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Generalised Holstein–Primakoff theory for anharmonic lattices

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Abstract. The spectrum of elementary excitations for scalar field theories on a lattice is calculated in the large-N approximation and is found to consist of two distinct branches, one of which may be interpreted as a collective mode. The method of calculation is based on a generalised Holstein–Primakoff theory for the real symplectic algebra.

1. Introduction

A unified approach to essentially all known semiclassical methods in quantum physics may be achieved through suitable generalisations of the Holstein–Primakoff (HP) theory which was originally developed in the context of ferromagnetism (Holstein and Primakoff 1940). While the HP approach is closely related to the theory of generalised coherent states and time-dependent Hartree–Fock approximations, it is more systematic in that higher-order calculations may be carried out without ordering ambiguities. Hence, aside from traditional calculations in magnetism and recent applications to the $1/N$ expansion in quantum mechanics and field theory (Mlodinow and Papanicolaou 1980, 1981, Papanicolaou 1981a, b), the HP theory was frequently used for the study of collective motion in nuclei (Marshalek 1980). The Bogoliubov theory of the Bose gas and random-phase approximations for Fermi systems may also be understood through suitable extensions of the HP theory (Mead and Papanicolaou 1983). In short, the generalised HP theory provides a rigorous alternative to collective-field and hydrodynamical approaches to many-body theory.

Although detailed explicit calculations have already been carried out in isolated cases, a good portion of the current technology is concerned with the group-theoretical foundations of the generalised HP theory (Deenen and Quesne 1981, 1982). On the other hand, it is obviously important to develop efficient calculational methods, especially for systems with a large (possibly infinite) number of degrees of freedom. This paper presents an explicit calculation of the spectrum of elementary excitations for a lattice field theory defined from the Hamiltonian

$$H=\tfrac{1}{2}\sum_n\left[\pi_n^j\pi_n^j+\kappa^2\sum_e(\phi_n^j-\phi_{n+e}^j)(\phi_n^j-\phi_{n+e}^j)+V(\phi_n^j\phi_n^j)\right], \tag{1.1}$$

where n denotes a site on a D-dimensional cubic lattice and the sum over the unit vectors collectively denoted by e extends over neighbouring sites. The repeated index j is summed over $j=1,2,\ldots,N$, so the theory is symmetric under O(N) rotations. π_n^j is

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the canonical momentum associated with ϕ_n^j and $V = V(x)$ is some single-site anharmonic potential.

The continuum limit of theories such as (1.1) was analysed in the large-N approximation by several authors (Dolan and Jackiw 1974, Schnitzer 1974, Coleman *et al* 1974, Abbott *et al* 1976, Halpern 1980). The emerging picture is troublesome because of the appearance of tachyonic poles in singlet correlation functions, the analogues of the Landau ghosts familiar from quantum electrodynamics. In fact, Gross and Neveu (1974) argued at length about the peculiarities arising in the continuum limit of non-asymptotically-free theories. However, instead of pathological Landau ghosts, we find that the *lattice* model (1.1) possesses a well defined spectrum of elementary excitations consisting of two distinct branches, one of which may be interpreted as a collective mode.

In the absence of the single-site potential in (1.1), the spectrum consists of the usual acoustic phonons. The first obvious consequence of the potential is that the phonons acquire a non-vanishing mass gap. A closer examination suggests that a second branch should arise in the spectrum, describing collective motion in the anharmonic potential. Notice, for instance, that in the extreme limit of strong anharmonicity the various degrees of freedom oscillate independently of each other in a common potential well. For moderate anharmonicity, a compromise is reached manifested by a twofold spectrum of excitations. The main burden of this paper is to exhibit that spectrum quantitatively. As it turns out, the general shape of the collective branch is fairly similar to the familiar optical modes. Nevertheless, the physical origin and characteristics of the collective mode are distinctly different, for it may occur in pure lattices (without a basis) and is a singlet under global $O(N)$ rotations. It should also be mentioned that the collective mode can coexist with optical modes, and that translation-invariant anharmonic terms may be included in (1.1) with no apparent qualitative consequences for the current discussion. Our aim is to exhibit the collective mode in the simplest possible situation.

The method of calculation adopted here is a Hamiltonian formulation of the $1/N$ expansion based on a generalised HP theory which is most suitable for the study of elementary excitations. Since the main algebraic results have already appeared in the literature, § 2 presents a brief survey of the relevant results. Section 3 is then devoted to the explicit calculation of the spectrum, exhibiting the two branches mentioned earlier, for typical choices of the potential.

2. Holstein–Primakoff theory

The algebraic aspects of the calculation are essentially independent of the effective dimensionality of the lattice D. For the sake of clarity, therefore, we first explain the procedure for the anharmonic chain ($D = 1$). The necessary generalisations to higher-dimensional lattices will be exhibited at the end of the calculation. A convenient set of operators is then introduced through the Fourier decomposition

$$\phi_n^j = \sum_p (2\Lambda\Omega_p)^{-1/2}[a_p^j \exp(ipn) + a_p^{j*} \exp(-ipn)],$$

$$\pi_n^j = \frac{1}{i}\sum_p \left(\frac{\Omega_p}{2\Lambda}\right)^{1/2} [a_p^j \exp(ipn) - a_p^{j*} \exp(-ipn)], \tag{2.1}$$

$$p = (2\pi/\Lambda)n, \qquad n = 0, \pm 1, \ldots, \pm K, \qquad \Lambda \equiv 2K + 1,$$

where Λ is the total number of sites in the periodic chain and is assumed odd for notational convenience. The frequencies Ω_p are at this point arbitrary except for the symmetry relation $\Omega_p = \Omega_{-p}$ which may be imposed without loss of generality.

The Hamiltonian may now be written in the form

$$\begin{aligned} H = \sum_p \left(\frac{1}{\Omega_p}(\omega_p^2 + \Omega_p^2) A_{pp} + \frac{1}{2\Omega_p}(\omega_p^2 - \Omega_p^2)(B_{p,-p} + B^*_{p,-p}) \right) \\ + \frac{1}{2}\sum_n V \left(\frac{1}{\Lambda} \sum_{pq} (\Omega_p \Omega_q)^{-1/2} \{ 2A_{pq} \exp[-\mathrm{i}(p-q)n] + B_{pq} \exp[\mathrm{i}(p+q)n] \right. \\ \left. + B^*_{pq} \exp[-\mathrm{i}(p+q)n] \} \right), \\ \omega_p = 2\kappa |\sin(p/2)|, \end{aligned} \tag{2.2}$$

which emphasises the dependence on the set of rotationally invariant bilocal operators

$$A_{pq} = \tfrac{1}{4}(a_p^{i*} a_q^i + a_q^i a_p^{i*}), \qquad B_{pq} = \tfrac{1}{2} a_p^i a_q^i, \qquad B^*_{pq} = \tfrac{1}{2} a_p^{i*} a_q^{i*}. \tag{2.3}$$

The above set of pseudospin operators is known to close the algebra of the real symplectic group $\mathrm{Sp}(2\Lambda, R)$. We shall often use matrix notation defined from $A = (A_{pq}), B = (B_{pq})$ and $B^* = (B^*_{pq})$. A is then a $\Lambda \times \Lambda$ Hermitian matrix whereas B and B^* are symmetric ($B^\dagger = B^*$).

In searching for eigenvalues of the Hamiltonian $H = H(A, B, B^*)$ defined from (2.2), it would be convenient first to disentangle the angular degrees of freedom as is normally done in few-body quantum mechanics. A similar task for (2.2) appears difficult because of the large number of degrees of freedom involved, and because it would be preferable to carry out the angular-momentum decomposition in the Heisenberg representation. Nevertheless, a concise answer to the above question is possible, noting that states in the Fock space with definite angular momentum but varying 'radial' quantum numbers may be placed within infinite-dimensional representations of the pseudospin algebra (2.3), sometimes called sectors. Our task is then to find suitable restrictions of the pseudospin algebra to each sector. This is accomplished by generalised HP representations.

A HP representation of the operators (2.3) suitable for the description of the singlet (or vacuum) sector is given by

$$A = \tfrac{1}{4}NI + \xi^* \xi, \qquad B = [\tfrac{1}{2}NI + (\xi^* \xi)^{\mathrm{T}}]^{1/2} \xi, \qquad B^* = \xi^* [\tfrac{1}{2}NI + (\xi^* \xi)^{\mathrm{T}}]^{1/2}, \tag{2.4}$$

where I is the $\Lambda \times \Lambda$ unit matrix and $\xi = (\xi_{pq})$ is a $\Lambda \times \Lambda$ symmetric matrix ($\xi_{pq} = \xi_{qp}$) whose entries are Bose operators:

$$[\xi_{pq}, \xi^*_{kl}] = \tfrac{1}{2}(\delta_{pk}\delta_{ql} + \delta_{pl}\delta_{qk}). \tag{2.5}$$

The symbol T in (2.4) stands for the usual transposition of matrices:

$$(\xi^* \xi)^{\mathrm{T}}_{pq} = \sum_k \xi^*_{qk} \xi_{kp}. \tag{2.6}$$

Notice, however, that $(\xi^* \xi)^{\mathrm{T}} \neq \xi \xi^*$ because the entries of ξ and ξ^* are non-commuting operators. Using (2.5) the correct identity is found to be

$$\xi \xi^* = (\xi^* \xi)^{\mathrm{T}} + \tfrac{1}{2}(\Lambda + 1) I, \tag{2.7}$$

which shows that in the special cases $\Lambda = 1$ and $\Lambda = 2$, equations (2.4) reduce to the HP representations employed by Mlodinow and Papanicolaou (1980, 1981) for the

discussion of one- and two-body Hamiltonians. Although the two forms are equivalent, equations (2.4) will be more convenient for the current calculation because Λ will eventually be taken to infinity. Enforcing the definition (2.6), the parameter Λ will never appear explicitly except as an overall factor in suitable Fourier transforms.

More detailed explanations and concise proofs of the preceding statements may be inferred from recent publications (Papanicolaou 1981b, Deenen and Quesne 1982), so our current effort will be directed toward explicit applications. Hence, an exact restriction of the Hamiltonian (2.2) to the vacuum sector may be obtained by the direct substitution $A \to A(\xi, \xi^*)$, etc, from equations (2.4), resulting in a Hamiltonian $H = H(\xi, \xi^*)$. The diagonalisation of $H(\xi, \xi^*)$ in the Fock space associated with (2.5) would yield the singlet spectrum of the original Hamiltonian. Is it then sufficient to consider only the restriction to the vacuum sector implied by (2.4)? As it turns out, the spectrum of $H(\xi, \xi^*)$ consists of genuinely singlet states (the collective mode), together with a two-body continuum of uncoupled angular-momentum-one states in suitable kinematical superpositions to form singlet states. Therefore, at least as far as elementary excitations are concerned, there is no apparent loss of generality. It should be mentioned, however, that direct HP restrictions to non-singlet sectors may also prove useful.

In practice, the representation (2.4) must be supplemented by some approximation procedure. We thus turn our attention to the explicit calculation of the spectrum of (2.2) in the large-N approximation, for which the HP theory is well adapted. If the potential V were treated as a small perturbation to the harmonic Hamiltonian, the undetermined frequencies Ω_p would be chosen equal to the phonon frequencies ω_p rendering the quadratic terms in (2.2) diagonal. We shall instead determine Ω_p from a variational argument so that $\xi = 0 = \xi^*$ becomes a stationary point of the Hamiltonian $H = H(\xi, \xi^*)$. The argument consists of three elementary steps. First, we set $\xi = 0 = \xi^*$ in (2.4) to obtain $A_{pq} = (N/4)\delta_{pq}$ and $B_{pq} = 0 = B^*_{pq}$, which are then inserted in (2.2) to yield

$$E \equiv H(\xi = 0, \xi^* = 0) = \sum_p \frac{N}{4\Omega_p}(\omega_p^2 + \Omega_p^2) + \tfrac{1}{2}\Lambda V(\sigma^2), \qquad \sigma^2 \equiv \frac{N}{2\Lambda}\sum_p \frac{1}{\Omega_p}. \tag{2.8}$$

Second, we minimise $E = E(\Omega_p)$ with respect to the unknown frequencies Ω_p:

$$\partial E/\partial \Omega_p = 0 \Rightarrow \Omega_p = [\omega_p^2 + V'(\sigma^2)]^{1/2} = [4\kappa^2 \sin^2(p/2) + V'(\sigma^2)]^{1/2}, \tag{2.9}$$

where $V'(x)$ is the derivative of the function $V = V(x)$. Recalling the definition of σ^2 from (2.8), we find that Ω_p is completely determined from (2.9) if σ^2 satisfies the algebraic gap equation

$$\sigma^2 = \frac{N}{2\Lambda}\sum_p \frac{1}{\Omega_p} = \frac{N}{2\Lambda}\sum_p [4\kappa^2 \sin^2(p/2) + V'(\sigma^2)]^{-1/2}. \tag{2.10}$$

The value of the function $E = E(\Omega_p)$ evaluated at frequencies determined from (2.9)–(2.10) is the large-N approximation to the ground-state energy which we denote by E_0.

The third and final step is to show that the point $\xi = 0 = \xi^*$ is a stationary point of the Hamiltonian if Ω_p is determined from equations (2.9)–(2.10). This may be done by a direct Taylor expansion of $H = H(\xi, \xi^*)$. To within harmonic terms, the HP representation (2.4) may be approximated by

$$A_{pq} = \tfrac{1}{4}N\delta_{pq} + \sum_k \xi^*_{pk}\xi_{kq}, \qquad B_{pq} = (N/2)^{1/2}\xi_{pq}, \qquad B^*_{pq} = (N/2)^{1/2}\xi^*_{pq}. \tag{2.11}$$

Insertion of (2.11) in (2.2) and further Taylor expansion produces the quadratic Hamiltonian:

$$H = E_0 + H_0 + \ldots,$$
$$H_0 = \sum_{pq} 2\Omega_p \xi^*_{pq} \xi_{qp} + \tfrac{1}{8} N V''(\sigma^2) \sum_n \left(\frac{1}{\Lambda} \sum_{pq} (\Omega_p \Omega_q)^{-1/2} \{ \xi_{pq} \exp[\mathrm{i}(p+q)n] + \xi^*_{pq} \exp[-\mathrm{i}(p+q)n] \} \right)^2. \tag{2.12}$$

Equations (2.9)–(2.10) were systematically enforced in obtaining (2.12). E_0 is the large-N approximation to the ground-state energy discussed earlier, whereas H_0 contains information about the normal modes of the system. Notice that linear terms do not appear in (2.12) which establishes that $\xi = 0 = \xi^*$ is indeed a stationary point. Whether the stationary point is a local minimum or not depends, of course, on the choice of the potential.

The general strategy should now be clear. The intended approximation procedure has been reduced to standard Rayleigh–Schrödinger perturbation theory in which H_0 plays the role of the fundamental approximation, and higher-order corrections are identified from a systematic $1/N$ expansion of (2.2) and (2.4). Our immediate concern will then be the diagonalisation of the quadratic Hamiltonian H_0, a task taken up in § 3 for typical choices of the potential.

3. Collective modes

In order to understand the kinematics associated with the quadratic Hamiltonian (2.12) we first examine the simple case of a harmonic potential

$$V(\phi^j_n \phi^j_n) = m^2 (\phi^j_n \phi^j_n), \tag{3.1}$$

so that $V(x) = m^2 x$, $V'(x) = m^2$, $V''(x) = 0$ and

$$H_0 = \sum_{pq} 2\Omega_p \xi^*_{pq} \xi_{qp}, \qquad \Omega_p = [4\kappa^2 \sin^2(p/2) + m^2]^{1/2}. \tag{3.2}$$

The gap equation (2.10) is trivialised and merely yields the vacuum-expectation value

$$\sigma^2 = \langle \phi^j_n \phi^j_n \rangle = \frac{N}{2\Lambda} \sum_p [4\kappa^2 \sin^2(p/2) + m^2]^{-1/2}. \tag{3.3}$$

The ground-state energy is then obtained setting $V(\sigma^2) = m^2 \sigma^2$ in (2.8) and replacing σ^2 from (3.3) to yield the expected result

$$E_0 = \tfrac{1}{2} N \sum_p \Omega_p. \tag{3.4}$$

The first excited state of H_0 is then given by

$$|pq\rangle = \xi^*_{pq} |0\rangle, \qquad H_0 |pq\rangle = (\Omega_p + \Omega_q) |pq\rangle \equiv E_{pq} |pq\rangle, \tag{3.5}$$

where we used the commutation relations (2.5). The spectrum consists of elementary excitations with mass gap m, to be referred to as quasiphonons. The eigenvalue in (3.5) is the sum of two quasiphonon frequencies because the current formulation addresses singlet states under global O(N) rotations.

In view of the symmetry relation $E_{pq} = E_{qp}$, there are $\Lambda(\Lambda+1)/2$ distinct normal modes, where $\Lambda = 2K+1$ is the total number of lattice sites. A useful labelling of the corresponding eigenstates is achieved by introducing the total crystal momentum, instead of the linear momentum $p+q$ which takes values in a double Brillouin zone. The crystal momentum denoted by s is defined from $s = p+q$ if $-K \leqslant p+q \leqslant K$, $s = p+q-\Lambda$ if $K < p+q \leqslant 2K$, and $s = p+q+\Lambda$ if $-2K \leqslant p+q < -K$. (For notational convenience, momenta are hereafter measured in units of $2\pi/\Lambda$.) The crystal momentum s takes values in the fundamental zone. For each s there are $K+1$ states with distinct energy eigenvalues $E_{pq} = \Omega_p + \Omega_q$. Figure 1($a$) displays the quasiphonon energies $E_{pq} = \Omega_p + \Omega_q$ against crystal momentum s for a small lattice ($\Lambda = 9$). Because energies corresponding to opposite crystal momentum ($\pm s$) are equal, only half of the Brillouin zone is depicted.

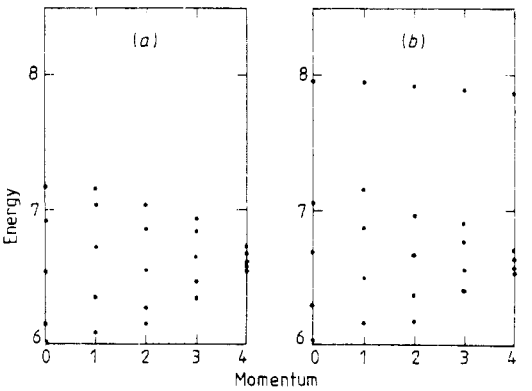

Figure 1. Normal frequencies for a small 1D lattice ($\Lambda = 9$, $\kappa = 1$, $m = 3$) plotted against the crystal momentum s (in units of $2\pi/\Lambda$) defined in the text. (a) Results for the harmonic potential. (b) Corresponding results for the anharmonic potential.

The preceding picture may be described in a more formal manner by introducing the translation operator

$$Q = \exp\left(i\sum_p p a_p^{j*} a_p^j\right) = \exp\left(i\sum_{pq} 2p\xi_{pq}^* \xi_{qp}\right). \tag{3.6}$$

The states $|pq\rangle$ are then eigenstates of Q:

$$Q|pq\rangle = \exp(is)|pq\rangle \tag{3.7}$$

where s takes values as described in the previous paragraph.

To be sure, this kinematical discussion is nearly academic as far as the harmonic potential (3.1) is concerned. Its merits become apparent in the study of anharmonic potentials which we consider next. Hence we study a typical example defined from

$$V(\phi_n^j \phi_n^j) = \tfrac{1}{2}g^2(\phi_n^j \phi_n^j)^2, \tag{3.8}$$

where g^2 is some positive coupling constant. The function $V(x)$ and its derivatives occurring in equations (2.8)–(2.12) are then given by $V(x) = \frac{1}{2}g^2x^2$, $V'(x) = g^2x$ and

$V'' = g^2$, and the gap equation (2.10) yields

$$m^2 = \frac{Ng^2}{2\Lambda} \sum_p \frac{1}{\Omega_p}, \qquad \Omega_p = [4\kappa^2 \sin^2(p/2) + m^2]^{1/2}, \tag{3.9}$$

where we have used the convenient mass parameter $m^2 \equiv g^2\sigma^2$. It is not difficult to establish that (3.9) possesses a unique solution m^2 for all g^2. In practice, equation (3.9) is used to express g^2 as a function of m^2, thus achieving a very convenient parametrisation.

We now turn our attention to the essential point of the calculation, the diagonalisation of the quadratic Hamiltonian (2.12). Setting $V'' = g^2$ and performing the summation over n, one finds that

$$H_0 = \sum_{pq} 2\Omega_p \xi^*_{pq} \xi_{qp} + \frac{\bar{g}^2}{4\Lambda} \sum_{pqkl} \frac{\Delta(p+q+k+l)}{(\Omega_p\Omega_q\Omega_k\Omega_l)^{1/2}} (\xi^*_{pq} + \xi_{-p,-q})(\xi^*_{kl} + \xi_{-k,-l}), \tag{3.10}$$

where $\bar{g}^2 = \frac{1}{2}Ng^2$ may be expressed in terms of the physical mass m^2 from (3.9), and

$$\Delta(p+q+k+l) = \frac{1}{\Lambda} \sum_{n=1}^{\Lambda} \exp[-i(p+q+k+l)n]. \tag{3.11}$$

It is important to note that Δ is not merely the Kronecker delta because of potential umklapp contributions, unless at least two of the momenta involved vanish. In general, Δ is equal to one if $p+q+k+l = 0$, or $\pm 2\pi$, and vanishes otherwise. No further umklapp contributions arise, however, because p, q, k and l all take values in the fundamental Brillouin zone.

It will be instructive to consider also the Heisenberg equation of motion deriving from the Hamiltonian (3.10) and the commutation relations (2.5):

$$i\dot{\xi}_{pq} = (\Omega_p + \Omega_q)\xi_{pq} + \frac{\bar{g}^2}{2\Lambda} \sum_{kl} \frac{\Delta(p+q+k+l)}{(\Omega_p\Omega_q\Omega_k\Omega_l)^{1/2}} (\xi^*_{kl} + \xi_{-k,-l}). \tag{3.12}$$

This already provides an important hint concerning the method of diagonalisation. Consider for instance the subset of operators ξ_{pq} and ξ^*_{pq} such that $p+q = 0$. Δ then becomes the usual Kronecker delta, establishing that the above subset of operators decouples from the rest. It is reasonable to expect that there may be a method for disentangling the various operators in (3.10) or (3.12) according to their total crystal momentum s, including $p+q = 0$ as a special case.

In order to systematise the preceding remarks, we introduce the more or less obvious identity

$$1 = \delta(p+q) + \sum_{s=1}^{K} (\delta(p+q-s) + \delta(p+q+s) + \delta(p+q-s+\Lambda) + \delta(p+q+s-\Lambda)), \tag{3.13}$$

which is valid if p and q takes values in the zone defined from equation (2.1). $\delta(x)$ is the Kronecker delta defined from $\delta(x=0) = 1$ and $\delta(x \neq 0) = 0$. Notice that the dummy index s takes only positive values so that terms with opposite crystal momentum are separately displayed. The above identity is inserted in (3.10), once in the first term and twice in the second, to disentangle the Hamiltonian into a sum of commuting operators each parametrised by the index s:

$$H_0 = H_{0,0} + \sum_{s=1}^{K} H_{0,s}, \tag{3.14}$$

where

$$H_{0,0} = \sum_{p=-K}^{K} 2\Omega_p \xi^*_{p,-p}\xi_{p,-p} + \frac{\bar{g}^2}{4\Lambda}\left(\sum_{p=-K}^{K}\frac{1}{\Omega_p}(\xi^*_{p,-p}+\xi_{p,-p})\right)^2, \tag{3.15}$$

$$H_{0,s} = \sum_{\substack{p+q=s \\ p+q=s-\Lambda}} (\Omega_p+\Omega_q)(\xi^*_{pq}\xi_{pq}+\xi^*_{-p,-q}\xi_{-p,-q}) + \tfrac{1}{2}\Gamma^*_s\Gamma_s,$$

$$\Gamma_s = \frac{\bar{g}}{\Lambda^{1/2}} \sum_{\substack{p+q=s \\ p+q=s-\Lambda}} \frac{\xi_{pq}+\xi^*_{-p,-q}}{(\Omega_p\Omega_q)^{1/2}}. \tag{3.16}$$

The sums in (3.16) extend over all values of p and q in the Brillouin zone which are compatible with $p+q=s$ or $p+q=s-\Lambda$, for fixed s in the range $1 \leqslant s \leqslant K$.

It is then sufficient to diagonalise each term in (3.14) separately, the corresponding eigenvalues being parametrised by s. To proceed with the diagonalisation we should first eliminate a minor redundancy occurring in (3.14)–(3.16) because of the symmetry $\xi_{pq} = \xi_{qp}$. For instance, the operator $\xi_{p,-p}$ with $p \neq 0$ occurs twice in (3.15), while ξ_{00} occurs only once. Define $C_0 = \xi_{00}$, and $C_p = \sqrt{2}\,\xi_{p,-p} = \sqrt{2}\,\xi_{-p,p}$ for $p \neq 0$, so the commutation relations (2.5) reduce to Bose commutators with standard normalisation: $[C_p, C^*_q] = \delta_{pq}$. Restriction of the sum in (3.15) to the range $[0, K]$ and suitable adjustment of the coefficients yields

$$H_{0,0} = \sum_{p=0}^{K} 2\Omega_p C^*_p C_p + \tfrac{1}{4}\left(\sum_{p=0}^{K} V_p(C_p + C^*_p)\right)^2,$$

$$V_p = \begin{cases} (2/\Lambda)^{1/2}\bar{g}/\Omega_p & \text{for } p \neq 0, \\ (1/\Lambda)^{1/2}\bar{g}/\Omega_0 & \text{for } p = 0. \end{cases} \tag{3.17}$$

There are $K+1$ normal frequencies associated with (3.17), which we denote by Ω, and are the roots of the algebraic equation

$$\sum_{p=0}^{K} \frac{2\Omega_p V_p^2}{\Omega^2 - (2\Omega_p)^2} = 1. \tag{3.18}$$

To obtain the generalisation of (3.18) to arbitrary crystal momentum s we must diagonalise the Hamiltonian (3.16). The calculation is slightly more complicated because of the umklapp terms present in (3.16). We state the final result which is a more or less obvious generalisation of (3.18). Thus, for even values of s, the eigenvalue equation reads

$$\sum_{p=0}^{K} \frac{f_p^2}{\Omega^2 - (\Omega_{p+s/2} + \Omega_{p-s/2})^2} = 1, \tag{3.19}$$

with

$$f_p^2 = \begin{cases} \dfrac{2\bar{g}^2}{\Lambda}\left(\dfrac{1}{\Omega_{p+s/2}} + \dfrac{1}{\Omega_{p-s/2}}\right) & \text{for } p \neq 0, \\ (2\bar{g}^2/\Lambda)\Omega_{s/2}^{-1} & \text{for } p = 0, \end{cases} \tag{3.20}$$

whereas for s odd the corresponding equations are

$$\sum_{p=0}^{K} \frac{f_p^2}{\Omega^2 - (\Omega_{p+(s+1)/2} + \Omega_{p-(s-1)/2})^2} = 1, \tag{3.21}$$

$$f_p^2 = \begin{cases} \dfrac{2\bar{g}^2}{\Lambda}\left(\dfrac{1}{\Omega_{p+(s+1)/2}} + \dfrac{1}{\Omega_{p-(s-1)/2}}\right) & \text{for } p \neq K, \\ \dfrac{\bar{g}^2}{\Lambda}\left(\dfrac{1}{\Omega_{p+(s+1)/2}} + \dfrac{1}{\Omega_{p-(s-1)/2}}\right) & \text{for } p = K. \end{cases} \tag{3.22}$$

The eigenvalue equations (3.18), (3.19) and (3.21) were solved numerically for various values of $\Lambda = 2K + 1$, noting that the roots of an algebraic equation of the form

$$\sum_p f_p^2/(\Omega^2 - \omega_p^2) = 1$$

are the eigenvalues of the $(K+1)\times(K+1)$ matrix

$$M = (\omega_p^2\delta_{pq} + f_p f_q) \Rightarrow \det[(\omega_p^2 - \Omega^2)\delta_{pq} + f_p f_q] = 0.$$

The lattice constant κ was taken equal to unity in all calculations. The only free parameter is then the physical mass m, because N and g^2 enter only through the combination $\bar{g}^2 = Ng^2/2$ which may be eliminated in favour of m by virtue of the gap equation (3.9). Figure 1(b) shows the results for a small lattice ($\Lambda = 9$) which should be compared with the corresponding results in figure 1(a) concerning the harmonic potential. In both cases the eigenvalues are plotted against the crystal momentum s, and the quasiphonon mass is taken equal to $m = 3$. While the total number of normal modes in figure 1(b) is exactly equal to the modes in figure 1(a), the formation of a collective branch separated from the two-body quasiphonon continuum is evident. We have repeated the calculation for a variety of values for Λ, up to $\Lambda = 29$. As it turned out, the mass gap of the collective branch (at $s = 0$) had stabilised to within five figures already at $\Lambda = 9$. The results for $\Lambda = 29$ are given in figure 2. The collective mode is drawn as a continuous curve whereas the shaded area corresponds to the two-body continuum. The shape of the collective branch is very similar to the more familiar optical modes. As was noted in the introduction, however, the physical origin of the collective mode is substantially different.

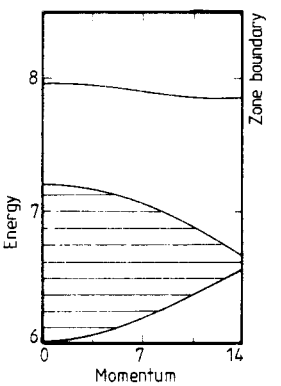

Figure 2. Normal frequencies for a large 1D lattice ($\Lambda = 29$, $\kappa = 1$, $m = 3$). The collective mode is drawn as a continuous curve, whereas the shaded area corresponds to the two-body continuum.

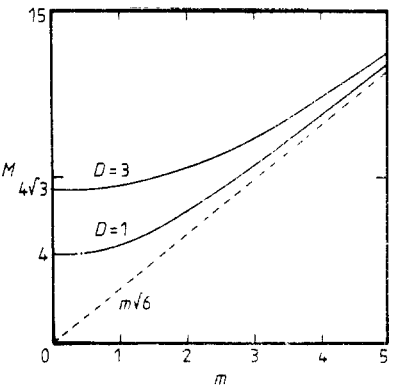

Figure 3. Mass gap of the collective mode against quasiphonon mass, for $D = 1$ and $D = 3$ ($\kappa = 1$, $\Lambda \to \infty$). Both curves are asymptotic to the strong-coupling limit $M \sim m\sqrt{6}$ which is independent of lattice dimension.

We further repeated the calculation for various values of m, which is equivalent to varying the coupling constant g^2. Large m corresponds to strong coupling g^2 while small m corresponds to weak coupling (see equation (3.9)). The picture is as follows. For small m, the collective branch falls into the two-body continuum, as expected in the limit of vanishing anharmonicity. For large m, the collective branch tends to a horizontal straight line at a distance $m\sqrt{6}$, and the two-body continuum also shrinks to a straight horizontal line at a distance $2m$. This provides an important check of consistency and sheds light on the nature of the collective excitation. In effect, the above limit corresponds to setting the lattice constant κ equal to zero. The system then reduces to Λ non-interacting particles each in the anharmonic potential (3.8). Notice that the gap equation (3.9) yields

$$m \sim (Ng^2/2)^{1/3} \tag{3.23}$$

in the strong-coupling limit. Furthermore, the large-N approximation to the spectrum in an anharmonic potential may be extracted from the work of Mlodinow and Papanicolaou (1980). Adjusting the conventions, one finds that

$$E = [g^2(l+\tfrac{1}{2}N)]^{1/3}[\tfrac{3}{4}(l+\tfrac{1}{2}N) + (n\sqrt{6}+\sqrt{\tfrac{3}{2}}-1)+\ldots] \tag{3.24}$$

where successive terms are organised in inverse powers of $(l+\frac{1}{2}N)$, l is the angular momentum, and n is the radial quantum number. Re-expanding (3.2) in inverse powers of N yields

$$E = m[\tfrac{3}{8}N + (l + n\sqrt{6}+\sqrt{\tfrac{3}{2}}-1) + O(N^{-1})], \tag{3.25}$$

where m is given by (3.23).

Therefore, the normal frequency for singlet oscillations is found to be equal to $m\sqrt{6}$ which is the coefficient of the radial quantum number n in equation (3.25). This is exactly equal to the limiting value of the collective mode discussed earlier. Furthermore, equation (3.25) implies that the frequency for angular excitations is equal to m which is the coefficient of the angular momentum l. The frequency for a two-body singlet state is then equal to $2m$ which again agrees with the limiting values for the two-body quasiphonon continuum found earlier. Aside from providing a check of consistency, the preceding remarks clarify the reason for the appearance of a singlet collective excitation in the full problem.

Our final task is to extend the calculation to a three-dimensional lattice ($D=3$), restricting ourselves to the calculation of the mass gap of the collective branch at vanishing crystal momentum. It is then sufficient to generalise (3.18) to $D=3$. First, we write out equation (3.18) in the thermodynamic limit $\Lambda \to \infty$ at $D=1$. Using the definition of the potential V_p from (3.17), and the gap equation (3.9) to express $\bar{g}^2 = Ng^2/2$ in terms of the physical mass m^2, one obtains

$$\begin{aligned} &\int_{-\pi}^{\pi} \frac{dp}{2\pi} \frac{1}{\Omega_p} \frac{1}{\Omega^2 - 4\Omega_p^2} = \frac{1}{2m^2} \int_{-\pi}^{\pi} \frac{dp}{2\pi} \frac{1}{\Omega_p}, \\ &\Omega_p = [4\kappa^2 \sin^2(p/2) + m^2]^{1/2}, \end{aligned} \tag{3.26}$$

which should be viewed as an algebraic equation for the frequency Ω. It possesses only one real root, in the region $\Omega^2 \geq 4(4\kappa^2 + m^2)$, which is equal to the mass gap of the collective branch. The two-body quasiphonon continuum appears to have been

lost in the thermodynamic limit, but it may be recovered by a suitable $i\varepsilon$ prescription in (3.26). The two-body continuum will not concern us at this point. Instead, we note that the generalisation of (3.26) to any lattice dimension D is straightforward. For $D=3$, the correct generalisation is obtained by the formal substitutions

$$\begin{aligned} &dp/2\pi \to d^3p/(2\pi)^3, \\ &\Omega_p \to \Omega_{\boldsymbol{p}} = \{4\kappa^2[\sin^2(p_1/2)+\sin^2(p_2/2)+\sin^2(p_3/2)]+m^2\}^{1/2}. \end{aligned} \tag{3.27}$$

The resulting algebraic equation for Ω is solved numerically for various values of the quasiphonon mass m. The real root is denoted by M and provides the mass of the collective branch at $D=3$. The results are summarised in figure 3 together with the corresponding results for $D=1$ obtained earlier. Note that M reaches the limiting value $m\sqrt{6}$ in the strong-coupling limit irrespectively of the lattice dimension D. This is as expected because for strong coupling (or $\kappa=0$) the system reduces to independent anharmonic oscillators. In the weak-coupling limit $m\to 0$, M reaches the value $4\kappa\sqrt{D}$ which is the energy of two uncoupled phonons at the zone boundary.

We conclude our discussion with a few remarks. The situation analysed here is probably too ideal to have applications in real crystals. Notice that we have assumed a global $O(N)$ symmetry. In real crystals the symmetry is reduced to a discrete subgroup of $O(N)$, resulting in additional terms in the Hamiltonian. These may alter the collective mode quite drastically, and possibly destroy it. From the methodological point of view, the generalised HP theory provides a rigorous alternative to collective-field or hydrodynamic formulations frequently encountered in many-body theory. Two related troublesome questions usually associated with the latter treatments are resolved by the HP theory. (i) Ordering ambiguities do not occur in higher-order calculations which may be systematically performed. (ii) Implicit in the diagonalisation of the Hamiltonian (3.10) is the construction of separate creation–annihilation operators for the collective mode and the two-body continuum. Double counting does not occur, however, as is best illustrated in figure 1. The total number of independent normal frequencies remains equal to $\Lambda(\Lambda+1)/2$ at all stages of the calculation, even though the frequencies are distributed over distinct branches.

There is little doubt that our results may be rederived using other methods. Independently of the method, the important conclusion is that the lattice ϕ^4-field theory possesses a spectrum of elementary excitations which is well defined and richer than what one would naively expect. We should emphasise, however, that our conclusions do not necessarily contradict the appearance of Landau ghosts in the spectrum of the continuum field theory, or in the context of other regularisation schemes. On the contrary, the current calculations may be used as a starting point for a careful study of the mechanism by which Landau ghosts emerge in the continuum limit. Such an exercise would be less than academic in view of the augmenting evidence that ϕ^4-couplings, an important ingredient in the Goldstone–Higgs mechanism, lead to either trivial or pathological continuum field theories outside weak-coupling perturbation theory.

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