $A = E_F - E$, $C = 2\Omega V_0$ and C_1 defines the magnitude of the superconducting current, $\underline{j}_s$.

When there are no currents, corresponding to the case when $C_1=0$, there are two main categories of solution to consider. Firstly, when $m^*>0$ the lowest exact solution is a mean field and if $A>0$ this describes the normal state whereas if $A<0$ we obtain the ordered superconducting state. In the case when $A<0$, just below the energy of the normal phase, one finds, with this approach, a discrete ladder of one-, two- etc. up to N-soliton states. If one assumes that the physical situation may be described by a nearly free soliton gas, then one can show that the N-soliton condensate is separated from the normal phase by a gap Δ. If, as is the case in the LG picture, the constant A is temperature dependent through the usual relation

$$A = \overline{a}\,(T - T_c) \quad , \tag{9}$$

then we find that the gap scales with temperature as

$$\Delta \sim (T - T_c)^{1/2} \quad , \tag{10}$$

exactly as it does for standard low temperature superconductors! In fact, between the mean field energy and disordered phase one finds a continuum of snoidal and dnoidal (of the Jacobi elliptic type) waves, the latter representing thermodynamically stable fluctuations. As the temperature approaches the critical point from above the normal phase becomes destabilised so that for $T<T_c$ soliton

energy levels become available to the system and dnoidal waves execute small oscillations about the mean superconducting energy.

Still describing the situation when $m^*>0$, but when <u>superconducting currents</u> $\underline{j}_s \neq 0$ are present, we may still solve the non-linear equation of motion exactly and above T_c all the solutions become unstable. However, below T_c, $\underline{j}_s$ breaks the topological solitons (or kinks) into pairs of bumps and the elliptic solutions become distorted. At a critical value of the current $\underline{j}_c$ both elliptic waves and bump solitons below them disappear and the superconducting state is destroyed. Remarkably, this critical condition enables us to deduce the correct scaling of the current with temperature as

$$\underline{j}_s \sim |T - T_c|^{3/2} \quad . \tag{11}$$

This is again as in standard superconductors [3].

The other main case is when $m^*<0$. This may arise due to band structure effects, re-dressing from higher order terms but in any case can happen if transport is by holes in an approximately two-dimensional system [9] as is the situation for high-temperature superconductivity. This situation is very different from that for $m^*>0$ and results in a ground state which is strongly modulated in space (cn-waves) and has a critical current whose square has a cubic dependences on T-T_c [10].

All the results above are consequences of the model <u>in the absence of spin</u> so it is legitimate to ask what difference its inclusion would produce. Following a similar procedure as outlined above, the starting point would be the analogue of equation (3) with spin components introduced, namely

$$H_1 = \sum_{\substack{\underline{k},\underline{\ell} \\ \sigma}} \omega_{\underline{k},\underline{\ell}}\, q^{\dagger}_{\underline{k}\sigma} q_{\underline{\ell}\sigma} + \sum_{\underline{k},\underline{\ell},\sigma',\sigma} \Delta_{\underline{k},\underline{\ell},\underline{m}} q^{\dagger}_{\underline{k}\sigma} q^{\dagger}_{\underline{\ell}\sigma'} q_{\underline{m}\sigma'} q_{(\underline{k}+\underline{\ell}-\underline{m})\sigma} \cdot \tag{12}$$

In equation (12) we have assumed for simplicity that the one- and two-body operators from which ω and Δ arise <u>do not</u> depend on spin. The labels σ, σ' refer to the components of spin, not necessarily for a spin $S=1/2$, and $q_{k\sigma}$ or $(q^{\dagger}_{k\sigma})$'s can refer to either Bosons or Fermions at this stage. If we take the case where the spins do refer to electrons, as an example, and denote spin components $\sigma = +1/2$ by '+' and $\sigma = -1/2$ by '−', then the Heisenberg equation of motion for $q_{\eta+}$ is given by

$$i\hbar\partial_t q_{\eta+} = \sum_{\underline{k}} \omega_{\underline{\eta},\underline{k}}\, q_{\underline{k}+} + \sum_{\underline{k},\underline{m}} \{\Delta_{\underline{\eta}\,\underline{k}\,\underline{m}} q^{\dagger}_{\underline{k}+} q_{\underline{m}+} q_{(\underline{\eta}+\underline{k}-\underline{m})+} - \Delta_{\underline{k}\,\underline{\eta}\,\underline{m}} q^{\dagger}_{\underline{k}+} q_{\underline{m}+} q_{(\underline{k}+\underline{\eta}-\underline{m})+}$$

$$+ \Delta_{\underline{\eta}\,\underline{k}\,\underline{m}} q^{\dagger}_{\underline{k}-} q_{\underline{m}-} q_{(\underline{\eta}+\underline{k}-\underline{m})+} - \Delta_{\underline{k}\,\underline{\eta}\,\underline{m}} q^{\dagger}_{\underline{k}+} q_{\underline{m}-} q_{(\underline{k}+\underline{\eta}-\underline{m})+}\} \quad , \tag{13}$$

with a corresponding equation for $i\hbar\,\partial_t q_{\eta -}$, obtained from (13) by interchanging '+' and '−'. These latter two equations may now be replaced by field equations involving, in this simple example, two spin-dependent fields defined by

$$\psi_+(\underline{r}) = \Omega^{-1/2}\sum_{\underline{k}} e^{-i\underline{k}\cdot\underline{r}}\, q_{\underline{k}+} \;, \qquad \psi_-(\underline{r}) = \Omega^{-1/2}\sum_{\underline{k}} e^{-i\underline{k}\cdot\underline{r}}\, q_{\underline{k}-} \tag{14}$$

using a similar procedure to that in the spinless field case. The field equation for ψ_+ may be obtained by making the following replacement in equation (5)

a) $q_{k\sigma} \rightarrow \psi_\sigma$

b) $k_x q_{k\sigma} \rightarrow \partial_{x_1}\psi_\sigma$ (15)

c) $\psi^{\dagger}\psi\,\nabla\psi \rightarrow \psi^{\dagger}_{+}\psi_+\psi_+ + \frac{1}{2}\psi^{\dagger}_{-}\psi_-\nabla\psi_+ + \frac{1}{2}\psi^{\dagger}_{-}\psi_+\nabla\psi_-$

d) $\psi^{\dagger}[\partial^2_{x_ix_j}\psi]\psi \rightarrow \psi^{\dagger}_{+}[\partial^2_{x_ix_j}\psi_+]\psi_+ + \frac{1}{2}\psi^{\dagger}_{-}[\partial^2_{x_ix_j}\psi_-]\psi_+ \;\frac{1}{2}\psi^{\dagger}_{-}[\partial^2_{x_ix_j}\psi_+]\psi_-$

and similar replacements by permutation of co-ordinates. An equation for the ψ_- field may also be obtained in this way but with '+' replaced by '−' in c) and d) of (15) and vice versa. A full calculation will confirm the relationships in (15). What one notices on writing down these equations of motion is that those terms which couple the ψ_+ and ψ_- fields together may all be written in terms of brackets of the form

$$[\psi_-\psi_+ + \psi_+\psi_-] \quad . \tag{16}$$

However, these all vanish due to the commutation relations for the quantum fields! Hence the equation of motion for ψ_+ becomes identical in form to the spinless case, with ψ_+ replaced by ψ. In a similar way the equation for ψ_- is also, on putting $\psi_- \rightarrow \psi$, exactly the same as in the spinless case. Hence, for Bosons with spin S=0 and Fermions with S=1/2 the equations of motion are of the <u>same</u> form, despite the fact that they apparently contain very complicated couplings between the spin component fields!

Even when the spin is greater than one-half for Fermions, a very similar argument, when the one-body and two-body terms involve sums over spin components, may be used to show that, for Fermions, for any total spin, the equation of motion for a field associated with one component of the spin is identical to that for any other component and has the same form as in the spinless case. This does take rather a lot of tedious algebra but is a remarkable result. The Boson case for $S \neq 0$, is a little more complicated but in this, although the equation of motion for any spin component has the same form, it is not identical to the spinless case and the two-body interaction terms become scaled by the spin degeneracy, $2S+1$. Thus, this result might lead to higher critical temperatures if the mechanism for superconductivity involved quasi-particles with a larger effective spin. In this connection we remark that the transition temperature for ^4He is much higher than in ^3He, provided we compare the two under the same conditions of pressure so this would agree with our deliberation above [11].

What we have presented in this paper is a nonlinear field-theoretic approach to superconductivity which is applicable to situations where a single phase exists. Depending on the case we may obtain a normal phase, a homogeneous superconducting phase, or indeed a host of modulated superconducting phases with periodically distributed regions of high and low concentration of superconducting charge. The regions with low concentrations of charge density will be easily penetrable by magnetic flux lines and may result in the formation of a flux lattice. Thus, this type of description appears fairly suitable for both type I and type II superconductors. However, in the case of the new ceramic type of superconductor the spatial ordering may be somewhat more complicated and the role of defects, twin boundaries and structural disorder should not be underestimated. Admittedly then, the model we have presented in this work would only be suitable for a single grain and interactions between the neighbouring domains of superconductivity would have to be modelled independently through the inclusion of Lawrence-Doniach terms, for example. We have made a first step in the direction of extending the present approach to embrace ceramic superconductors [12]. Interesting phenomena appear to be already incorporated, for instance the associated vortex arrays form from the order parameter phases of the domains and may or may not be commensurate with the structure of the island or domain envelopes. This may explain the experimentally observed glassy features of these materials [13].

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