Dynamical Group Model of the CDW State

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Abstract

The dynamical group for a one-dimensional model of a many-electron system exhibiting a charge-density wave is obtained. The corresponding Lie algebra in a physical model is U(2); it is used to obtain the spectrum and coherent ground state, and to define a corresponding order parameter.

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Many intermetallic compounds of the form A_3B, known as β-tungstens, undergo a structural transformation in their crystalline lattices from the cubic to the tetragonal state [1]. This phase transition is often referred to as a martensitic transition, after its observation in the iron-carbon system called martensite. This structural transition was predicted to occur in one-dimensional systems by Peierls [2]; in recent times the effect has been much studied in quasi-one-dimensional conductors such as the organic TCNQ salts [3]. The aspect of the phenomenon which interests us in this note is the occurrence of a charge-density wave (CDW) having wave vector $Q = 2k_F$, where k_F is the Fermi surface wave vector; a simple model incorporating an impressed wave of this nature is exactly solvable, and lends itself to a group theoretic treatment. It turns out that for the model we use, the spectrum-generating Lie algebra is not semi-simple, but for a model with real and constant coupling it is essentially U(2). However, it is straightforward to obtain the spectrum and generalized Bogoliubov transformation. The coherent ground state is also easily obtainable, and gives rise to the appearance of a non-vanishing order parameter in the CDW state.

Our starting point is a Fröhlich-type hamiltonian describing lattice electrons interacting with phonons

$$H = \sum_{k,\sigma} \varepsilon(k)\, a^{\dagger}_{k\sigma}\, a_{k\sigma} + \Big(\sum_{q,k,\sigma} g_{q,k} b_q\, a^{\dagger}_{k+q\sigma}\, a_{k\sigma} + \text{h.c.} \Big)$$

The $a_{k,\sigma}$ are the destruction operators for electrons in the Bloch state of wave-vector k and spin σ ($\sigma = \uparrow$ or $\downarrow$) having corresponding energy $\varepsilon(k)$; b_q is the phonon destruction operator and $g_{q,k}$ the electron-phonon coupling constant. The CDW assumption is that the dominating term in the interaction is with the phonon of wave vector Q, and we neglect all other terms. In the spirit of the BCS [5] and Bogoliubov [6] (superfluid He^4) linearisation tricks, we replace the remaining phonon operator b_Q by its "average value" -a c-number-

$$g_{Q,k}\, b_Q \sim \langle g_{Q,k}\, b_Q \rangle = \gamma_k$$

to obtain the reduced hamiltonian

$$H^{red} = \sum \varepsilon(k)\, a^{\dagger}_{k\sigma}\, a_{k\sigma} + \left(\sum \gamma_k\, a^{\dagger}_{k+Q\sigma}\, a_{k\sigma} + \text{h.c.}\right) \qquad (1)$$

where the summation is over wave vectors k and spin σ.

Just as in the superfluid cases where this type of replacement destroys a conserved quantity (number) and gives rise to a corresponding order parameter in the superfluid phase, here too we have destroyed momentum conservation and expect to see a corresponding order parameter appear in the CDW phase.

Determination of the spectrum-generating algebra (SGA) is achieved by decoupling the reduced hamiltonian (1) into a sum of commuting terms

$$H^{red} = \sum_k H(k).$$

The SGA for H^{red}, g, will be of the form

$$g = \oplus_k g_k$$

in the sense of a direct sum of Lie algebras where each g_k is isomorphic to a fixed Lie algebra (which we often loosely refer to as the SGA of H^{red}). This process is analogous to that carried out for superfluid systems [7]. This decoupling is achieved as follows: We assume that only states for which $|k| \leq Q = 2k_F$ can participate in the reduced hamiltonian (1). This leads to

$$H^{red} = \sum_{-k_F}^{k_F} H(k) \tag{2}$$

where

$$H(k) = H_{(+)}(k) \quad \text{for } k \in [0,k_F]$$

and

$$H(k) = H_{(-)}(k) \quad \text{for } k \in [-k_F,0).$$

[Note that we have now implicitly taken a <u>linear</u> model with this domain of k.]

Here

$$H_{(\pm)}(k) = E_{(\pm)}(k) + V_{(\pm)}(k)$$

with

$$E_{(\pm)}(k) = \varepsilon(k)\ (a^{\dagger}_{k\uparrow}\, a_{k\uparrow} + a^{\dagger}_{-k\downarrow}\, a_{-k\downarrow}) + \varepsilon(k_{+}^{-}Q)\ (a^{\dagger}_{k_{+}^{-}Q\uparrow}\, a_{k_{+}^{-}Q\uparrow} + a^{\dagger}_{-(k_{+}^{-}Q)\downarrow}\, a_{-(k_{+}^{-}Q)\downarrow}) .$$

The interaction terms are

$$V_{(+)}(k) = \gamma_{k-Q}\, a^{\dagger}_{k\uparrow}\, a_{k-Q\uparrow} + \gamma_{-k}\, a^{\dagger}_{-(k-Q)\downarrow}\, a_{-k\downarrow} + \text{h.c.}$$

and

$$V_{(-)}(k) = \gamma_{-(k+Q)}\, a^{\dagger}_{-k\downarrow}\, a_{-k-Q\downarrow} + \gamma_{k}\, a^{\dagger}_{k+Q\uparrow}\, a_{k\uparrow} + \text{h.c.}$$

Having achieved the requisite decoupling, we now note that the terms in $H_{(\pm)}(k)$ can be written as hermitian bilinear forms of the four operators $A_{(\pm)i}(k)$, $i = 1,2,3,4$,

$$\{A_{(\pm)1}(k),\ A_{(\pm)2}(k),\ A_{(\pm)3}(k),\ A_{(\pm)4}(k)\} =$$

$$\{a_{k\uparrow},\ a^{\dagger}_{-k\downarrow},\ a_{k\mp Q\uparrow},\ a^{\dagger}_{-(k\mp(Q)\downarrow}\}\ .$$

Since the 16 operators $X_{ij} = A^{\dagger}_{i} A_{j}$ generate a representation of the algebra $g\ell(4,R)$ [8] (we have dropped the $(\pm)$ suffix and the explicit k dependence in our notation - these remarks are clearly true for both + and - sectors and all k) we see that the SGA of H is a subalgebra of U(4), the algebra of the hermitian elements of $g\ell(4,R)$. We may determine the subalgebra in question by choosing an explicit 4 x 4 representation of X_{ij}

$$\hat{X}_{ij} = e_{ij} \qquad (i,j = 1,\ 2,\ 3,\ 4)$$

where each e_{ij} matrix has elements

$$(e_{ij})_{\ell m} = \delta_{i\ell}\, \delta_{jm}$$

In this representation, each H(k) of the sum in (2) is given by a 4x4 matrix

$$\hat{H} = \left[\begin{array}{cc|cc} \varepsilon & & \gamma & \\ & -\varepsilon & & -\gamma' \\ \hline \gamma^* & & \varepsilon' & \\ & -\gamma'^* & & -\varepsilon' \end{array}\right]$$

with

$$\varepsilon = \varepsilon(k),\ \varepsilon' = \varepsilon(k-Q),\ \gamma = \gamma_{k-Q},\ \gamma' = \gamma_{-k} \quad \text{for } k\in[0,k_F];$$

$$\varepsilon = \varepsilon(k),\ \varepsilon' = \varepsilon(k+Q),\ \gamma = \gamma_k^*,\ \gamma' = \gamma^*_{-(k+Q)} \quad \text{for } k\in[-k_F,0) \tag{3}$$

Define the matrices

$$\underline{L} = 1/2\ \underline{\tau} \times \tau_0$$
$$\underline{K} = 1/2\ \underline{\tau} \times \tau_3$$
$$S = 1/2\ \tau_0 \times \tau_3$$

in terms of the Pauli-spin matrices

$$\{\tau_0, \underline{\tau}\} \equiv \left\{\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}, \begin{bmatrix} & 1 \\ 1 & \end{bmatrix}, \begin{bmatrix} & -i \\ \underline{i} & \end{bmatrix}, \begin{bmatrix} 1 & \\ & -\underline{1} \end{bmatrix}\right\},$$

and note that $\hat{H}$ above can be written

$$\hat{H} = \lambda S + \underline{a} \cdot \underline{L} + \underline{b} \cdot \underline{K} \tag{4}$$

where

$$\lambda = \varepsilon + \varepsilon', \ \underline{a} = ((\alpha - \alpha'), -(\beta - \beta'), 0) ,$$
$$\underline{b} = ((\alpha + \alpha'), -(\beta + \beta'), (\varepsilon - \varepsilon'))$$

(with $\gamma \equiv \alpha + i\beta$).

Since

$$[L_i, L_j] = i\, e_{ijk}\, L_k$$
$$[L_i, K_j] = i\, e_{ijk}\, K_k$$
$$[K_i, K_j] = i\, e_{ijk}\, L_K$$

and

$$[S, \underline{L}\,] = [S, \underline{K}] = 0$$

We have in (4) explicitly described $\hat{H}$ as an element of the $U(1) \oplus SO(4)$ algebra generated by $(S, \underline{L}, \underline{K})$. Thus the SGA of this CDW model is $g = \oplus_k g_k$ and $g_k \sim U(1) \oplus SO(4)$.

Since under automorphisms of this algebra the terms

$$\lambda, \ a^2 + b^2, \ \underline{a} \cdot \underline{b}$$

are invariant, diagonalisation involves transforming

$$\hat{H} \rightarrow R\hat{H}R^{-1} = \lambda S + \mu L_3 + \nu K_3 \qquad (5)$$

where

$$\lambda = \varepsilon + \varepsilon' ,$$
$$\mu^2 + \nu^2 = 2(|\gamma|^2 + |\gamma'|^2) + (\varepsilon - \varepsilon')^2 ,$$
$$\mu\nu = |\gamma|^2 - |\gamma'|^2 .$$

When account is taken of the symmetry of the electron-phonon scattering term in the original Fröhlich hamiltonian, we see that in a physical model $\gamma = \gamma'$, and so there is a degeneracy of the spectrum.

The corresponding energy spectrum has the form

$$1/2\ (\varepsilon + \varepsilon') \pm 1/2\ [4|\gamma|^2 + (\varepsilon - \varepsilon')^2]^{1/2}$$

where the k-dependence of the above quantities is given by (3). Note that at the Fermi surface $k = k_F$ where $\varepsilon = \varepsilon' = \varepsilon_F$, the corresponding energies are

$$\varepsilon_F \pm |\gamma| \ ,$$

showing an energy discontinuity of magnitude $2|\gamma|$. (Whether or not there is an energy gap in the sense of a forbidden range of energies depends on satisfying the inequality, for constant γ,

$$\text{Max}\ (\varepsilon + \varepsilon') - \text{Min}\ (\varepsilon + \varepsilon') < 4|\gamma|$$

For a model with $\varepsilon(k) = 1/2\ W\ (1 - \cos k)$ this condition is $W \cos k_F < 2|\gamma|$.)

The Bogoliubov transformation is related to the transformation T in Hilbert space which corresponds to the matrix R which implements the diagonalisation (5). R may be readily obtained for the U(1)⊕ SO(4) hamiltonian (4); however, it is more instructive to exhibit it for a simplified model in which γ is real. In this case our hamiltonian becomes

$$\hat{H} = \lambda S + \underline{\mu} \cdot \underline{J}$$

where

$$\underline{\mu} = (2\gamma,\ 0,\ \varepsilon - \varepsilon') \ ; \ \underline{J} = (K_1,\ L_2,\ K_3)$$

and so $\hat{H}$ has the SGA: $U(1) \oplus SO(3) \sim U(2)$, whence T involves

only a single rotation angle. Explicitly, the diagonalizing rotation in the 4x4 representation is given by

$$R = \exp(2i\phi \; J_2)$$

where

$$\tan 2\phi = 2\gamma/(\varepsilon-\varepsilon');$$

this corresponds in Fock space to

$$T_{(k)} = \exp \phi_k \{a^{\dagger}_{k\uparrow} a_{k-Q\uparrow} + a_{-k\downarrow} a^{\dagger}_{-(k-Q)\downarrow} - \text{h.c.}\}$$

(for $k \geq 0$; an entirely analogous expression with $Q \to -Q$ holds for $k < 0$), where we have explicitly put back the k dependence in the second expression to emphasize that the corresponding transformation on the reduced hamiltonian (2) would be given by

$$H^{red} \to T \, H^{red} \, T^{-1}$$

where

$$T = \prod_{k=-k_F}^{k_F} T_{(k)}$$

The Bogoliubov transformation is precisely that unitary transformation on the operators $a_{k\sigma}$ in terms of which H^{red} is (unchanged and) diagonal. This clearly has the form

$$a_{k\uparrow} \to T^{+} a_{k\uparrow} T = \cos \phi_k \, a_{k\uparrow} + \sin \phi_k \, a_{k-Q\uparrow} \qquad (k \geq 0)$$

with similar expressions for the other operators.

Coherent states are obtained by the action of elements of the dynamical group corresponding to the SGA on a fixed state [9]; the most important example is the ground coherent state $|g\rangle$ corresponding to the Fermi sea $|f\rangle$,

$$|g\rangle = T|f\rangle$$

where

$$|f\rangle = \prod_{\substack{-k_F \leq k \leq k_F \\ \sigma=\uparrow,\downarrow}} a^{\dagger}_{k\sigma} \, |0\rangle$$

for vacuum state $|0\rangle$.

We conclude by exhibiting the appearance of an order parameter in the ground state $|g\rangle$ of the CDW phase, as we expected at the beginning. First note that the operator $a_{k\sigma} \, a^{\dagger}_{k-Q\sigma}$ vanishes in the normal (Fermi-sea) ground state;

$$\langle f| \, a_{k\sigma} \, a^{\dagger}_{k-Q\sigma} \, |f\rangle = 0 \ .$$

However

$$\begin{aligned} \langle g| \, a_{k\sigma} \, a^{\dagger}_{k-Q\sigma} \, |g\rangle &= \langle f| \, T^{\dagger} a_{k\sigma} \, a^{\dagger}_{k-Q\sigma} \, T \, |f\rangle \\ &= \langle f| \, n_{k\sigma} - n_{k-Q,\sigma} \, |f\rangle \cos\phi_k \sin\phi_k \\ &= 1/2 \sin 2\phi_k, \text{ for } k \in [0, k_F] \ , \end{aligned}$$

where $n_{k\sigma}$ is the number operator in state $k\sigma$.
We deduce that the relevant order parameter for characterizing the CDW phase is $\langle a_{k\sigma} \, a^{\dagger}_{k'\sigma} \rangle$, (where $k' = k \mp Q$ for $k = \pm |k|$).

Elsewhere [10] we discuss the dynamical group of a mean-field model of coexistence of superconductivity and charge density waves; work is also in progress to include magnetic effects in the dynamical group formalism.

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