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Coherent structures in strongly interacting many-body systems: I. Derivation of dynamics

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Abstract. Numerous examples in condensed matter physics possess an effective Hamiltonian structure involving two-body anharmonic interactions between elementary excitations. The effective second-quantised Hamiltonian used to model these systems is essentially of the same form except for the particulars of the interaction parameters and the statistics of the particles which are interacting. In this paper we investigate such systems in the limit of strongly anharmonic interactions which may possibly lead to symmetry breaking. We introduce quantum field operators and calculate their equations of motion. The interaction coefficients are expanded in a Taylor series about the critical mode to second order to illustrate the method, but we give the expansion to infinite order for completeness. It is demonstrated that both in first and second order the equations of motion are reduced to a system of highly non-linear coupled partial differential equations (PDE) for the field operator. We show that the form of our second-order equation is exact due to renormalisation theory, in the case where the Hamiltonian coefficients represent operators in real space which are isotropic, and incorporates symmetries and topologies which would appear in an expansion to infinite order. This special situation arises in a very wide range of physical examples. These equations can be solved exactly using a particular ansatz in conjunction with recent mathematical developments in the field of non-linear analysis. In particular, the method of symmetry reduction for PDE provides a complete set of symmetry variables for the type of equations used in our study.

1. Introduction

The method of second quantisation (Berezin 1966, Judd 1967) is not only a very convenient and succinct approach to the study of many-particle systems but a representation in which elementary excitations appear naturally (Nakajima *et al* 1980). To a first approximation it also diagonalises Hamiltonians of numerous many-particle systems when interactions are weak. Interactions between the resulting quasiparticles can be readily incorporated using standard perturbation methods developed in quantum mechanics such as Green function techniques (Economu 1983), the deployment of Feynmann diagrams (Fetter and Walecka 1971) or projection operators (Stevens 1976). This often leads to modified dispersion relations for the quasiparticles with effective masses which differ from those of free particles as a result of the emergence of some sort of self-consistent potential to which the particles are subjected. However, when interparticle interactions are sufficiently strong, a new phenomenon often occurs which cannot be treated perturbatively with elementary excitations used as a zeroth-order approximation, e.g. the harmonic approximation. The new phenomenon is the so-called symmetry breaking effect (Anderson 1984, Makhankov and Fedyanin 1984) whereby

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the new degenerate ground state of the total Hamiltonian is not invariant with respect to an application of one or more symmetry operations of the total Hamiltonian, e.g. parity or gauge invariance. Such systems exhibit extraordinary properties such as Bose condensation, long-range order, the existence of soft (Goldstone) modes and coherence as can be seen in such phenomena as superconductivity, superfluidity or structural phase transitions, to name but a few.

In this paper we intend to present a unified approach to a many-particle problem near a critical point. By a critical point we are to understand the occurrence of a singularity in the thermodynamic potential of the system (Ma 1976). In § 2 we give a very wide range of physically important examples and show that all of them lead to the same form of effective Hamiltonian. This, of course, does not mean that all these systems possess identical physical states but only that a single mathematical procedure can be adopted to solve these problems. In § 3 we derive an equation of motion for the field operator using the effective Hamiltonian and analyse the form of the interactions. The two sections which follow this are devoted to deriving two general cases of non-linear equations of motion. In the first we expand to first order and in the second we include second order which will incorporate those cases where the first-order coefficients vanish identically.

Our method differs markedly from standard perturbation approaches due to the fact that in the critical region anharmonic terms dominate and drive the system. As a consequence the equations of motion we find are highly non-linear and perturbative expansions are not adequate. In this paper we construct these non-linear equations. In a second paper we will treat these equations classically and solve them analytically. Subsequently quantum corrections will be added to the classical solutions, following standard methods due to Jackiw (1977), and correspond either to the elementary excitations of the system or scattering states when stability is lost.

2. Examples of many-particle Hamiltonians

2.1. Conduction electrons in a metal

One of the simplest models which is used to understand the behaviour of conduction electrons in a metal is a system of N spinless electrons in unit volume interacting by means of Coulombic electrostatic repulsion in a uniform positive background to take account of the overall charge neutrality of the metal. The Hamiltonian for this model, when second quantised using a plane wave complete set, takes the form (Taylor 1970, Callaway 1976)

$$H_1 = \sum_k \varepsilon_k c_k^+ c_k + \sum_{k,k',q\neq 0} \frac{2\pi e^2}{q^2} c_{k-q}^+ c_{k'+q}^+ c_{k'} c_k \tag{1}$$

where ε_k represents the kinetic energy of the electrons and is given by

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \delta_{k,k} .$$

The interaction strength $2\pi e^2/q^2$ is the Fourier transform of the interparticle interaction e^2/r with $r = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ and the $\boldsymbol{q} = \boldsymbol{0}$ term has been cancelled by the corresponding terms for the uniform positive background. A Hamiltonian of this form may be obtained for electrons moving in the fields of fixed nuclei and interacting via a screened Coulomb

interaction (Raimes 1963, 1972, Dixon 1978) (which may be obtained by unitary transformation from a bare Coulomb two-body operator).

2.2. Electrons in an atom

Electrons interacting not only with each other but with only one nucleus provides an interesting special case of another system with an effective Hamiltonian of the form in (1). However, a plane wave basis is not the most appropriate one to use for the bound states of an atom! In this case we would probably use a complete set of single-particle orbital angular momentum eigenstates, each with spin labels and the Hamiltonian resulting would have the form

$$H_2 = \sum_{\alpha} \varepsilon_\alpha a_\alpha^+ a_\alpha + \tfrac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ a_\delta a_\gamma \tag{2}$$

where each of the subscripts α, β, γ, δ refers to one set of four quantum numbers n, l, m_l, m_s (Judd 1967) and

$$\varepsilon_\alpha = \left\langle \alpha \left| \frac{p^2}{2m} - \frac{Ze^2}{r} \right| \alpha \right\rangle.$$

In the second term of (2) the coefficient $V_{\alpha\beta\gamma\delta}$ would be defined by

$$V_{\alpha\beta\gamma\delta} = \left\langle \alpha, \beta \left| \frac{e^2}{r_{12}} \right| \gamma, \delta \right\rangle.$$

As the Coulomb interaction conserves orbital angular momentum just as it does linear momentum in (1), the labels on the second quantised operators (and indeed $V_{\alpha\beta\gamma\delta}$) may be rewritten to make this more explicit.

2.3. The electron-phonon Hamiltonian

An analysis of the interactions between electrons and phonons is fraught with difficulties and is extremely complicated but there is a simple model, due to Fröhlich (Taylor 1970), which we can use to describe such systems. In this model the ions are assumed to interact with one another and with electrons via a short-range screened potential. The electrons, on the other hand, are considered to be essentially independent fermions and this leads to a Hamiltonian of the form

$$H_3 = \sum_{k} \varepsilon_k C_k^+ C_k + \sum_{q} \hbar\omega_q b_q^+ b_q + \sum_{k,k'} M_{k,k'} (b_{-q}^+ + b_q) C_k^+ C_{k'}. \tag{3}$$

The first term in (3) describes the electrons, the second the phonons and the third the interaction between them. To obtain this specific form of interaction certain simplifying assumptions are made, e.g. that the phonon spectrum is isotropic and that only longitudinal modes enter the third term. A canonical transformation $\exp(s)$, followed by truncation of the series in s by omitting terms of order s^3 and higher, results in another effective Hamiltonian $H_{\text{eff}}^{(2)}$ given by (Taylor 1970)

$$H_{\text{eff}}^{(3)} = \sum_{k} \varepsilon_k C_k^+ C_k + \sum_{q} \hbar\omega_q b_q^+ b_q + \sum_{k,k'q} W_{k,k'q} C_{k'+q}^+ C_{k-q}^+ C_k C_{k'}$$

$$+ (\text{other terms involving only two-body electron-electron operators}) \tag{4}$$

where

$$W_{kk'q} = |M_q|^2 \hbar\omega_q / [(\varepsilon_k - \varepsilon_{k-q})^2 - (\hbar\omega_q)^2].$$

In a recent paper (Dixon and Wardlaw 1986), concerned with the calculation of crystal fields in metals, it was shown that the total electrostatic potential energy of a system of interacting electrons and ions (not rigid), all with the same nuclear charge $Z|e|$, may be written in the form

$$\sum_k \frac{2\pi e^2}{k^2} (\rho_k^+ \rho_k - n)$$

where n is a constant self-energy and ρ_k is a one-body operator defined by

$$\rho_k = \sum_i \exp(-i\boldsymbol{k} \cdot \boldsymbol{r}_i) - Z \sum_n \exp(-i\boldsymbol{k} \cdot \boldsymbol{R}_n)$$

and $\boldsymbol{r}_i$, $\boldsymbol{R}_n$ are the position vectors of the electrons and ions, respectively. If the first term of ρ_k is second quantised and the second expanded about the equilibrium positions of the ions $\boldsymbol{R}_n^0$, retaining only the terms linear in the nuclear displacements $\boldsymbol{U}(\boldsymbol{R}_n)$, then the effective Hamiltonian, when $\boldsymbol{U}(\boldsymbol{R}_n)$ is written in the usual way using Bose operators, takes the form

$$H_4 = \sum_k b_k^+ b_k (\hbar\omega_k + \tfrac{1}{2}) + \sum_k \varepsilon_k' C_k^+ C_k + \sum_{k,l,m,n} V_{k,l,m} C_k^+ C_l^+ C_m C_{k+l-m} + \sum_{k,k',q} M_{kk'q} (b_{-q}^+ + b_q) C_k^+ C_k + \text{HC}. \tag{5}$$

With the exception of the electron-electron term in (5) this is of exactly the same form as the Fröhlich Hamiltonian in (3). As is well known, under certain circumstances electrons can become trapped in the potential generated by lattice displacements leading to the formation of a polaron. Notice again that the electronic component of $H_{\text{eff}}^{(3)}$ is of the same form as (1).

2.4. *The BCS Hamiltonian*

The Hamiltonian in (4) may be used as a starting point for the derivation of the BCS Hamiltonian of superconductivity. In special types of materials it is well known that the effective two-body operator in (4), i.e. the term in $W_{kk'q}$ and purely electron-electron terms, provide a net attractive potential interaction leading to the formation of Cooper pairs in the ground state provided the temperature and external fields do not exceed certain critical values. The ground state is separated in energy from the excited continuum states by what can be a large energy gap, which is a function of these fields. The possibility of coexistence between normal and superconducting phases leads to the formation of domain walls which are solutions of the Landau-Ginzburg equation. Moreover, similarly to superfluids, the superconducting state exhibits vorticity which is required to bring about the Meissner effect. Under these circumstances

$$H_{\text{BCS}} = \sum_k \varepsilon_k (C_{k\uparrow}^+ C_{k\uparrow} + C_{-k\downarrow}^+ C_{-k\downarrow}) - \sum_{k,k'} V_{kk'} C_{k'\uparrow}^+ C_{-k'\downarrow}^+ C_{-k\downarrow} C_{k\uparrow} \tag{6}$$

where $V_{kk'} = -2W_{-k,k,k'-k} - U_{kk'}$ and the arrow subscripts describe the spin component for the particular wavevector $\boldsymbol{k}$. $U_{kk'}$ is a screened Coulomb repulsion term similar to the electron-electron terms in braces in (4). Notice again the similarity of H_{BCS} to our first Hamiltonian in (1).

2.5. Superfluidity

A very similar Hamiltonian to that in (1) appears in the theory of liquid ^{4}He where the atoms are treated as a system of interacting bosons with a Hamiltonian of the form

$$H_5 = \sum_k \varepsilon_k b_k^+ b_k + \tfrac{1}{2} \sum_{k,k',q} V_q b_{k-q}^+ b_{k'+q}^+ b_{k'} b_k \tag{7}$$

where $\varepsilon_k = \hbar^2 k^2/2m$ and V_q is a Fourier transform of a short-range potential and b_k^+ creates a boson from the vacuum. By assuming that there was a macroscopic number of particles in the zero-momentum state Bogoliubov showed how excitations arise as a modification of the single-particle excitation spectrum and a dispersion relation of the form

$$\hbar\omega_k \simeq \varepsilon_k^2 + 2\varepsilon_k N_0 V_k$$

arises, where N_0 is the number of particles in the zero-momentum state (Taylor 1970). It can be further shown that below a critical temperature a macroscopic number of quasiparticles undergo Bose condensation into a superfluid phase.

2.6. Anharmonic lattice vibrations

A different physical example which exhibits an effective Hamiltonian like (1) is the simple case of a strongly anharmonic lattice consisting of identical masses M which has as its Hamiltonian

$$H_6 = \sum_l \frac{p_l^2}{2M} + V(\{\boldsymbol{r}_l\}) \tag{8}$$

where $\{\boldsymbol{r}_l\}$ includes all instantaneous positions of ion sites. The anharmonic potential $V(\{\boldsymbol{r}_l\})$ may be expanded, in the usual way, in a Taylor series about an equilibrium position. Subsequent application of second quantisation results in a rather complicated form for the Hamiltonian. However, in the vicinity of a structural phase transition it is sufficient to consider the following effective Hamiltonian (Bruce and Cowley 1981, Aubry 1975)

$$H_{\text{eff}}^{(6)} = \sum_{q,s} \hbar\omega_{qs}(b_{qs}^+ b_{qs} + \tfrac{1}{2}) + \frac{1}{4!}\frac{1}{N}\left(\frac{\hbar}{2M}\right)^2 \sum_{\substack{qq'q''q''' \\ ijkl \\ ss's''s'''}} (\omega_{qs}\omega_{q's'}\omega_{q''s''}\omega_{q'''s'''})^{-1/2} s^i (s')^j (s'')^k (s''')^l$$

$$\times V_{qq'q''q'''}^{ijkl} \Delta(\boldsymbol{q}+\boldsymbol{q}'+\boldsymbol{q}''+\boldsymbol{q}''') b_{-qs}^+ b_{-q's'}^+ b_{q''s''} b_{q'''s'''}. \tag{9}$$

In (9), $\boldsymbol{q}$, $\boldsymbol{q}'$, $\boldsymbol{q}''$ and $\boldsymbol{q}'''$ are reciprocal lattice vectors, s, s', s'', s''' are polarisation vectors and i, j, k, l label their components. The symbol $V_{qq'q''q'''}^{ijkl}$ is the Fourier transform of the fourth derivative of the original potential at the equilibrium position (Taylor 1970) and Δ is a function to preserve linear momentum in the terms of the summation. The squares of the angular frequencies ω_{qs}^2 are the eigenvalues of the dynamical matrix. The striking similarity of (9) to (1) is again quite apparent.

A particular mode of lattice vibration labelled $\boldsymbol{k}_0$ in the critical region will predominantly determine both the dynamical and static properties of the crystal lattice. It has been referred to as a 'soft mode' and is characterised by a vanishing frequency as the critical temperature is approached, i.e. $\omega_{k_0} \to 0$ as $T \to T_c$. Depending on the particular regime of parameters it may either be a so-called 'kink' or a 'bump', both of which are solutions of non-linear PDE (Aubry 1975).

2.7. Spin waves

Another example of the type of system we wish to study is provided by the Heisenberg model of a ferromagnet (White 1983) in which the interaction between spins is assumed to be a scalar type and

$$H_7 = -\sum_{l} \boldsymbol{s}(l) \cdot \left(\boldsymbol{\omega}_0 + \sum_{l'} J_{ll'} \boldsymbol{s}(l') \right) \tag{10}$$

where $J_{ll'}$ is an interaction constant, being a scalar function of the vectorial positions of the spin sites l, l', and $\boldsymbol{\omega}_0$ is proportional to an externally applied magnetic field. Boson operators are then introduced using the Holstein–Primakoff transformation and if the expectation values of the boson number operators n_i are assumed unity, a diagonal operator

$$\sum_{q} \hbar \omega_q b_q^+ b_q \tag{11}$$

results where

$$\omega_q = \omega_0 + 2\hbar \sum_{l'} J_{ll'} \sin^2[\tfrac{1}{2}\boldsymbol{q} \cdot (\boldsymbol{l} - \boldsymbol{l}')].$$

However, when the operators n_i have an expectation value close to but not actually unity, the magnons described by (11) begin to interact and the effective Hamiltonian resulting from (10) becomes

$$H_{\text{eff}}^{(7)} = \varepsilon_0 + \sum_{q} \hbar \omega_q b_q^+ b_q + \frac{\hbar^2}{2N} \sum_{q,q',p} (J_{q'} + J_{q'+p} - 2J_{q'+p-q}) b_{q-p}^+ b_{q'+p}^+ b_{q'} b_q \tag{12}$$

where it has been assumed that $J_{ll'} = J_{l-l'}$.

2.8. The Fröhlich biological model

Fröhlich (1968) proposed a model intended to describe the transition to a metabolic state occurring in living cells. The Hamiltonian put forward by Wu and Austin (1977) involves a membrane's dipolar modes described by operators (a_i^+, a_i), a heat bath's modes (b_i^+, b_i) and energy pumping annihilators and creators (P_i^+, P_i). It takes the form

$$H = \sum_i \omega_i a_i^+ a_i + \sum_i \Omega_i b_i^+ b_i + \sum_i \theta_i P_i^+ P_i + \tfrac{1}{2} \sum_{i,j,k} (\chi a_i^+ a_j b_k^+ + \chi^* a_j a_i^+ b_k) + \sum_{i,j} (\lambda b_i a_j^+ + \lambda^* b_i^+ a_j)$$
$$+ \sum_{i,j} (\xi P_i a_j^+ + \xi^* P_i^+ a_j). \tag{13}$$

It has been recently demonstrated (Tuszyński *et al* 1984), with a series of canonical transformations, that the effective Hamiltonian, in terms of the membrane dipoles, may be written as

$$H_{\text{eff}}^{(8)} = \sum_k W_k a_k^+ a_k + \sum_{k,k',q} \Delta_{kk'q} a_{k'+q}^+ a_{k-q}^+ a_k a_{k'}$$

where the Hamiltonian parameters are explicitly given (Tuszyński *et al* 1984). The result of a symmetry breaking non-equilibrium transition in the system is the establishment of long-range dynamical order, non-zero electric polarisation and a Bose-like condensation of dipole oscillations.

2.9. The Davydov model

The Davydov model has recently been used as a basis for an investigation into the problem of energy transfer in one-dimensional molecular chains (Davydov 1982). Here the relevant Hamiltonian may be expressed as

$$H' = \sum_m \hbar\Omega_m a_m^+ a_m + \sum_q \hbar\omega_q (b_q^+ b_q + \tfrac{1}{2}) + \sum_{q,m} \chi_{qm} (b_q^+ + b_{-q}) a_m^+ a_m$$

where b_q^+ (b_q) are phonon ladder operators and a_m^+ (a_m) are exciton creators (annihilators). It has been demonstrated (Tuszyński 1986), using a unitary transformation that the effective Hamiltonian of the system can be written in the now familiar form

$$H'_{\text{eff}} = \sum_{m,n} (E_{mn}\delta_{m,n} + J_{m,n}) a_m^+ a_n + \sum_q \hbar\omega_q (b_q^+ b_q + \tfrac{1}{2}) + \sum_{m,n,q} \Delta_{mnq} a_{n+q}^+ a_{n-q}^+ a_m a_n$$

except that the first term in $a_m^+ a_n$ is not completely diagonal but can be made so by a suitable transformation. The two-body term constant Δ_{mnq} is defined by

$$\Delta_{mnq} = 4\chi_{mn}^2 \omega_q^2 / [(\Omega_m - \Omega_n)^2 - \omega_q^2].$$

The resultant behaviour of the system may, under special circumstances, be characterised by soliton formation, which is claimed to explain the almost lossless energy transfer in living systems.

It is apparent from the examples we have given that a large number of diverse physical phenomena may be described by a single form of effective second quantised Hamiltonian, namely

$$H_{\text{eff}} = \sum_{k,l} \omega_{k,l} q_k^+ q_l + \sum_{k,l,m} \Delta_{k,l,m} q_k^+ q_l^+ q_m q_{k+l-m} \tag{14}$$

where the second quantised operators may obey either Fermi–Dirac or Bose–Einstein statistics with their attendant commutation relations. The details of the interaction coefficients in (14) are model dependent. Their symmetries depend on the properties of a general class of systems exemplified by the particular model, e.g. rotational symmetries, parity or time reversal of the operators which give rise to the terms in (14). Without loss of generality the first term of (14) can be made diagonal by unitary transformation.

It is our objective to investigate the prototype effective Hamiltonian in (14) making no specific assumptions about the strength of the interactions between the quasiparticles concerned. We shall be interested, in particular, in the vicinity of a symmetry breaking phenomenon and associated dynamical and static structures which arise there. We have seen in the examples presented that seemingly unrelated physical effects (pairing, condensation, mode softening, coherence, solitons) can in fact be traced to a unified second-quantised formalism so it is of very great interest to study them in the above more general scheme. We shall be concerned not only with the critical point itself but the regime close to it which warrants the use of various expansion techniques around a variety of solutions to highly non-linear equations of motion. We first find the equations of motion of the $q_k(q_k^+)$ operators in (14) using Heisenberg's equation. A field operator is then defined and the equations of motion rewritten in terms of this field. Our approach is to first seek exact classical solutions to these highly non-linear equations of motion. In this procedure we will make full use of the recently published studies of Winternitz and co-workers (Winternitz *et al* 1987, Gagnon and Winternitz 1988a) which found exact solutions of the types of non-linear PDE that appear remarkably in our study. The great value of their results lies in the fact that the solutions are

obtained non-trivially in multidimensional spacetime and they possess exact symmetries of the original Hamiltonian. Subsequently semiclassical quantisation methods will be employed to obtain the internal excitation structure following the pioneering work of Jackiw (1977). This will provide us with the exact symmetries and approximate forms of the coherent structures that result from spontaneous symmetry breaking occurring in this type of system.

3. Derivation of the non-linear field equations

We shall consider (14) as our model Hamiltonian for the class of systems described earlier. We take into account both Bose-Einstein commutation relations:

$$[q_k^+, q_l^+]_- = [q_k, q_l]_- = 0 \qquad [q_k, q_l^+]_- = \delta_{k,l} \tag{15}$$

and Fermi-Dirac relations:

$$[q_k^+, q_l^+]_+ = [q_k, q_l]_+ = 0 \qquad [q_k, q_l^+]_+ = \delta_{k,l}. \tag{16}$$

The next step is to use Heisenberg's equation of motion for a general operator A, namely

$$i\hbar\partial_t A = -[H, A]_- \tag{17}$$

where H is the Hamiltonian. The equations of motion for the Bose annihilator and creator are

$$\begin{aligned} i\hbar\partial_t q_\eta &= \sum_k \omega_{\eta,k} q_k + \sum_{k,m} (\Delta_{\eta km} + \Delta_{k\eta m}) q_k^+ q_m q_{k+\eta-m} \\ i\hbar\partial_t q_\eta^+ &= -\sum_k \omega_{k,\eta} q_k^+ - \sum_{k,m} (\Delta_{km\eta} + \Delta_{mk\eta}) q_k^+ q_m^+ q_{k+m-\eta} \end{aligned} \tag{18}$$

where the general Hamiltonian in (14) has been used. Similarly for the Fermi-Dirac case

$$\begin{aligned} i\hbar\partial_t q_\eta &= \sum_k \omega_{\eta,k} q_k - \sum_{k,m} (\Delta_{k\eta m} - \Delta_{\eta km}) q_k^+ q_m q_{k+\eta-m} \\ i\hbar\partial_t q_\eta^+ &= -\sum_k \omega_{k,\eta} q_k^+ + \sum_{k,m} (\Delta_{km\eta} - \Delta_{mk\eta}) q_k^+ q_m^+ q_{k+m-\eta}. \end{aligned} \tag{19}$$

We see that for bosons, interchange of q_k^+ and q_l^+ in the two-body operator of (14) results in the operator remaining the same. Thus

$$\Delta_{klm} = \Delta_{lkm}$$

for bosons. Similarly, for fermions $\Delta_{klm} = -\Delta_{lkm}$. Hence, (18) for bosons and (19) for fermions may be written in identical form:

$$i\hbar\partial_t q_\eta = \sum_k \omega_{\eta,k} q_k + 2\sum_{k,m} \Delta_{\eta km} q_k^+ q_m q_{k+\eta-m} \tag{20a}$$

$$i\hbar\partial_t q_\eta^+ = -\sum_k \omega_{k,\eta} q_k^+ - 2\sum_{k,m} \Delta_{mk\eta} q_k^+ q_m^+ q_{k+m-\eta}. \tag{20b}$$

In the standard way (Haken 1976) we define a quantum field operator ψ by

$$\psi(\mathbf{r}) = \Omega^{-1/2} \sum_k \exp(-i\mathbf{k}\cdot\mathbf{r}) q_k. \tag{21}$$

In the context of critical phenomena the classical part of this field operator plays the role of an order parameter, namely above the critical point the classical part vanishes

while below it is non-zero. We will demonstrate later that it provides an effective potential for quantum excitations. Multiplying both sides of (20*a*) by $\exp(-i\boldsymbol{\eta}\cdot\boldsymbol{r})$, summing over η and dividing by the root volume $\Omega^{+1/2}$ we obtain

$$\begin{aligned} i\hbar\partial_t\psi(\boldsymbol{r}) &= \frac{1}{\Omega^{1/2}}\Bigg(\sum_{k,\eta}\exp(-i\boldsymbol{\eta}\cdot\boldsymbol{r})\omega_{\eta,k}q_k + 2\sum_{k,m,\eta}\Delta_{\eta km} \\ &\quad\times\exp(i\boldsymbol{k}\cdot\boldsymbol{r})q_k^+\exp(-i\boldsymbol{m}\cdot\boldsymbol{r})q_m\exp[-i(\boldsymbol{k}+\boldsymbol{\eta}-\boldsymbol{m})\cdot\boldsymbol{r}]q_{k+\eta-m}\Bigg) \\ &= \frac{1}{\Omega^{1/2}}\Bigg(\sum_{k,\eta}\exp(-i\boldsymbol{\eta}\cdot\boldsymbol{r})\omega_{\eta,k}q_k + 2\sum_{km\eta}\Delta_{\eta+m-k,k,m}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})q_k^+ \\ &\quad\times\exp(-i\boldsymbol{m}\cdot\boldsymbol{r})q_m\exp(-i\boldsymbol{\eta}\cdot\boldsymbol{r})q_\eta\Bigg). \end{aligned} \tag{22}$$

The dispersion relation $\omega_{\eta,k}$ is, of course, model dependent, but can always be chosen to be diagonal using a unitary transformation. Our objective is to re-express (22) using only field operators and their derivatives. However, in general, the interaction coefficients $\omega_{\eta,k}$ and $\Delta_{\eta+m-k,k,m}$ depend on $\boldsymbol{k}$, $\boldsymbol{\eta}$ and $\boldsymbol{m}$. Therefore, the simplest way to proceed is to Taylor expand these coefficients about some point in the space spanned by $\boldsymbol{\eta}$, $\boldsymbol{k}$ and $\boldsymbol{m}$. This 'point', in a nine-dimensional space, could be an arbitrary point and our analysis proceeds as if it were, but later it will be convenient to consider it to correspond to a local minimum of the Hamiltonian treated as a function of these momenta. In fact, in the theory of critical phenomena (Ma 1976) it is common to use a plane wave representation for the order parameter (which may correspond to our quantum field ψ) and apply renormalisation group methods to find the so-called 'fixed point' of the model Hamiltonian as a particular value of the interaction parameters. Having found this point we could then minimise the Hamiltonian with respect to the momentum coordinates (or the field operator ψ) to obtain a local energy minimum. Suppose this corresponds to $(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0)$. If we could use these values of the momentum parameters as the expansion centre then we might expect the best convergence properties for the expansion.

For convenience and to simplify such an expansion, we define

$$f(\boldsymbol{\eta}, \boldsymbol{k}, \boldsymbol{m}) = 2\Delta_{\eta+m-k,k,m}.$$

Thus, to all orders we have

$$\omega_{\eta,k} = \delta_{\eta,k}\left(\omega_{\eta_0} + \sum_{s=1}^{\infty}\frac{[(\boldsymbol{\eta}-\boldsymbol{\eta}_0)\cdot\nabla_\eta]^s\omega_0}{s!}\right). \tag{23}$$

Similarly the interaction constant may be expanded in deviations from the expansion centre to give

$$\begin{aligned} f(\boldsymbol{\eta}, \boldsymbol{k}, \boldsymbol{m}) &= f(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0) + (\boldsymbol{\eta}-\boldsymbol{\eta}_0)\cdot(\nabla_\eta f)_0 + (\boldsymbol{k}-\boldsymbol{k}_0)\cdot(\nabla_k f)_0 + (\boldsymbol{m}-\boldsymbol{m}_0)\cdot(\nabla_m f)_0 \\ &\quad + \sum_{s=2}^{\infty}\sum_{r=0}^{s}\sum_{t=0}^{s-r}\frac{{}^sC_r\,{}^{s-r}C_t}{s!} \\ &\quad\times[(\boldsymbol{\eta}-\boldsymbol{\eta}_0)\cdot\nabla_\eta]^r[(\boldsymbol{k}-\boldsymbol{k}_0)\cdot\nabla_k]^t[((\boldsymbol{m}-\boldsymbol{m}_0)\cdot\nabla_m)^{s-r-t}f_0]. \end{aligned} \tag{24}$$

In (23) and (24) the subscript 0 on both f and ω means that the corresponding gradient(s) of f and ω is (are) to be evaluated at the centre of expansion $(\boldsymbol{\eta}_0\boldsymbol{k}_0\boldsymbol{m}_0)$. For example, $\nabla_k f$ means $\boldsymbol{i}\partial_{k_x}f + \boldsymbol{j}\partial_{k_y}f + \boldsymbol{k}\partial_{k_z}f$ where $\boldsymbol{i}$, $\boldsymbol{j}$ and $\boldsymbol{k}$ are unit vectors in the k_x, k_y and k_z directions, respectively, and $(\nabla_k f)_0$ is the value of the gradient at

$(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0)$. In the fifth term of (24) the ${}^sC_r$ are binomial coefficients and f_0 indicates that the three partial gradients $\nabla_{\boldsymbol{\eta}}$, $\nabla_{\boldsymbol{k}}$ and $\nabla_{\boldsymbol{m}}$ are to operate *only* on f and then the net result is to be evaluated at $(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0)$. It is easy to see that the first four terms of (24) correspond to $s=0$ and $s=1$ in the summation of the fifth term. To make the terminology clearer consider (23) and the term with $s=2$ in the sum. This will be understood to mean

$$(\eta_x-\eta_{0x})^2\left(\frac{\partial^2\omega}{\partial\eta_x^2}\right)_0+(\eta_y-\eta_{0y})^2\left(\frac{\partial^2\omega}{\partial\eta_y^2}\right)_0+(\eta_z-\eta_{0z})^2\left(\frac{\partial^2\omega}{\partial\eta_z^2}\right)_0$$
$$+2(\eta_x-\eta_{0x})(\eta_y-\eta_{0y})\left(\frac{\partial^2\omega}{\partial\eta_x\,\partial\eta_y}\right)_0$$
$$+2(\eta_x-\eta_{0x})(\eta_z-\eta_{0z})\left(\frac{\partial^2\omega}{\partial\eta_x\,\partial\eta_z}\right)_0$$
$$+2(\eta_y-\eta_{0y})(\eta_z-\eta_{0z})\left(\frac{\partial^2\omega}{\partial\eta_y\,\partial\eta_z}\right)_0$$

where each derivative is evaluated at $(\boldsymbol{\eta}_0\boldsymbol{k}_0\boldsymbol{m}_0)$ and *only* second-order derivatives appear.

Using (23) and (24) in (22) we give below the equations of motion up to second order in the Taylor expansions. For comparison we begin with the equation for the case of non-interacting particles, then consider two special cases, namely zeroth and first order with a non-zero interaction. Finally, we give the most general second-order expansion.

3.1. Non-interacting particles

Expanding $\omega_{\boldsymbol{\eta},\boldsymbol{k}}$ to second order in $\boldsymbol{\eta}-\boldsymbol{\eta}_0$ and putting the interaction $f=0$ we readily obtain

$$\mathrm{i}\hbar\partial_t\psi=\lambda_0\psi+\mathrm{i}\boldsymbol{\lambda}_1\cdot(\nabla\psi)-\tfrac{1}{2}\sum_{i,j}(\boldsymbol{\lambda}_2)_{ij}\partial^2_{x_ix_j}\psi \tag{25}$$

where

$$\lambda_0=\omega(\boldsymbol{\eta}_0)-\boldsymbol{\eta}_0\cdot(\nabla_{\boldsymbol{\eta}}\omega)_0+\tfrac{1}{2}\sum_{i,j}\eta_{0i}\eta_{0j}(\partial^2_{\eta_i\eta_j}\omega)_0$$

and

$$(\boldsymbol{\lambda}_1)_i=-\sum_j\eta_{0j}(\partial^2\eta_i\eta_j\omega)_0+(\partial\eta_i\omega)_0$$
$$(\boldsymbol{\lambda}_2)_{ij}=(\partial^2_{\eta_i\eta_j}\omega)_0.$$

We have used the notation where $(x_1x_2x_3)\equiv(x,y,z)$ and the summations run over $i,j=1,2,3$. The last term in (25) is inconvenient in its present form so we apply a coordinate transformation a_{ij} so that the new coordinates are x_j. This term becomes diagonal and the second term remains in the same form since it is a scalar product, i.e. $x_j\to a_{ij}x_i$ and $(\boldsymbol{\lambda}_2)_{ij}$ becomes

$$(\boldsymbol{\lambda}_2)_{ij}a_{ik}a_{jl}=\delta_{kl}\Lambda_k.$$

Since Λ_k $(k=1,2,3)$ may have different magnitudes and signs we apply a subsequent scaling transformation, namely

$$x_i'=x_i/(|\Lambda_i|)^{1/2}.$$

Using the definition, $\nabla_\varepsilon^2 = \varepsilon_1\partial_{xx}^2 + \varepsilon_2\partial_{yy}^2 + \varepsilon_3\partial_{zz}^2$, of a Laplace-Beltrami operator in three dimensions, where ε_i $(i = 1, 2, 3)$ are defined by

$$\varepsilon_i = \mathrm{sgn}(\Lambda_i)$$

we recast (25) in the form

$$\mathrm{i}\hbar\partial_t\psi = \nu_0\psi + \mathrm{i}\boldsymbol{\nu}_1 \cdot (\nabla_\varepsilon\psi) - \tfrac{1}{2}\nabla_\varepsilon^2\psi \tag{26}$$

where

$$(\boldsymbol{\nu}_1)_i = \frac{\varepsilon_i}{(|\Lambda_i|)^{1/2}}(\boldsymbol{\lambda}_1)_i$$

and $\nu_0 = \lambda_0$.

This is clearly in the form of a linear Schrödinger equation for the 'free' field ψ which propagates in a dispersive medium.

3.2. Zeroth order

Here we keep the same expansion of $\omega_{\eta,k}$ as in § 3.1 but include now the zeroth-order or constant term, $f(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0)$, from the interaction. Our field equation becomes

$$\mathrm{i}\hbar\partial_t\psi = \nu_0\psi + \mathrm{i}\boldsymbol{\nu}_1 \cdot (\nabla_\varepsilon\psi) - \tfrac{1}{2}\nabla_\varepsilon^2\psi + \Omega f(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0)\psi^+\psi\psi \tag{27}$$

provided we perform the same transformations as in § 3.1. This takes the form of the standard non-linear Schrödinger equation in Euclidean or Minkowski space provided the term in $\boldsymbol{\nu}_1$ is transformed away by an appropriate Galilean transformation.

3.3. First order

Expanding $f(\boldsymbol{\eta}, \boldsymbol{k}, \boldsymbol{m})$ to first order in $\boldsymbol{\eta} - \boldsymbol{\eta}_0$, $\boldsymbol{k} - \boldsymbol{k}_0$ and $\boldsymbol{m} - \boldsymbol{m}_0$ but retaining all the terms of $\omega_{\eta,k}$ to second order we can use the definition in (21), as well as its time and space derivatives, to derive an equation of motion for the quantum field ψ. Thus, (22) yields

$$\begin{aligned}\mathrm{i}\hbar\partial_t\psi = {} & \lambda_0\psi + \mathrm{i}\boldsymbol{\lambda}_1 \cdot (\nabla\psi) - \tfrac{1}{2}\sum_{i,j}(\boldsymbol{\lambda}_2)_{ij}\partial_{x_i x_j}^2\psi \\ & + \Omega[f(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0) - \boldsymbol{\eta}_0 \cdot (\nabla_\eta f)_0 - \boldsymbol{k}_0 \cdot (\nabla_k f)_0 - \boldsymbol{m}_0 \cdot (\nabla_m f)_0]\psi^+\psi\psi \\ & + \Omega[\mathrm{i}(\nabla_\eta f)_0 \cdot \psi^+\psi(\nabla\psi) + \mathrm{i}(\nabla_m f)_0 \cdot \psi^+(\nabla\psi)\psi - \mathrm{i}(\nabla_k f)_0 \cdot (\nabla\psi^+)\psi\psi].\end{aligned} \tag{28}$$

Following a similar coordinate transformation and scaling procedure to that in §§ 3.1 and 3.2, (28) becomes transformed to

$$\begin{aligned}\mathrm{i}\hbar\partial_t\psi = {} & \gamma_0\psi + \mathrm{i}\boldsymbol{\gamma}_1 \cdot (\nabla_\varepsilon\psi) - \tfrac{1}{2}\nabla_\varepsilon^2\psi + \gamma_2\psi^+\psi\psi + \mathrm{i}\boldsymbol{\gamma}_3 \cdot \psi^+\psi(\nabla\psi) \\ & + \mathrm{i}\boldsymbol{\gamma}_4 \cdot \psi^+(\nabla\psi)\psi + \mathrm{i}\boldsymbol{\gamma}_5 \cdot (\nabla\psi^+)\psi\psi\end{aligned} \tag{29}$$

where $\gamma_0 = \nu_0$, $\boldsymbol{\gamma}_1 = \boldsymbol{\nu}_1$ and

$$\gamma_2 = \Omega[f(\boldsymbol{\eta}_0, \boldsymbol{k}_0, \boldsymbol{m}_0) - \boldsymbol{\eta}_0 \cdot (\nabla_\eta f)_0 - \boldsymbol{k}_0 \cdot (\nabla_k f)_0 - \boldsymbol{m}_0 \cdot (\nabla_m f)_0]$$

$$(\boldsymbol{\gamma}_3)_i = \Omega(\partial_{\eta_i} f)_0 \frac{\varepsilon_i}{(|\Lambda_i|)^{1/2}} \qquad (\boldsymbol{\gamma}_4)_i = \Omega(\partial_{m_i} f)_0 \frac{\varepsilon_i}{(|\Lambda_i|)^{1/2}}$$

and

$$(\boldsymbol{\gamma}_5)_i = \Omega(\partial_{k_i} f)_0 \frac{\varepsilon_i}{(|\Lambda_i|)^{1/2}}.$$

We show later in § 3.4 that $\boldsymbol{\gamma}_5 = 0$ and $\boldsymbol{\gamma}_3 = \boldsymbol{\gamma}_4$.

3.4. Second order

In certain physical systems the first-order approximation is not expected to be sufficient since the interactions between the particles may be an even function of the wavevectors and hence some of the first-order expansion coefficients vanish identically. Hence, it is important to retain only the first non-vanishing terms in the expansion but here, for completeness we include all first-order terms. This is a very tedious calculation but the result is given below for the reader to verify!

$$\begin{aligned}
\mathrm{i}\hbar\partial_t\psi = {} & \lambda_0\psi + \mathrm{i}\boldsymbol{\lambda}_1 \cdot (\nabla\psi) - \tfrac{1}{2}\sum_{i,j} (\boldsymbol{\lambda}_2)_{ij}\partial^2_{x_i x_j}\psi + \gamma_2\psi^+\psi\psi \\
& + \Omega[\mathrm{i}(\nabla_{\boldsymbol{\eta}} f)_0 \cdot \psi^+\psi(\nabla\psi) + \mathrm{i}(\nabla_{\boldsymbol{m}} f)_0 \cdot \psi^+(\nabla\psi)\psi - \mathrm{i}(\nabla_{\boldsymbol{k}} f)_0 \cdot (\nabla\psi^+)\psi\psi] \\
& + \frac{\Omega}{2!}\sum_{i,j}\{\psi^+[-\partial^2_{x_i x_j}\psi(\partial^2_{m_i m_j} f)_0 - 2\mathrm{i}(\partial_{x_i}\psi)m_j^0(\partial^2_{m_i m_j} f)_0 + \psi m_i^0 m_j^0(\partial^2_{m_i m_j} f)_0]\psi \\
& + [-\partial^2_{x_i x_j}\psi^+(\partial^2_{k_i k_j} f)_0 + 2\mathrm{i}(\partial_{x_i}\psi^+)k_j^0(\partial^2_{k_i k_j} f)_0 + \psi^+ k_i^0 k_j^0(\partial^2_{k_i k_j} f)_0]\psi\psi \\
& + \psi^+\psi[-\partial^2_{x_i x_j}\psi(\partial^2_{\eta_i \eta_j} f)_0 - 2\mathrm{i}(\partial_{x_i}\psi)\eta_j^0(\partial^2_{\eta_i \eta_j} f)_0 + \psi\eta_i^0\eta_j^0(\partial^2_{\eta_i \eta_j} f)_0] \\
& + 2[(-\mathrm{i}\partial_{x_i}\psi^+ - k_i^0\psi^+)(\mathrm{i}\partial_{x_j}\psi - m_j^0\psi)(\partial^2_{k_i m_j} f)_0]\psi \\
& + 2\psi^+[(\mathrm{i}\partial_{x_i}\psi - m_i^0\psi)(\mathrm{i}\partial_{x_j}\psi - \eta_j^0\psi)(\partial^2_{m_i \eta_j} f)_0] \\
& + 2[(-\mathrm{i}\partial_{x_i}\psi^+ - k_i^0\psi^+)\psi(\mathrm{i}\partial_{x_j}\psi - \eta_j^0\psi)(\partial^2_{k_i \eta_j} f)_0]\}. \qquad (30)
\end{aligned}$$

Equation (30) is inconvenient to use since any symmetries which may be present are not immediately apparent. In order to simplify this equation we can apply a succession of coordinate transformations to obtain a canonical form. However, it is first necessary to use a symmetry of the various $\Delta_{\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{k},\boldsymbol{m}}$ to afford a marked simplification. In usual second-quantisation terminology these coefficients may be written as

$$f(\boldsymbol{\eta}, \boldsymbol{k}, \boldsymbol{m}) = 2\Delta_{\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{k},\boldsymbol{m}} = 2\langle \boldsymbol{\eta} + \boldsymbol{m} - \boldsymbol{k}, \boldsymbol{k}| V(\boldsymbol{r}_1, \boldsymbol{r}_2)|\boldsymbol{\eta}, \boldsymbol{m}\rangle \qquad (31)$$

where each vector represents a set of quantum numbers and the integers in rounded brackets indicate that that particular state has as arguments the position vector of that particle, e.g. $\boldsymbol{k}(2)$ means that the state $\boldsymbol{k}$ has the position vector $\boldsymbol{r}_2$ of particle 2 as its argument.

It is clear from (31) that $\Delta_{\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{k},\boldsymbol{m}}$ is unchanged when particles 1 and 2 are interchanged, provided the interaction $V(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in configuration space is symmetric with respect to interchange of particle position vectors. That is

$$\Delta_{\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{k},\boldsymbol{m}} = \langle \boldsymbol{k}, \boldsymbol{\eta} + \boldsymbol{m} - \boldsymbol{k}| V(\boldsymbol{r}_1, \boldsymbol{r}_2)|\boldsymbol{m}, \boldsymbol{\eta}\rangle. \qquad (32)$$

From (31) and (32)

$$\Delta_{\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{k},\boldsymbol{m}} = \Delta_{\boldsymbol{k},\boldsymbol{\eta}+\boldsymbol{m}-\boldsymbol{k},\boldsymbol{\eta}}. \qquad (33)$$

Using the definition of f (above (23)), this relationship reduces to

$$f(\boldsymbol{\eta}, \boldsymbol{k}, \boldsymbol{m}) = f(\boldsymbol{m}, \boldsymbol{\eta} + \boldsymbol{m} - \boldsymbol{k}, \boldsymbol{\eta}). \tag{34}$$

By partially differentiating (34), it is now simple to demonstrate that

$$\nabla_{\boldsymbol{k}} f = \mathbf{0} \qquad \nabla_{\boldsymbol{\eta}} f = \nabla_{\boldsymbol{m}} f \neq 0 \tag{35}$$

where the subscript on the gradient indicates that the derivatives are with respect to the vector components. As a consequence of this symmetry $\gamma_5 = 0$ and $\gamma_3 = \gamma_4$ in (29). Hence from (35) we have

$$\partial^2_{k_i k_j} f = \partial^2_{k_i \eta_j} f = \partial^2_{k_i m_j} f = 0 \tag{36a}$$

and

$$\partial^2_{\eta_i \eta_j} f = \partial^2_{\eta_i m_j} f = \partial^2_{m_i m_j} f \neq 0 \tag{36b}$$

and in general we have a different value for each pair i and j.

Using these symmetries (30) becomes

$$\begin{aligned} \mathrm{i}\hbar\partial_t \psi = {} & \lambda_0 \psi + \mathrm{i}\boldsymbol{\lambda}_1 \cdot (\nabla\psi) - \tfrac{1}{2}\sum_{i,j} (\boldsymbol{\lambda}_2)_{ij} \partial^2_{x_i x_j} \psi + \gamma_2 \psi^+ \psi\psi \\ & + \Omega[\mathrm{i}(\nabla_{\boldsymbol{\eta}} f)_0 \cdot \psi^+ \psi(\nabla\psi) + \mathrm{i}(\nabla_{\boldsymbol{m}} f)_0 \cdot \psi^+ (\nabla\psi)\psi - \mathrm{i}(\nabla_{\boldsymbol{k}} f)_0 \cdot (\nabla\boldsymbol{\psi}^-)\boldsymbol{\psi}\boldsymbol{\psi}] \\ & + \frac{\Omega}{2!}\sum_{i,j} (\partial^2_{m_i m_j} f)_0 \{\psi^+[-\partial^2_{x_i x_j}\psi - 2\mathrm{i}(\partial_{x_i}\psi) m_j^0 + \psi m_i^0 m_j^0]\psi \\ & + \psi^+\psi[-\partial^2_{x_i x_j}\psi - 2\mathrm{i}(\partial_{x_i}\psi)\eta_j^0 + \eta_i^0 \eta_j^0 \psi] \\ & + 2\psi^+[(\mathrm{i}\partial_{x_i}\psi - m_i^0\psi)(\mathrm{i}\partial_{x_j}\psi - \eta_j^0\psi)]\}. \end{aligned} \tag{37}$$

The cross derivatives in (37) make it very awkward for further calculations so we transform to a different set of coordinates to remove them. This is readily done as follows. Suppose the transformation is represented by the non-singular matrix α_{ij} so that the new coordinates x_j are related to the original ones x_i by

$$x_j \to \alpha_{ij} x_i. \tag{38}$$

The derivatives then transform as

$$\partial_{x_i} \to \alpha_{ij} \partial_{x_j}. \tag{39}$$

We have three general tensorial types of terms of second rank in (37) which are of the form

$$A_{ij} \partial^2_{x_i x_j} \psi \tag{40a}$$

$$2B_{ij}(\partial_{x_i}\psi)(\partial_{x_j}\psi) \tag{40b}$$

$$-B_{ij}(\partial^2_{x_i x_j}\psi). \tag{40c}$$

The transformation (39) is now applied to each expression in (40) in turn and the transformation is so chosen to make the terms in (40c) diagonal, i.e. $i' = j'$, where the primed symbols are those appearing after the transformation. We thus obtain

$$-B_{ij}\alpha_{ik}\alpha_{jl} = \delta_{kl} b_k \tag{41}$$

where the b_k are the eigenvalues of the 3×3 matrix $-\boldsymbol{B} = -(B_{ij})$. Obviously, this will also diagonalise the term in (40b) since the coefficients of these two types of term are proportional. However, this cannot be said in general about the term in (40a).

In order to be able to use ∇_ε and ∇_ε^2 symbols for the diagonalised terms in (40*a*, *b*) we may apply a subsequent scaling transformation, namely

$$x_i'' = x_i'/(|b_i|)^{1/2} \tag{42}$$

using the definition of a Laplace-Beltrami operator in three dimensions where the ε_i ($i = 1, 2, 3$) are defined by

$$\varepsilon_i = \operatorname{sgn}(b_i). \tag{43}$$

It will be convenient to represent the term in (40*a*) as a linear combination of a Laplace-Beltrami operator acting on ψ and remaining terms which do not conform to the new signature in the transformed components of (40*b*) and (40*c*). However, this decomposition can be made in an arbitrary way but we wish to minimise the magnitude of the residual terms. Therefore, we shall use the following decomposition:

$$\tilde{A}_{ij} \equiv \Upsilon(I_\varepsilon)_{ij} + [\tilde{A}_{ij} - \Upsilon(I_\varepsilon)_{ij}] \tag{44}$$

where I_ε is a signatured identity matrix given by

$$(I_\varepsilon)_{ij} = \varepsilon_i \delta_{ij}$$

and $\tilde{A}$ is the transformed matrix A after rotation and scaling. The coefficient Υ is to be chosen such that the residue matrix in the square brackets of (44) attains the minimum of its norm for a value of $\Upsilon = \mu_2$. Hence, we rewrite (44) as

$$\tilde{A}_{ij} \equiv \mu_2 (I_\varepsilon)_{ij} + R_{ij}$$

where

$$R_{ij} \equiv \tilde{A}_{ij} - \mu_2 (I_\varepsilon)_{ij}.$$

Thus, we can recast equation (37) in the form

$$\begin{aligned} \mathrm{i}\hbar\partial_t\psi = {} & \mu_0\psi + \mathrm{i}\boldsymbol{\mu}_1 \cdot (\nabla_\varepsilon\psi) + \mu_2\nabla_\varepsilon^2\psi + \sum_{ij} R_{ij}\partial^2_{x_i x_j}\psi - 2(\nabla_\varepsilon\psi^\top)\psi(\nabla_\varepsilon\psi) + \mu_3\psi^\top\psi\psi \\ & + \mathrm{i}[\psi^+\psi(\boldsymbol{\mu}_4 \cdot \nabla_\varepsilon)\psi + \psi^+((\boldsymbol{\mu}_4 \cdot \nabla_\varepsilon)\psi)\psi] + ((\nabla_\varepsilon^2\psi^+)\psi\psi + \psi^+\psi\nabla_\varepsilon^2\psi) \end{aligned} \tag{45}$$

where $\mu_0 = \lambda_0$,

$$\mu_{1i} = \lambda_{1i}\frac{\varepsilon_i}{(|b_i|)^{1/2}} \qquad \mu_3 = \gamma_2 + \Omega\sum_{i,j}(\partial^2_{m_i m_j} f)_0 (m_i^0 m_j^0 + \eta_i^0\eta_j^0 + 2m_i^0\eta_j^0)$$

and

$$\mu_{4i} = \Omega\left((\partial_{\eta_i} f)_0 \frac{\varepsilon_i}{(|b_i|)^{1/2}} - 2\sum_{s,t}(\partial^2_{\eta_s\eta_t} f)_0 \frac{\alpha_{si}}{(|b_i|)^{1/2}}(\eta_t^0 + \eta_s^0)\right).$$

It is worth noting that, due to the last transformation in (42), the space of independent variables x, y, z may have arbitrary signatures, as is reflected in the use of the Laplace-Beltrami operator, and also in the use of generalised scalar products between gradients and vectors, i.e.

$$(\boldsymbol{a} \cdot \nabla)_\varepsilon\psi \equiv \sum_i \varepsilon_i a_i \,\partial\psi/\partial x_i.$$

However, all the possible cases may be convered by two generic cases, namely $(+++)$ and $(++-)$; all the other possibilities may be obtained through a sign reversal. The first possibility means that the space of independent variables is Euclidean while the second is a Minkowski-type space. This will have important repercussions on the solutions of the above field equations.

The fourth term in (45) deserves further comment. This has been obtained from the third term in (37). We have separated it from the third term of (45) to consistently use the operators that reflect the signatures of the space of independent variables. However, in many important physical applications, e.g. for the electrostatic two-body Coulomb interaction, we expect the potential energy to be isotropic, which implies that $b_1 = b_2 = b_3$ and hence the matrix R_{ij} would vanish identically. In any case, at the critical point $\nabla_{\eta}^2 \omega = 0$ and, once again, these apparently unsymmetrical terms become insignificant at or near a symmetry breaking point. In the second part of the paper we will present a number of solutions to the equations of motion we have derived here. The solutions which will be presented pertain to the isotropic interaction case where we put $R_{ij} = 0$. If this assumption should not be entirely justified, e.g. being at a finite distance from the expansion point, these terms then distort the symmetry and lead to charge or mass dissipation along preferential directions or else to rotational flows. In any of the cases where R_{ij} is not negligible the method of solving the problem would be to perturb the isotropic solutions, assuming that the term in R_{ij} is a small distortion.

4. Summary and conclusions

In this paper we have presented a number of important examples of condensed matter systems which can all be described using an effective Hamiltonian involving two-body interactions between quasiparticles. Our interest concentrated on the strong interaction regime which is often manifested by symmetry breaking effects, such as Cooper pair formation, Bose condensation, long-range coherence and soft mode behaviour. In order to investigate the prototype Hamiltonian we have used a non-perturbative approach where the Heisenberg equations of motion for ladder operators were transformed into highly non-linear PDE for quantum field operators. This was accomplished through a Taylor expansion of the interaction coefficients. We have explicitly demonstrated the form of these equations up to second order. However, an infinite-order expansion, in principle, may easily be obtained.

Our model Hamiltonian may be written in terms of the fields ψ^+ and ψ using a similar ansatz as we have employed for the equation of motion. This would result in the following types of terms.

(i) The one-body part of the Hamiltonian in equation (14) will yield four types of term:

(*a*) those which do not depend on any wavevector component having the form $\psi^+\psi$;

(*b*) some components will be linear in a wavevector component k_ν and give rise to $(\partial_\nu \psi^+)\psi$ and $\psi^+(\partial_\nu \psi)$ and similarly for other components and wavevectors;

(*c*) in the resulting expansion some parts which are proportional to k_ν^2 and produce $(\partial_{\nu\nu}^2 \psi^+)\psi$, $(\partial_\nu \psi^+)(\partial_\nu \psi)$, $\psi^+(\partial_{\nu\nu}^2 \psi)$: clearly, by changing the wavevector or component, similar terms of the same type will be obtained;

(*d*) lastly, those contributions in the expansion involving two different wavevector components like k_ν and k_γ will lead to $(\partial_{\nu\gamma}^2 \psi^+)\psi$, $(\partial_\gamma \psi^+)(\partial_\nu \psi)$, $(\partial_\nu \psi^+)(\partial_\gamma \psi)$, $\psi^+(\partial_{\nu\gamma}^2 \psi)$.

(ii) The two-body part of the Hamiltonian can be analysed in the same way and also produces four groups of terms:

(a) $\psi^+\psi^+\psi\psi$;

(b) $(\partial_x\psi^+)\psi^+\psi\psi$, $\psi^+(\partial_x\psi^+)\psi\psi$, $\psi^+\psi^+(\partial_x\psi)\psi$, $\psi^+\psi^+\psi(\partial_x\psi)$;

(c) $(\partial^2_{xx}\psi^+)\psi^+\psi\psi$, $(\partial_x\psi^+)(\partial_x\psi^+)\psi\psi$, $(\partial_x\psi^+)\psi^+(\partial_x\psi)\psi$,
$(\partial_x\psi^+)\psi^+\psi(\partial_x\psi)$, $\psi^+(\partial^2_{xx}\psi^+)\psi\psi$, $(\partial_x\psi^+)\psi^+(\partial_x\psi)\psi$,
$\psi^+(\partial_x\psi^+)(\partial_x\psi)\psi$,
$\psi^+\psi^+(\partial^2_{xx}\psi)\psi$, $\psi^+\psi^+(\partial_x\psi)(\partial_x\psi)$, $(\partial_x\psi^+)\psi^+\psi(\partial_x\psi)$,
$\psi^+(\partial_x\psi^+)\psi(\partial_x\psi)$, $\psi^+\psi^+\psi(\partial^2_{xx}\psi)$;

(d) $(\partial^2_{xy}\psi^+)\psi^+\psi\psi$, $(\partial_x\psi^+)\psi^+(\partial_y\psi)\psi$,
$(\partial_y\psi^+)(\partial_x\psi^+)\psi\psi$, $\psi^+(\partial^2_{xy}\psi^+)\psi\psi$, $\psi^+(\partial_x\psi^+)(\partial_y\psi)\psi$,
$(\partial_y\psi^+)\psi^+(\partial_x\psi)\psi$, $\psi^+(\partial_x\psi^+)(\partial_x\psi)\psi$, $\psi^+\psi^+(\partial^2_{xy}\psi)\psi$,
$\psi^+\psi^+(\partial_x\psi)(\partial_y\psi)$,
$(\partial_y\psi^+)\psi^+\psi(\partial_x\psi)$, $\psi^+(\partial_y\psi^+)\psi(\partial_x\psi)$, $\psi^+\psi^+\psi(\partial^2_{xy}\psi)$.

We have only selected k_x and k_y terms because these are representative of other wavevectors. This Hamiltonian would subsequently be subjected to symmetry requirements imposed by the form of interactions present. Of particular interest would be the case of isotropic interactions which are expected to greatly reduce and simplify the number of terms. From the two (a) types nothing is changed, namely $\psi^+\psi$ and $\psi^+\psi^+\psi\psi$. Those in type (b) will produce contributions like $(\nabla\psi^+)\psi$, $(\nabla\psi^+)\psi^+\psi\psi$, $\psi^+(\nabla\psi^+)\psi\psi$ and their Hermitian conjugates. Components in (c) and (d) will give rise to $(\nabla^2\psi^+)\psi$, $(\nabla\psi^+)\cdot(\nabla\psi)$, $(\nabla^2\psi^+)\psi^+\psi\psi$ and all terms arising from the permutation of the Laplacian operator, $(\nabla\psi^+)\cdot(\nabla\psi^+)\psi\psi$ with permutations in the positions of the two gradients. It is worth noting that a Landau-Ginzburg Hamiltonian density would be of the form

$$H_{LG} = a\psi^+\psi + b\psi^+\psi^+\psi\psi + c\nabla\psi^+\cdot\nabla\psi \tag{46}$$

which has played a very prominent role in the development of field theoretical approaches to critical phenomena (Amit 1978, Rajaraman 1987). It is apparent that our Hamiltonian will contain H_{LG} as a special case. It is also evident that the quantum field ψ is analogous to the order parameter field used in generalised Landau-Ginzburg theories. The quantum nature of ψ is, at this stage, still manifest, provided the operators appearing are kept in their original order. We therefore see a further generalisation of Landau-Ginzburg concepts at criticality and also a direct link between microscopic and phenomenological approaches.

Moreover, extensive analysis of the so-called 'ϕ^n' field theories using renormalisation have been performed for which H_{LG} is the model Hamiltonian (Amit 1978). Their conclusion is that a particular ϕ^n model is renormalisable when the number of independent space (or spacetime) variables N_c is given by

$$N_c = \frac{2n}{n-2}.$$

Therefore, the ϕ^4 model of H_{LG} is renormalisable when $N_c = 4$ while an analogous ϕ^6 model is renormalisable when $N_c = 3$. These two particular examples are also important

as prototypes of second-order and first-order phase transitions, respectively. Using the language of catastrophe theory, the former (ϕ^4) exhibits a 'cusp' catastrophe whereas the latter a 'butterfly' castastrophe (Poston and Stewart 1978). For a particular ϕ^n theory, higher powers are called irrelevant operators since they can, at most, affect critical amplitudes but not critical exponents. An important link between these general statements and our second-order study could be obtained by setting $\nabla\psi = g(\psi)$ for the solutions of our equation of motion. With a polynomial expansion of the *a priori* arbitrary vector function g our second-order result embraces both the ϕ^4 and ϕ^6 phenomena and this is sufficiently general, because of renormalisation theorems, to effectively ignore higher-order corrections. The latter can, at best, modify the parameters of our second-order theory, but will not affect in any way the symmetries and topologies of the system under examination. Thus, our general equations for the field ψ, for the isotropic case, are exact in form and may describe an enormous range of physical phenomena.

Obviously, it is imperative to provide, at least special solutions of the equations of motion which we have derived for this model to be useful. This is, in fact, the objective for part II of this paper. We shall make full use of recent studies carried out on just this type of equation. The method employed is the very powerful symmetry reduction method for PDE, which makes full use of continuous symmetries (Winternitz *et al* 1987, Gagnon and Winternitz 1988a, b, 1989a, b). This, of course, requires or implies that we treat the field operator, at least initially, as a classical dependent variable. Quantum corrections are subsequently accounted for through various well known semiclassical quantisation approaches (Jackiw 1977, Rajaraman 1987). The result of applying this method is, first of all, a classical coherent structure (Klauder and Skagerstam 1985) which is localised in space and elementary quantum excitations whose spectrum we wish to study. The classical solution acts as an effective potential for the elementary excitations whose nature therefore reflects the symmetries of the coherent structure. The fact that an effective one-body-like potential exists is supported by the excellent results obtained, for example, from density functional approaches (Hohenberg and Kohn 1964, Kohn and Sham 1965, Kohn 1986).

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