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Inclusion of fermionic degrees of freedom in the lattice dynamics shell model

A Greco† and O Zandron‡

Departamento de Física, Facultad de Ciencias Exactas Ingeniería y Agrimensura, UNR, Avenida Pellegrini 250, 2000 Rosario, Argentina

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Abstract. We present a model which allows us to describe not only the interaction of electrons with rigid ions, but also the interaction between electrons and the deformation of the electronic clouds of the ions due to atomic displacements. To this purpose the usual shell model is extended by incorporating a finite set of fermionic coordinates (Grassmann variables), which represent the fermionic degrees of freedom. The pseudomechanics and the quantum statistical mechanics of the model are studied. The perturbative formalism for a general interacting potential and the Feynman rules are given. This perturbative method is useful to evaluate several physical properties in solid state physics at finite temperature.

1. Introduction

The Fröhlich's Hamiltonian (e.g. see [1]) is frequently used to treat the electron–phonon interaction. In this model the electrons interact with rigid ions vibrating around their equilibrium positions. Effects of the electronic polarizability of ions can be taken into account at most by introducing the high-frequency dielectric constant in the electron–phonon coupling constant. If the electronic shells of the ions are deformed by the vibration of ionic cores, additional interactions between these deformations and other electrons arise. Recently, some authors have considered this problem [2]. In lattice dynamics, a model which takes into account effects of ionic polarizabilities is the well known shell model [3]. The electronic polarizability effects have been incorporated in the shell model by means of massless charge shells with empirical potentials between shells and between cores and shells. Thus, the description of these electronic effects through the shell model is quite different to the Born–von Karman approach, where the electrons are considered only implicitly in the adiabatic potential [4].

In a recent paper [5] we have obtained the quantum partition function of a general anharmonic shell model by using the Dirac theory of constrained Hamiltonian systems [6]. The shell model constitutes a constrained Hamiltonian system in which all the constraints are of second class. Therefore the path integral formalism developed by Senjanovic [7] was used to construct the quantum partition function. Starting from this quantum partition function, an anharmonic perturbation theory was developed [8]. This perturbative formalism allowed us to compute the phonon response function

† Fellow of the Consejo de Investigaciones de la UNR.
‡ Fellow of the Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina.

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and thermodynamic properties of solids described by an anharmonic shell model. The previous formalism treats the electronic shells as bosonic degrees of freedom.

On the other hand, if additional electrons are to be considered as fermionic degrees of freedom, it is well known that these can be treated at a classical level by introducing Grassmann variables. The classical treatment of Bose–Fermi dynamical systems is known as pseudomechanics [9, 10].

In this paper a model is presented which takes into account not only the electron interactions with rigid ions, but also the interactions between electrons and the electronic deformability of ions. These types of electronic effects cannot be described by using only shell coordinates; therefore, we generalize the shell model to an extended one. The generalization is performed by considering a finite set of fermionic coordinates (Grassmann variables). Thus, our extended shell model (ESM), in addition to the usual bosonic coordinates of shells and cores, also has fermionic dynamical variables.

As the shell model is a constrained Hamiltonian system, the electronic degrees of freedom cannot be treated at a quantum level in a simple way as in the Fröhlich model. Therefore, first we must study the ESM in the framework of Hamiltonian constrained systems before carrying out the quantization.

The paper is organized as follows. In section 2, the model is presented and we analyse it in the framework of constrained Hamiltonian systems. In section 3, the quantization of the model via Dirac brackets is considered and also the quantum path integral method is applied. In section 4 a perturbative theory for the model is constructed. In section 5, we find the connection between our model and that of the Fröhlich formalism for the electron–phonon interaction. Also, we point out that in the general case the two models provide very different information. In section 6, some possible applications of the ESM are briefly summarized. Finally, in section 7 the conclusions are given.

2. The ESM: constraints and first-class Hamiltonian

The shell model frequently used in the lattice dynamics of ionic crystals is described by the following Lagrangian:

$$L(u, \dot{u}, v) = \tfrac{1}{2}\dot{u}^i M_{ij} \dot{u}^j - \Phi(u, v) \tag{2.1}$$

where u and v denote the cores and shells displacements, respectively. The cartesian components, cell and ionic site are summarized in the indices $i, j, \ldots$ The quantities M_{ij} are the matrix elements of the mass matrix and $\Phi(u, v)$ is a general interacting potential. We will use the convention of summation over repeated indices.

The Euler–Lagrange equations obtained from equation (2.1) are

$$M_{ij}\ddot{u}^j + \frac{\partial \Phi}{\partial u^i} = 0 \tag{2.2a}$$

$$\frac{\partial \Phi}{\partial v_i} = 0 \tag{2.2b}$$

where equation (2.2b) is the so-called adiabatic condition.

Equation (2.2b) defines an implicit functional relation $v = v(u)$. When this relation is nonlinear in the v-variable, $v = v(u)$ cannot be explicitly known.

As mentioned above, our purpose is to take into account not only the interaction between electrons and rigid ions, but also the interaction between electrons and the deformation of the electronic clouds due to atomic displacements. Therefore, we extend the shell model by introducing classically the fermionic degrees of freedom by means of a finite set of complex Grassmannian coordinates ξ^α [11]. Thus, we start from the following Lagrangian:

$$L=\tfrac{1}{2}\dot{u}^i M_{ij}\dot{u}^j+\frac{\mathrm{i}}{2}(\xi^+_\alpha\dot{\xi}^\alpha-\dot{\xi}^+_\alpha\xi^\alpha)-\Phi(u, v, \xi, \xi^+) \tag{2.3}$$

where the complex Grassmann coordinates ξ^α and ξ^+_α verify the anticommutation relations

$$\{\xi^\alpha, \xi^\beta\}=\{\xi^+_\alpha, \xi^+_\beta\}=\{\xi^+_\alpha, \xi^\beta\}=0. \tag{2.4}$$

The index α is a generic one and can represent, for example, site, orbital or momentum, according to the representation used. This index can also carry information about the spin of the electrons.

The Grassmann variables allow us to describe electronic effects, such as the conductivity, which are not taken into account by means of shell displacements v. Thus, the second term on the right-hand side of equation (2.3) corresponds to the kinetic terms in the fermionic variables [10]. The general potential of interaction $\Phi(u, v, \xi, \xi^+)$ will depend on the bosonic variables u^i and v_j, and on the fermionic variables ξ^α and ξ^+_α.

Before giving the quantum description of the model, we analyse it in the framework of constrained Hamiltonian systems.

First, we consider the canonical momenta corresponding to the bosonic variables v_j and the fermionic variables ξ^α and ξ^+_α given by

$$P_{v_j}\equiv\frac{\partial L}{\partial\dot{v}_j}=0 \tag{2.5}$$

$$\Pi^+_\alpha\equiv\frac{\partial L}{\partial\dot{\xi}^\alpha}=-\frac{\mathrm{i}}{2}\xi^+_\alpha \tag{2.6}$$

$$\Pi^\alpha\equiv\frac{\partial L}{\partial\dot{\xi}^+_\alpha}=-\frac{\mathrm{i}}{2}\xi^\alpha. \tag{2.7}$$

These momenta define the following primary constraints:

$$\phi^j\equiv P_{v_j}\approx 0 \tag{2.8}$$

$$\psi^+_\alpha\equiv\Pi^+_\alpha+\frac{\mathrm{i}}{2}\xi^+_\alpha\approx 0 \tag{2.9}$$

$$\psi^\alpha\equiv\Pi^\alpha+\frac{\mathrm{i}}{2}\xi^\alpha\approx 0. \tag{2.10}$$

In equations (2.6) and (2.7) we use the right-hand derivatives when the derivation is performed with respect to the Grassmann variables [11]. The symbol $\approx$ is used to indicate a weakly zero equation [6].

After some algebraic manipulations, the canonical Hamiltonian is written as

$$H_{\mathrm{can}}=\tfrac{1}{2}P_{u^i}(M^{-1})^{ij}P_{u^j}+\Phi(u, v, \xi, \xi^+). \tag{2.11}$$

The Hamiltonian (2.11) is not univocally determined; therefore, we must define the following bosonic quantity as the total Hamiltonian:

$$H_T = H_{can} + \phi^i B_i + F_\alpha^{1+}\psi^\alpha + \psi_\alpha^+ F^{2\alpha}. \tag{2.12}$$

The set B_i are bosonic Lagrange multipliers and the sets $F^{1\alpha}$ and $F^{2\alpha}$ are fermionic Lagrange multipliers.

The consistency conditions of the formalism require the preservation in time of the constraints (2.8)-(2.10). This leads to the equations

$$\dot{\phi}^j = \{\phi^j, H_T\}_{PB} = -\frac{\partial \Phi}{\partial v_j} \approx 0 \tag{2.13}$$

$$\dot{\psi}_\alpha^+ = \{\psi_\alpha^+, H_T\}_{PB} = -\frac{\partial \Phi}{\partial \xi^\alpha} + iF_\alpha^{1+} \approx 0 \tag{2.14}$$

$$\dot{\psi}^\alpha = \{\psi^\alpha, H_T\}_{PB} = -\frac{\partial \Phi}{\partial \xi_\alpha^+} - iF^{2\alpha} \approx 0. \tag{2.15}$$

We have used the symbol $\{,\}_{PB}$ to indicate the graded Poisson brackets which were defined in [9].

Equations (2.14) and (2.15) univocally determine the fermionic multipliers F_α^{1+} and $F^{2\alpha}$:

$$F_\alpha^{1+} = -i\frac{\partial \Phi}{\partial \xi^\alpha} \tag{2.16a}$$

$$F^{2\alpha} = i\frac{\partial \Phi}{\partial \xi_\alpha^+} \tag{2.16b}$$

while equation (2.13) defines the secondary constraints:

$$\chi^j \equiv -\frac{\partial \Phi}{\partial v_j} \approx 0. \tag{2.17}$$

Moreover, from equation (2.16) we can see that $F^{1\alpha} = F^{2\alpha} = F^\alpha$.

Requiring the preservation in time of the secondary constraints (2.17) we find

$$\dot{\chi}^j = \{\chi^j, H_T\}_{PB} = -T^j{}_i (M^{-1})^{ik} P_{u^k} - B_i S^{ij} - F_\alpha^+ U^{\alpha j} - U_\alpha^{+j} F^\alpha \approx 0 \tag{2.18}$$

where we have defined the following matrix elements:

$$T_i^j \equiv \frac{\partial \Phi}{\partial u^i \partial v_j} \tag{2.19a}$$

$$S^{ij} \equiv \frac{\partial \Phi}{\partial v_i \partial v_j} \tag{2.19b}$$

$$U^{\alpha j} \equiv \frac{\partial \Phi}{\partial \xi_\alpha^+ \partial v_j} \qquad U_\alpha^{+j} \equiv \frac{\partial \Phi}{\partial \xi^\alpha \partial v_j}. \tag{2.19c}$$

Equation (2.18) univocally defines the bosonic Lagrange multipliers B_k which are given by

$$B_k = -(S^{-1})_{kj}(M^{-1})^{ji} T_i^l P_{u^l} - (S^{-1})_{kj} U_\alpha^{+j} F^\alpha - (S^{-1})_{kj} F_\alpha^+ U^{\alpha j} \tag{2.20}$$

where F^α and F_α^+ are given in equations (2.16).

Finally, the total Hamiltonian H_T, which is a first-class dynamical quantity, becomes

$$H_T = \tfrac{1}{2}P_{u^j}(M^{-1})^{ji}P_{u^i} + \Phi(u, v, \xi, \xi^+) - (S^{-1})_{kj}(M^{-1})^{ji}T_i{}^l P_{u^l}P_{v_k} + i(S^{-1})_{kl}F^+_\alpha U^{\alpha l}P_{v_k}$$
$$- i(S^{-1})_{kj}U^{+j}_\alpha F^\alpha P_{v_k} - iF^+_\alpha\left(\Pi^\alpha + \frac{i}{2}\xi^\alpha\right) + i\left(\Pi^+_\alpha + \frac{i}{2}\xi^+_\alpha\right)F^\alpha. \tag{2.21}$$

The constraints given by equations (2.8)–(2.10) and (2.17) are second-class ones. In this sense, the dynamical system under consideration differs from the quantum electrodynamics formalism in which there are first- and second-class constraints [12].

The next step is to compute the graded Dirac brackets. The graded Dirac brackets $\{,\}^*$ between two quantities O_1 and O_2 are obtained by means of the definition

$$\{O_1, O_2\}^* = \{O_1, O_2\}_{PB} - \{O_1, \phi_a\}_{PB}\Delta^{ab}\{\phi_b, O_2\}_{PB}. \tag{2.22}$$

In equation (2.22) all the possible second-class constraints ϕ_α are given as the components of the following vector:

$$\phi = \begin{pmatrix} P_{v_j} \\ \chi^j \\ \psi^\alpha \\ \psi^+_\alpha \end{pmatrix}. \tag{2.23}$$

The supermatrix Δ is the inverse of the supermatrix constructed with the elements $\{\phi_a, \phi_b\}_{PB}$, i.e.

$$\Delta^{ab}\{\phi_b, \phi_c\}_{PB} = \delta^a{}_c. \tag{2.24}$$

The matrix Δ^{-1} is given by

$$\Delta^{-1} = \begin{pmatrix} 0 & S^{ij} & 0 & 0 \\ -S^{ij} & 0 & -U^{\alpha i} & -U^{+i}_\alpha \\ 0 & U^{\alpha j} & 0 & -i\delta^\alpha{}_\beta \\ 0 & U^{+j}_\alpha & -i\delta^\alpha{}_\beta & 0 \end{pmatrix} \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{2.25}$$

The name 'supermatrix' is applied to a matrix containing bosonic and fermionic elements. To work with these supermatrices we follow the supermatrix algebra given in [13]. Computing the supermatrix Δ it can be written as

$$\Delta = \begin{pmatrix} A' & B' \\ C' & D' \end{pmatrix} \tag{2.26}$$

whose Bose-Bose parts A' and Fermi-Fermi parts D' are even elements of a Grassmann algebra and whose Bose-Fermi parts B' and Fermi-Bose parts C' are odd elements. The explicit expressions for these four matrices are:

$$A' = \begin{pmatrix} -i(S^{-1})_{ij}[U^{+j}_\alpha U^{\alpha k} - U^{+k}_\alpha U^{\alpha j}](S^{-1})_{kl} & -(S^{-1})_{il} \\ (S^{-1})_{il} & 0 \end{pmatrix} \tag{2.27}$$

$$B' = \begin{pmatrix} -i(S^{-1})_{ij}U^{+j}_\alpha & -i(S^{-1})_{ij}U^{\alpha j} \\ 0 & 0 \end{pmatrix} \tag{2.28}$$

$$C' = \begin{pmatrix} -iU^{+j}_\alpha(S^{-1})_{ji} & 0 \\ -iU^{\alpha j}(S^{-1})_{ji} & 0 \end{pmatrix} \tag{2.29}$$

$$D' = \begin{pmatrix} 0 & i\delta^\alpha{}_\beta \\ i\delta^\alpha{}_\beta & 0 \end{pmatrix}. \tag{2.30}$$

The time evolution of all relevant physical quantities and the equations of motion are written in terms of Dirac brackets. The equations of motion are valid for both Dirac and Poisson brackets because H_T defined in equation (2.21) is a first-class dynamical quantity.

3. Quantization

Let us begin by using the canonical method in the quantization procedure of the ESM. The second-class constraints may be eliminated by means of the graded Dirac brackets. Consequently, we must take the commutations relations corresponding to the graded Dirac brackets (2.22) and consider the second-class constraints as strong equations between operators. From equation (2.22) and after some algebraic manipulation we find

$$\{\xi^\alpha, \xi^+_\beta\}^* = -\mathrm{i}\delta^\alpha{}_\beta \tag{3.1}$$

$$[u^i, P_{u^j}]^* = \delta^i_j \tag{3.2}$$

$$[v_i, P_{v_i}]^* = 0 \tag{3.3}$$

$$[u^i, \xi^\alpha]^* = [u^i, \xi^+_\alpha]^* = 0 \tag{3.4}$$

$$[v_i, \xi^\alpha]^* = \mathrm{i}(S^{-1})_{ik}U^{\alpha k} \tag{3.5}$$

$$[v_i, \xi^+_\alpha]^* = \mathrm{i}(S^{-1})_{ik}U^{+k}_\alpha. \tag{3.6}$$

Subsequently, by defining the graded commutation relation between two operators $\hat{O}_1$ and $\hat{O}_2$,

$$\{\hat{O}_1, \hat{O}_2] = \mathrm{i}\hbar\{O_1, O_2]^* \tag{3.7}$$

we find

$$\{\hat{\xi}^\alpha, \hat{\xi}^+_\beta\} = \hbar\delta^\alpha{}_\beta \tag{3.8}$$

$$[\hat{u}^i, \hat{P}_{u^j}] = \mathrm{i}\hbar\delta^i_j \tag{3.9}$$

$$[\hat{v}_i, \hat{P}_{v_i}] = 0 \tag{3.10}$$

$$[\hat{u}^i, \hat{\xi}^\alpha] = [\hat{u}^i, \hat{\xi}^+_\alpha] = 0 \tag{3.11}$$

$$[\hat{v}_i, \hat{\xi}^\alpha] = -\hbar(S^{-1})_{ik}U^{\alpha k} \tag{3.12}$$

$$[\hat{v}_i, \hat{\xi}^+_\alpha] = -\hbar(S^{-1})_{ik}U^{+k}_\alpha. \tag{3.13}$$

From equation (3.8) we see that the operators $\hat{\xi}^\alpha$ and $\hat{\xi}^+_\alpha$ verify a Clifford algebra. This equation corresponds to the anticommutation relation between creation and annihilation operators of electrons. Subsequently, when we take the second-class constraints (2.8)–(2.10) as strongly equal to zero, the total Hamiltonian is written

$$\hat{H}_T = \tfrac{1}{2}\hat{P}_{u^i}(M^{-1})^{ij}\hat{P}_{u^j} + \Phi(\hat{u}, \hat{v}, \hat{\xi}, \hat{\xi}^+). \tag{3.14}$$

Thus, the quantum formalism of our model remains defined by the Hamiltonian operator (3.14), the graded commutation relations (3.8)–(3.13) and the secondary constraints (2.17), taking these last constraints as strongly equal to zero quantities. The commutation relation (3.10) clearly shows that the variable v is not a true dynamical variable.

Moreover, we note that the non-trivial commutation relations (3.12) and (3.13) can be obtained only by means of the Dirac formalism.

An alternative quantization method is the path integral one. It is a powerful method which allows us to extend the results to quantum statistical mechanics and to construct the perturbative method for the ESM.

As already mentioned in the introduction, we will use the path integral formalism developed by Senjanovich [7] because the system under consideration has second-class constraints. The probability amplitude for the system initially at $|u_0, v_0, \xi_0, \xi_0^+\rangle$ and in state $|u, v, \xi, \xi^+\rangle$ at time T can be written as

$$\begin{aligned}\langle u, v, \xi, \xi^+|u_0, v_0, \xi_0, \xi_0^+\rangle &= \int \mathcal{D}u\mathcal{D}P_u\mathcal{D}v\mathcal{D}P_v\mathcal{D}\xi^+\mathcal{D}\Pi^+\mathcal{D}\xi\mathcal{D}\Pi(\mathrm{sdet}\,\Delta^{-1})^{1/2} \\ &\times\delta(P_v)\delta(\chi)\delta\left(\Pi^+ + \frac{\mathrm{i}}{2}\xi^+\right)\delta\left(\Pi + \frac{\mathrm{i}}{2}\xi\right) \\ &\times\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^T (\dot{u}^i P_{u^i} + \dot{v}_j P_{v^j} - \Pi_\alpha^+\dot{\xi}^\alpha + \dot{\xi}_\alpha^+\Pi^\alpha - H_T)\,\mathrm{d}t\right). \end{aligned} \tag{3.15}$$

In equation (3.15) $(\mathrm{sdet}\,\Delta^{-1})$ is the superdeterminant of Δ^{-1} [13] and is equal to

$$(\mathrm{sdet}\,\Delta^{-1}) = (\det A)\det{}^{-1}(D - CA^{-1}B) \tag{3.16}$$

therefore

$$(\mathrm{sdet}\,\Delta^{-1})^{1/2} = \mathrm{i}(\det S). \tag{3.17}$$

Using this last result, and integrating in the P_u, P_v, Π and Π^+ momenta, the probability amplitude is given by

$$\begin{aligned}\langle u, v, \xi, \xi^+|u_0, v_0, \xi_0, \xi_0^+\rangle &= \mathrm{i}\int \mathcal{D}u\mathcal{D}v\mathcal{D}\xi\mathcal{D}\xi^+ \det S\,\delta(\chi) \\ &\times\exp\left[\frac{\mathrm{i}}{\hbar}\int_0^T \left(\tfrac{1}{2}\dot{u}^i\bar{M}_{ij}\dot{u}^j + \frac{\mathrm{i}}{2}(\xi_\alpha^+\dot{\xi}^\alpha - \dot{\xi}_\alpha^+\xi^\alpha) - \Phi(u, v, \xi, \xi^+)\right)\mathrm{d}t\right]. \end{aligned} \tag{3.18}$$

From equation (3.18) it can be seen that the path integral in the Grassmann variables has the same expression as that obtained for a fermionic system in the holomorphic representation [14].

4. Perturbative method and Feynman rules

In this section we give a perturbative method which allows us to obtain the Green functions of the ESM. Our starting point is the expression (3.18).

The quantum partition function is obtained from equation (3.18) by integrating over all the periodic paths in the bosonic variables, over all the antiperiodic paths in the fermionic ones and making the change of variable $it = \tau$ [15]. Thus we have

$$Z = \int \mathcal{D}u\mathcal{D}v\mathcal{D}\xi\mathcal{D}\xi^+\mathcal{D}\eta\mathcal{D}\eta^+\mathcal{D}\lambda\,\exp\left(-\frac{1}{\hbar}S'(u, v, \lambda, \xi, \xi^+, \eta^+)\right) \tag{4.1}$$

where

$$S' = S_E(u, v, \xi, \xi^+) + \int_0^{\beta\hbar} d\tau(\lambda_i \chi^i + \eta_i^+ S^{ij} \eta_j) \tag{4.2}$$

and the Euclidean action S_E is given by

$$S_E(u, v, \xi, \xi^+) = \int_0^{\beta\hbar} d\tau[\tfrac{1}{2}(\xi_\alpha^+ \dot{\xi}^\alpha - \dot{\xi}_\alpha^+ \xi^\alpha) + \tfrac{1}{2}\dot{u}^i M_{ij} \dot{u}^j + \Phi(u, v, \xi, \xi^+)]. \tag{4.3}$$

In equation (4.3) $\dot{\xi} = d\xi/d\tau$ and $\dot{u} = du/d\tau$.

To arrive at expression (4.1) we have used the δ-function integral representation and det S was written as a path integral over Grassmann numbers η.

The general interacting potential $\Phi(u, v, \xi, \xi^+)$ must be understood as the following expansion in the ξ and ξ^+ Grassmann variables:

$$\Phi(u, v, \xi, \xi^+) = \overset{(0)}{\Phi}(u, v) + \xi_\alpha^+ \overset{(1)}{\Phi}{}^\alpha{}_\beta(u, v)\xi^\beta + \text{higher-order terms in } \xi^+\xi. \tag{4.4}$$

Since the potentials $\overset{(0)}{\Phi}(u, v)$ and $\overset{(1)}{\Phi}{}^\alpha{}_\beta(u, v)$ will be, in general, polynomials in the u^i and v_j variables the last term on the right-hand side of equation (4.2) will also be a polynomial in the u, v, λ, ξ, ξ^+, η and η^+ variables.

Analogously to [8], we can define the quantity

$$X(i) = \begin{pmatrix} u^i \\ v_i \\ \lambda_i \end{pmatrix}. \tag{4.5}$$

Expression (4.2) can be written in terms of the quantity $X(i)$ and therefore the action S' contains terms of the form

$$A_{\mu\nu\ldots\rho}(i, j, \ldots, k)X^\mu(i)X^\nu(j)\ldots X^\rho(k) \tag{4.6}$$

$$B_{\mu\nu\ldots\rho}(i, j, \ldots, k, h, p)X^\mu(i)X^\nu(j)\ldots X^\rho(k)\eta_h^+\eta_p \tag{4.7}$$

$$C(\alpha, \beta, \ldots, \gamma)\xi_\alpha^+\xi^\beta\ldots \tag{4.8}$$

$$D(h, p, \alpha, \beta, \ldots, \gamma)\eta_h^+\eta_p\xi_\alpha^+\xi^\beta\ldots \tag{4.9}$$

$$E_{\mu\nu\ldots\rho}(i, j, \ldots, k, \alpha, \beta, \ldots, \gamma)X^\mu(i)X^\nu(j)\ldots X^\rho(k)\xi_\alpha^+\xi^\beta\ldots \tag{4.10}$$

$$F_{\mu\nu\ldots\rho}(i, j, \ldots, k, h, p, \alpha, \beta, \ldots, \gamma)X^\mu(i)X^\nu(j)\ldots X^\rho(k)\eta_h^+\eta_p\xi_\alpha^+\xi^\beta\ldots. \tag{4.11}$$

The convention of summation on repeated indices for both Greek and italic characters is used. The Greek superscripts $\mu, \nu, \ldots, \rho$ run from 1 to 3. The Greek indices $\alpha, \beta, \ldots, \gamma$ run from 1 to the number of fermionic degrees of freedom. Moreover, an integral from 0 to $\beta\hbar$ in the continuum variable τ must be understood. We will use this convention whenever the integral on τ is not explicitly written.

The quantities $A_{\mu\nu\ldots\rho}$, $B_{\mu\nu\ldots\rho}$, C, D, $E_{\mu\nu\ldots\rho}$ and $F_{\mu\nu\ldots\rho}$ appearing in the terms (4.6)-(4.11) are constructed following a similar prescription to that used in [8].

To obtain the Feynman rules we proceed in the usual manner [16]. The propagators are given by the bilinear (harmonic) components of the action and the remaining anharmonic pieces are represented by vertices.

The function $\overset{(0)}{\Phi}(u, v)$ has the bilinear component plus anharmonic terms. To obtain the propagator of the bosonic field we must take into account the bilinear part, i.e.

$$\overset{(0)}{\Phi}_{\mathrm{H}}(u, v) = \tfrac{1}{2}R_{ij}u^i u^j + T_i^j u^i v_j + \tfrac{1}{2}S^{ij}v_i v_j. \tag{4.12}$$

On the other hand, the function $\overset{(1)}{\Phi}{}^{\alpha}{}_{\beta}(u, v)$ can be expanded as follows:

$$\overset{(1)}{\Phi}{}^{\alpha}{}_{\beta}(u, v) = C^{\alpha}{}_{\beta} + D^{\alpha}{}_{\beta i}u^i + E^{\alpha}{}_{\beta}{}^{j}v_j + \ldots. \tag{4.13}$$

To obtain the fermionic field propagator we consider only the first term of the expansion (4.13), which leads us to the term $\xi_{\alpha}^{+}C^{\alpha}{}_{\beta}\xi^{\beta}$ in the action, bilinear in the fermionic field. Thus, the complete bilinear part S_0' of the expression (4.2) for the action takes the form

$$\begin{aligned} S_0'(u, v, \lambda, \xi, \xi^+, \eta, \eta^+) &= \int_0^{\beta\hbar} (\tfrac{1}{2}\dot{u}^i M_{ij}\dot{u}^j + \tfrac{1}{2}R_{ij}u^i u^j + T_i^j u^i v_j + \tfrac{1}{2}S^{ij}v_i v_j + T_i^j u^i \lambda_j + S^{ij}v_i\lambda_j \\ &\quad + S^{ij}\eta_i^+\eta_j + \tfrac{1}{2}(\xi_{\alpha}^{+}\dot{\xi}^{\alpha} - \dot{\xi}_{\alpha}^{+}\xi^{\alpha}) + \xi_{\alpha}^{+}C^{\alpha}{}_{\beta}\xi^{\beta})\,\mathrm{d}\tau \end{aligned} \tag{4.14}$$

which by using definition (4.5) can be written in a more compact form:

$$S_0' = \tfrac{1}{2}X^{\mu}(i)[G^{-1}(i, j)]_{\mu\nu}X^{\nu}(j) + \eta_i^+ S^{ij}\eta_j + \tfrac{1}{2}(\xi_{\alpha}^{+}\dot{\xi}^{\alpha} - \dot{\xi}_{\alpha}^{+}\xi^{\alpha}) + \xi_{\alpha}^{+}C^{\alpha}{}_{\beta}\xi^{\beta}. \tag{4.15}$$

The matrix G^{-1} appearing in equation (4.15) and whose elements are $[G^{-1}(i, j)]_{\mu\nu}$ is given by

$$G^{-1} = \begin{pmatrix} g^{-1} & T & T \\ T^{+} & S & S \\ T^{+} & S & 0 \end{pmatrix}. \tag{4.16}$$

Computing its inverse we find

$$G = \begin{pmatrix} g & gC^{+} & 0 \\ Cg & CgC^{+} & S^{-1} \\ 0 & S^{-1} & -S^{-1} \end{pmatrix} \tag{4.17}$$

where

$$D_{ij} = R_{ij} - T_i^j(S^{-1})_{kl}(T^{\mathrm{T}})^l{}_j \tag{4.18}$$

$$C_{ij} = -(S^{-1})_{ik}(T^{\mathrm{T}})^k{}_j \tag{4.19}$$

and

$$g_{ij}(\tau) = (M_{ij}\,\partial_{\tau}^2 + D_{ij})^{-1}. \tag{4.20}$$

The matrix D whose elements are defined in equation (4.18) is the dynamical matrix of the shell model. The quantity g defined in equation (4.20) is the free phonon propagator defined in [8].

Looking at the expression (4.15) we see that there are three propagators associated with the fields X^{μ}, η and ξ. The first and the second terms on the right-hand side of equation (4.15) define the propagators $[G(i, j)]_{\mu\nu}$ and $(S^{-1})_{ij}$ for the fields X^{μ} and η_i respectively. These two propagators are equal to those given in [8]. The last two terms

in equation (4.15) allow us to write the quantity

$$\mathcal{G}^{\alpha}{}_{\beta} = (\mathrm{i}\delta^{\alpha}{}_{\beta}\,\partial_{\tau} + C^{\alpha}{}_{\beta})^{-1} \tag{4.21}$$

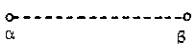
which is the well known expression for the fermionic field propagator [14].

In summary, the Feynman rules for a general interacting potential are:

(i) Propagators. We associate with the propagator $G_{\mu\nu}(i,j)$ a line connecting the two points i and j:

$G_{\mu\nu}(i,j)$ 

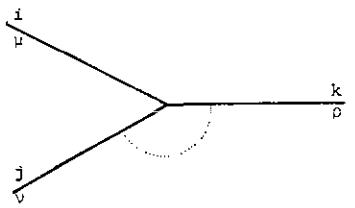
We associate with the propagator $\mathcal{G}^{\alpha}{}_{\beta}$ a dashed line connecting two generic points α and β (i.e. sites, orbitals):

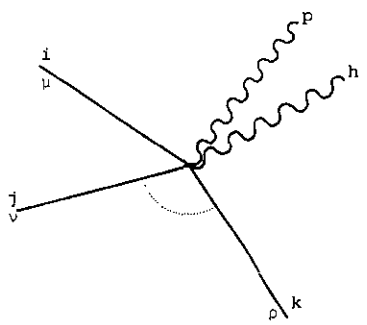
$\mathcal{G}^{\alpha}{}_{\beta}$ 

We associate with the propagator S_{ij}^{-1} a wavy line connecting the two points i and j:

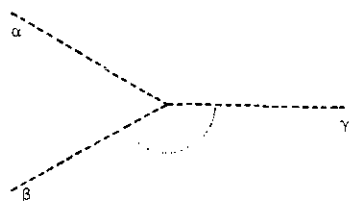
S_{ij}^{-1} 

(ii) Vertices. The generic vertices (of n legs $X^{\mu}(i)$) are represented by

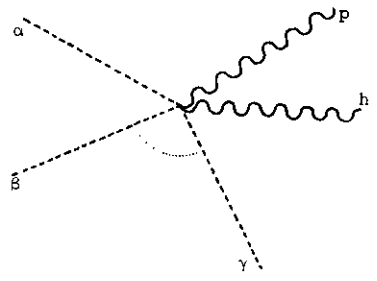
$(-1)\dfrac{1}{n!}A_{\mu\nu\ldots\rho}(i,j,\ldots,k)$ 

$(-1)\dfrac{1}{n!}B_{\mu\nu\ldots\rho}(i,j,\ldots,k,h,p)$ 

The generic vertices (of $2m$ legs ξ) are represented by

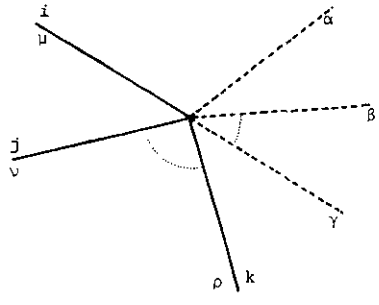
$(-1)C(\alpha,\beta,\ldots,\gamma)$ 

$(-1)D(h, p, \alpha, \beta, \ldots, \gamma)$

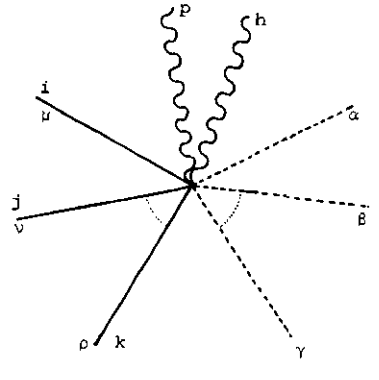


The generic vertices (of n legs $X^{\mu}(i)$ and $2m$ legs ξ) are represented by

$(-1)\frac{1}{n!}E_{\mu\nu\ldots\rho}(i, j, \ldots, k, \alpha, \beta, \ldots, \gamma)$



$(-1)\frac{1}{n!}F_{\mu\nu\ldots\rho}(i, j, \ldots, k, h, p, \alpha, \beta, \ldots, \gamma)$



(iii) A minus sign must be added to each closed loop built up to ξ and η fields, owing to its Grassmannian character.

(iv) Each diagram must be multiplied by the corresponding topological factor.

(v) The summation over all internal indices, both Greek and italic characters, must be carried out.

(vi) The external legs can take only the value $\mu = 1$ corresponding to the first component of the field X^{μ}.

Finally, as in the many-body theory [17], the sum of the vacuum-connected diagrams allows us to compute up to a given order the partition function Z and therefore thermodynamical properties can be obtained.

5. The connection of the ESM with the Fröhlich Hamiltonian

It is interesting to see in what case our model can be confronted with the Fröhlich Hamiltonian, and also in which cases the essential differences are found. To this

purpose we must consider the expansions (4.12) and (4.13), the latter up to first order in the fields u and v. Therefore, under these conditions the general interacting potential (4.4) remains

$$\Phi(u, v, \xi, \xi^+) = \tfrac{1}{2}R_{ij}u^iu^j + T_i^ju^iv_j + \tfrac{1}{2}S^{ij}v_iv_j + \xi_\alpha^+C^\alpha{}_\beta\xi^\beta + \xi_\alpha^+B^\alpha{}_{\beta i}u^i\xi^\beta + \xi_\alpha^+D^\alpha{}_\beta{}^jv_j\xi^\beta. \quad (5.1)$$

For the interacting potential (5.1) the adiabatic condition is written as

$$\frac{\partial\Phi}{\partial v_j} = T_i^ju^i + S^{ij}v_i + \xi_\alpha^+D^\alpha{}_\beta{}^j\xi^\beta = 0. \quad (5.2)$$

As equation (5.2) is linear in the v-variable, it can be solved for v and replaced in equation (5.1), thus we obtain

$$\Phi(u, \xi, \xi^+) = \tfrac{1}{2}[R_{ij} - T_i^l(S^{-1})_{lk}T^k{}_j]u^iu^j + \xi_\alpha^+C^\alpha{}_\beta\xi^\beta + \xi_\alpha^+[B^\alpha{}_{\beta i} - D^\alpha{}_\beta{}^l(S^{-1})_{lk}T_i^k]u^i\xi^\beta$$
$$-\tfrac{1}{2}\xi_\alpha^+D^\alpha{}_\beta{}^k\xi^\beta(S^{-1})_{kl}\xi_\gamma^+D^\gamma{}_\delta{}^l\xi^\delta. \quad (5.3)$$

Taking $D = 0$ in equation (5.3), the resulting expression for the interacting potential reduces to that used in the Fröhlich model. This situation implies that the interaction between the electrons and the shell displacements is not taken into account, i.e. the interaction between electrons and the electronic deformability of atoms is neglected. As we can see from equation (5.3), for D different from zero, two new terms are present in the potential. One of these is a Fröhlich-type electron–phonon interaction term. The other term gives rise to electron–electron interaction. Thus, in our model it is shown how the inclusion of interactions between electrons and shell displacements gives rise to effective electron–phonon and electron–electron interactions.

Finally, we remark that the attainment of the effective potential (5.3) was possible because the adiabatic condition (2.2*b*) is linear in the variable v. For more general cases in which the adiabatic condition is not linear in v, it is not possible to obtain $v = v(u)$ explicitly. It is for these cases that the perturbative method developed in section 4, takes its full relevance.

6. Some possible applications of the ESM

As has been already pointed out, the ESM contains explicitly the interaction between mobile electrons and electronic degrees of freedom corresponding to deformabilities of ionic electron clouds. Therefore, the usefulness of the ESM should be apparent in cases where these interactions are relevant and cannot be appropriately incorporated in the Fröhlich Hamiltonian.

At present we have envisaged several possible applications of the ESM. Among them we mention the following:

(i) It is well known that intermediate valence compounds such as SmS, present pronounced anomalies in the phonon dispersion curves [18]. Several such anomalies can be satisfactorily explained by means of a breathing shell model [19], or a damped breathing shell model [20].

In a breathing shell model, variations of ionic radius of the intermediate valence ions are simulated by using a variable shell radius as a degree of freedom. A damping term accounts for the strong coupling between f and band electrons.

The ESM can also be used for the case in which the shell coordinate is a breathing one. Thus, we think that the presence of electron–shell interaction terms in the ESM

can more naturally account for such anomalies than the *ad hoc* introduction of an energy dispersion mechanism.

(ii) The inelastic neutron scattering in La_2CuO_4 shows a non-phononic extra branch [21]. In the framework of a nonlinear breathing shell model with a double-well core–shell interaction it has been recently shown that the extra excitation is due to valence fluctuations of the copper ions [22].

On the other hand it has been observed that the anomalous excitation is the only one significantly affected by the injection of carriers through doping [23]. In these conditions we can expect the dressing of the double-well interaction, owing to the interaction of the shell with carriers, thus leading to renormalization of the extra branch.

(iii) Another important problem was considered recently by Overhauser [24], who has shown how the transverse collective shell vibration mechanism might contribute significantly to the quest for a high-Tc superconductor. The ESM could also be useful in the examination of this problem.

It is well known that starting from the usual electron–phonon interaction theory, the phononic degrees of freedom can be eliminated by means of a unitary transformation [25]. Thus an effective Hamiltonian where the electrons interact attractively can be found. This concept leads to conventional low-temperature superconductivity.

Now, looking at the expression (5.3) for the potential we see that the first three terms on the right-hand side are of the same type as those appearing in the usual electron–phonon interaction theory. Therefore, these terms, once the degree of freedom of the phonons are eliminated, will give an attractive electron–electron interaction. The last term appearing in equation (5.3) gives rise to an additional attractive interaction between electrons, which reinforces the interaction arising from the first three terms. As Tc depends significantly on attractive electron–electron interaction, we can expect that the presence of this term in the potential (5.3) yields a higher allowable Tc content. Investigations in this direction are under consideration.

7. Conclusions

In this paper we have presented an ESM in which, besides the interaction between electrons and rigid ion vibrations, we have considered the interaction of electrons and ionic shell deformations. To simulate this effect in the shell model we allow for the interaction of cores and shells with electronic degrees of freedom.

Since the shell model is a constrained Hamiltonian system, the electronic degrees of freedom cannot be incorporated at a quantum level in a simple way, as is done in the Fröhlich model. Thus, we have constructed our model by incorporating these degrees of freedom at a classical level as Grassmann variables. We have analysed the classical dynamics of the model and later on its quantization via Dirac brackets was carried out. The non-trivial commutation relations (3.12) and (3.13) reveal the difficulty for the quantum treatment of the model.

Subsequently, by starting with the path integral representation of the model partition function, a perturbative method was constructed. This method is useful to evaluate several properties in solid state physics at finite temperature. The use of the perturbative method is essential in the case in which the presence of anharmonic coupling in the interaction potential Φ does not allow the use of the adiabatic condition to solve for the shell coordinate v.

Moreover, for a particular expression of the interaction potential we can recover the Fröhlich model. When the shell coordinate is removed, terms of the form $\xi^{+}u\xi$ which reinforce the Fröhlich ones appear. Also, electron–electron interaction terms are present in this simplest case.

Finally, some possible applications of our formalism were highlighted.

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