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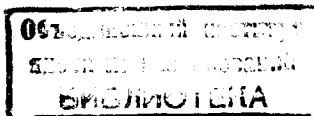J-23

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D. Janssen, R.V. Jolos

GENERATOR COORDINATE METHOD AND DERIVATION OF THE COLLECTIVE HAMILTONIAN

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I. INTRODUCTION

Recently a great deal of experimental information has been accumulated about low-lying collective quadrupole states in spherical, translational and deformed nuclei on the basis, in general, of studying the (HI, xn) reactions, Coulomb excitation and two-nucleon transfer reactions.

This information may be splitted into two parts, though not always strictly enough. The first one concerns the collective states constructed on the nucleus ground state. Though it is difficult to formulate the experimental criteria the use of which enables one to say surely that a given state is built up from the ground one, by the latter we will mean that this state is based on the same self-consistent field as the ground state of a nucleus. The complication of description of such states, especially in transitional nuclei, is due to that the nature of the collective motion in them is transitional between vibrational and rotational one.

The second part includes the information on collective quadrupole states constructed from two-quasiparticle states or those with an equilibrium deformation different from that of the ground state. To describe such states it is necessary to introduce explicitly the two-quasiparticle degrees of freedom or collective quadrupole variables of a structure other than those which specify the collective quadrupole excitation constructed from the ground state.

It is not excluded, however, that even in the states we have related to the first group there occurs, with increasing excitation energy, a gradual change of microscopic structure of the collective quadrupole variable.

A method we shall propose makes it possible to construct the collective Hamiltonian in the case of small change of the microscopic structure of the collective variable with increasing excitation energy. As will be shown, this collective Hamiltonian possesses a simple structure and depends on a small number of coefficients which can be calculated microscopically. Having a sufficient experimental information on properties of the collective excitations we can test the validity of the assumption about invariability of the microscopic structure of the collective variable. In the case of a noticeable change of the above structure with increasing excitation energy one can make use of the constructed below boson images of Fermi operators together with the proposed in /1/ method for constructing the corrections to the collective Hamiltonian.

Moreover, in the cases when it is important to allow for the two-quasiparticle excitations, our method permits these new degrees of freedom to be included in a natural way into consideration.

II. MATRIX ELEMENTS OF QUADRUPOLE FERMION OPERATORS

1. Basic Assumption

As a wave function of the collective states we assume to employ the wave function of the method of generator coordinates. The general form of such a function is as follows:

$$\psi = \int \prod_i dx_i \, F(x) \, \exp\{\sum_{\alpha\beta} f_{\alpha\beta}(x) \, a_\alpha^+ a_\beta^+ \} \, | 0>\ , \qquad (1)$$

where a_α^+, a_β^+ are the Fermi quasiparticle operators, $a_\alpha | 0> = 0$. The equation for the weight function $F(x)$ can be found by using the variational principle

$$\delta <\psi | \hat{H} - E | \psi> = 0\ . \qquad (2)$$

If the number of parameters x_i equals the number of all possible two-quasiparticle excitations, i.e., all the coefficients $f_{\alpha\beta}$ are independent, then a solution of eq. (2) is equivalent to the exact solution of the Schrödinger equation.

If the number of parameters x_i is considerably smaller and we use, e.g., the deformation variables β and γ only, eq. (2) is equivalent to diagonalization of the Hamiltonian just in the space of internal collective states.

Note also that to solve numerically eq. (2) with the wave functions (1) dependent on two parameters requires very much calculations, thus effective approximate methods for calculating such functions are necessary.

To describe the spherical and transitional nuclei one should employ the generator functions with five parameters β, γ and three Euler angles or, the same, as five parameters the components of the quadrupole tensor $a_{2\mu}$ may be used.

Then the wave function can be searched in the following form

$$\psi = \int da_{-2} \ldots da_2 F(a) \, \exp\{\sum_\mu a_\mu^* A_\mu^+ \} \, | 0>\ , \qquad (3)$$

where

$$A_\mu^+ = \sum_{a,b} \phi_{a,b} <j_a m_a j_b m_\beta | 2\mu> a_\alpha^+ a_\beta^+\ .$$

That the amplitudes $\phi_{a,b}$ are independent of a_μ corresponds to the assumed constancy of the microscopic structure of the excitation collective branch. If as $\phi_{a,b}$ the following amplitudes

$$\phi_{a,b} = \frac{1}{\sqrt{5}} \frac{<a || r^2 Y_2 || b> (u_a v_b + v_a u_b)}{E_a + E_b}$$

are taken and the parameters a_μ are fixed as follows: $a_{\mu \neq 0} = 0$, $a_0 = \delta$ then $\exp\{\sum_\mu a_\mu^* A_\mu^+ \} | 0>$ will be the Nilsson wave function of small values of the deformation parameter δ.

When using the Tamm-Dankoff method for determining structure of the collective variables the coefficients $\phi_{a,b}$ are of the form

$$\phi_{a,b} = \frac{1}{\sqrt{5}} \frac{<a \| r^2 Y_2 \| b> (u_a v_b + v_a u_b)}{E_a + E_b - \omega},$$

where ω is the frequency of the collective vibrations.

The fact that we have taken the form (3) of the wave function means that we try to diagonalize the Hamiltonian not in the whole fermion space but only in that constructed from the binary quadrupole fermion operators A_μ^+. Since this space is rather important for the proposed method we would like to consider it in more detail.

2. The Space of Quadrupole Fermion Operators and the Pauli Principle

First we briefly consider properties of the space of states of quadrupole boson operator $b_{2\mu}^+$. These operators obey the following commutation relations:

$$[b_{2\mu}, b_{2\mu'}^+] = \delta_{\mu\mu'}, \quad [b_\mu, b_{\mu'}] = 0.$$

Each boson state is determined uniquely by five quantum numbers. In problems of nuclear theory as these ones it is suitable to use the eigenvalues of the following five operators:

$$\hat{N}_B = \sum_\mu b_{2\mu}^+ b_{2\mu}, \quad \hat{I}_B^2 = 10 \sum_\mu (-)^\mu (b_2^+ b_2)_{1\mu} (b_2^+ b_2)_{1-\mu}$$

$$(\hat{I}_B)_z = \sqrt{10} \, (b_2^+ b_2)_{10}$$

$$\hat{T}_B^2 = 2 \{\sum (b_2^+ b_2)_{3\mu} (b_2^+ b_2)_{3-\mu}(-)^\mu + \sum (b_2^+ b_2)_{1\mu} (b_2^+ b_2)_{1-\mu}(-)^\mu\}$$

$$\hat{\Omega} = \sum ((b_2^+ b_2)_3 (b_2^+ b_2)_1)_{2\mu} ((b_2^+ b_2)_3 (b_2^+ b_2)_1)_{2\mu} (-)^\mu$$

the physical meaning of the operators $\hat{N}_B$, $\hat{I}_B^2$, $(\hat{I}_B)_z$ is well-known. The eigenvalues of $\hat{T}_B^2$ can be written as follows:

$$v(v+3),$$

where v is a positive integer called seniority. The operator $\hat{T}_B^2$ commutes with the Bohr-Mottelson collective Hamiltonian provided the potential energy does not depend on γ. In this case the seniority is a good quantum number. The operator $\hat{\Omega}_B$ is of need only for complete defining of physical boson states. The states thus constructed will be written in the following manner

$$\psi_B = | N \, v \, \omega \, I M). \tag{4}$$

In the basic (4) one may find the analytical form for matrix elements $(N v \omega I M | b_{2\mu}^+ | N' v' \omega' I'M)$[2].

Consider now the state space constructed from the quadrupole fermion operators

$$|0>, \quad A_{\mu_1}^+ |0>, \quad A_{\mu_1}^+ A_{\mu_2}^+ |0>, \quad A_{\mu_1}^+ A_{\mu_2}^+ A_{\mu_3}^+ |0>, \ldots$$

As all the operators A_μ^+ commute with each other and all the five ones are independent then we in principle can define uniquely the operators $\hat{N}_F$, $\hat{I}_F^2$, $(\hat{I}_F)_z$, $\hat{T}_F^2$, $\hat{\Omega}_F$ from the requirement that they operate on the fermion states $|\mu_1 \mu_2 \cdots \mu_n> \equiv A_{\mu_1}^+ A_{\mu_2}^+ \ldots A_{\mu_n}^+ |0>$ in the same way as the operators $\hat{N}_B$, $\hat{I}_B^2$, $(\hat{I}_B)$, $\hat{T}_B^2$, $\hat{\Omega}_B$ on the corresponding boson states $|\mu_1 \mu_2 \cdots \mu_n) = b_{2\mu_1}^+ b_{2\mu_2}^+ \ldots b_{2\mu_n}^+ |0)$, i.e., the set of the fermion states $|\mu_1 \mu_2 \cdots \mu_n>$ is equivalent to that of the fermion states $|N v \omega I M>$. Thus a correspondence can be established between the fermion and boson vectors of states.

However, a profound difference exists between the fermion and boson basis. The number of boson states $|N v \omega I M>$ is infinite while that of fermion states constructed from quadrupole fermion operators is limited if the space of one-particle fermion states is finite. This is a result of the Pauli principle. So, to every fermion state $|N v \omega I M>$ one can make correspond a boson state, but not vice versa. The boson states to which one can make correspond the fermion states form the physical subspace in the whole boson space. The boundaries of the physical subspace depend on the amplitudes $\phi_{a,b}$.

The next section is devoted to determination of these boundaries for arbitrary amplitudes $\phi_{a,b}$ and to calculation of matrix elements of the Fermi operators.

3. Calculation of Matrix Elements of the Fermi Operators

a. The wave function ψ is searched in the following form:

$$\psi = \int \prod_\mu d a_\mu F(a) |a>,$$

where

$$|a> = \exp\{\sum_\mu a_\mu^* A_\mu^+\} |0>.$$

The variational principle (2) results in the following equation

$$\int \prod_\mu d a_\mu' <a|H-E|a'> F(a') = 0. \qquad (5)$$

If we could be able to write $<a|H|a'>$ in the form

$$\hat{h}(a_\mu, \frac{d}{d a_\mu}) <a|a'>$$

then instead of eq. (5) we would obtain:

$$\{\hat{h}(a_\mu, \frac{d}{da_\mu}) -E\} \int \prod_\mu d a_\mu' F(a') <a|a'> = 0.$$

Thus, we have found the Schrödinger equation for the collective Hamiltonian $\hat{h}(a_\mu, d/da_\mu)$. The function

$$\int \prod_\mu d a_\mu' F(a') <a|a'> = \phi_{coll}(a)$$

serves as the collective wave function.

Next we proceed to construction of $\hat{h}(a_\mu, \frac{d}{da_\mu})$. First consider the matrix elements:

$$<a|A_\mu|a'> \quad \text{and} \quad <a|A_\mu^+|a'>$$

$$<a|A_\mu|a'> = <0| \exp\{\sum_\nu a_\nu A_\nu\} A_\mu |a'> = \frac{d}{da_\mu} <a|a'>$$

$$<a|A_\mu^+|a'> = <0 \exp\{\sum_\nu a_\nu A_\nu\} A_\mu^+ |a'>$$

$$= a_\mu <a|a'> + \frac{1}{2} \sum_{\nu\nu'} a_\nu a_{\nu'} <a|[A_\nu,[A_{\nu'},A_\mu^+]]|a'>$$

$$= (a_\mu - (\frac{1}{L} + \frac{1}{K+L}) a_\mu \sum_\nu a_\nu \frac{d}{da_\nu} - \frac{1}{2L(K+1)} \sum_\nu (-)^\nu a_\nu a_{-\nu} (-)^\mu \frac{d}{da_{-\mu}}$$

$$+ \frac{1}{R} [a_\mu, \hat{1}^2] + \dots) <a|a'>,$$

where the coefficients K, L and R are expressed via the amplitudes ϕ_{ab}*. The explicit form of these coefficients will be found below.

So we have derived the following boson representations of A_μ and A_μ^+:

$$A_\mu \rightarrow \frac{d}{da_\mu} \qquad (6)$$

$$A_\mu^+ \rightarrow a_\mu - (\frac{1}{L} + \frac{1}{K+1}) a_\mu \sum_\nu a_\nu \frac{d}{da_\nu} - \frac{1}{2L(K+1)} \sum_\nu (-)^{\nu+\mu} a_\nu a_{-\nu} \frac{d}{da_{-\mu}}$$

$$+ \frac{1}{R} [a_\mu, \hat{1}^2] + \dots \qquad (7)$$

In what follows we shall make use of the change

$$a_\mu \rightarrow b_{2\mu}^+, \quad \frac{d}{da_\mu} \rightarrow b_{2\mu}, \qquad (8)$$

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* The normalization $\sum_{a,b} (\phi_{ab})^2 = \frac{1}{2}$ has been used here.

where $b_{2\mu}^+$, $b_{2\mu}$ are the boson operators, which keeps valid the commutation relations. The expression obtained by substituting (8) into (7) is denoted as $B_{2\mu}^+$. Boson representations (6) and (7) are representations of the Dyson type. These do not conserve Hermitean conjugation of the operators A_μ and A_μ^+ in the usual boson metric, since $b_{2\mu}^+ \neq B_{2\mu}^+$. However, as will be shown, the hermitean conjugation of the boson images of A_μ and A_μ^+ can be easily reproduced.

Since $[A_\mu^+ , A_{\mu'}^+] = 0$ we require that $[B_{2\mu}^+ , B_{2\mu'}^+] = 0$. (9)

In the infinite series (7) in addition to the first four terms we keep only the terms which are necessary for fulfilling condition (9)

If $K \to \infty$ and $R \to \infty$ then, as can be easily checked, the expression

$$B_{2\mu}^+ = b_{2\mu}^+ \{ 1 - \frac{1}{L} \sum_\nu b_{2\nu}^+ b_{2\nu} \} \tag{10}$$

obeys the condition (9).

If $R \to \infty$ only, then the condition (9) also can be satisfied by keeping in (7) a finite number of terms:

$$B_{2\mu}^+ = b_{2\mu}^+ - (\frac{1}{L} + \frac{1}{K+1}) b_{2\mu}^+ \sum_\nu b_{2\nu}^+ b_{2\nu} - \frac{1}{2L(K+1)} \sum_\nu (-)^{\nu+\mu} b_{2\nu}^+ b_{2-\nu}^+ b_{2-\mu}$$

$$+ \frac{1}{L(K+1)} b_{2\mu}^+ (\sum_\nu b_{2\nu}^+ b_{2\nu})^2 - \frac{1}{2L(K+1)} \sum_\nu (-)^\nu b_{2\nu}^+ b_{2-\nu}^+ \sum_{\nu'} b_{\nu'}^+ b_{\nu'} (-)^\mu b_{2-\mu}$$

$$\equiv B_{2\mu}^+ (L,K). \tag{11}$$

If all the three coefficients L, K and R are finite, then the condition (9) cannot be satisfied by taking (7) as a finite series. Nevertheless, as is verified easily, this condition can be satisfied by writing $B_{2\mu}^+$ in the form:

$$B_{2\mu}^+ = F^{-1} (\frac{\hat{I}^2}{R}) B_{2\mu}^+ (K,L) F (\frac{\hat{I}^2}{R}) \frac{1}{F(6/R)}, \tag{12}$$

where F is an arbitrary function.

The factor $1/F(6/R)$ is inserted in order that the coefficient for $b_{2\mu}^+$ remains to be equal to unity.

The operator $B_{2\mu}^+ (K,L)$ can be represented in the form

$$B_{2\mu}^+ (K,L) = \Phi^{-1} b_{2\mu}^+ \Phi , \tag{13}$$

where Φ is the Hermitean operator diagonal in basis (4) which matrix elements depend on N and ν only. These matrix elements can be found if one calculates and compares the matrix elements from expressions (11) and (13). As a result we arrive of the following relations

$$\frac{\Phi(N,\nu)}{\Phi(N+1,\nu+1)} = (1 - \frac{(N+\nu)}{2K}) (1 - \frac{N}{L})$$

$$\tag{14}$$

$$\frac{\Phi(N,\nu)}{\Phi(N+1,\nu-1)} = (1 - \frac{N}{L}) (1 - \frac{N-\nu-3}{2K})$$

From relations (14) the shape of Φ can be restored.

Thus, we have found the following boson representations of A_μ^+ and A_μ :

$$A_\mu \to b_{2\mu}$$

$$A_\mu^+ \to F^{-1} \Phi^{-1} b_{2\mu}^+ \Phi F . \tag{15}$$

As was noted above, this representation does not maintain the Hermitean conjugation properties of these operators. The latter requirement is satisfied by the following boson representation

$$A_\mu \to F^{1/2} \Phi^{1/2} b_{2\mu} \Phi^{-1/2} F^{-1/2}$$

$$\tag{16}$$

$$A_\mu^+ \to F^{-1/2} \Phi^{-1/2} b_{2\mu}^+ \Phi^{1/2} F^{1/2}$$

If we consider the quantity R to be large relative to the nucleus spin I then we may expand F into a series and from (16), (14) we obtain the following expressions of matrix elements of A_μ^+

$$\langle I+2,v+1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I+2,v+1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1 - \frac{N}{L})(1-\frac{(N+v)}{2K})(1-\frac{2I}{R})}$$

$$\langle I+1,v+1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I+1,v+1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1 - \frac{N}{L})(1-\frac{(N+v)}{2K})(1-\frac{(2I-1)}{2R})}$$

$$\langle Iv+1,N+1 | A_\mu^+ | IvN \rangle = (I,v+1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1-\frac{N}{L})(1-\frac{(N+v)}{2R})}$$

$$\langle I-1,v+1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I-1,v+1,N+1 | b_{2\mu}^+ (IvN)\sqrt{(1 - \frac{N}{L})(1-\frac{(N+v)}{2K})(1-\frac{(2I-3)}{2R})}$$

$$\langle I-2,v+1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I-2,v+1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1-\frac{N}{L})(1-\frac{(N+v)}{2K})(1-\frac{(2I-4)}{R})}$$

$$\langle I+2,v-1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I+2,v-1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1-\frac{N}{L})(1-\frac{N-v-3}{2K})(1-\frac{2I}{R})}$$

$$\langle I+1,v-1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I+1,v-1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1 - \frac{N}{L})(1 - \frac{(N-v-3)}{2K})(1-\frac{(2I-1)}{2R})}$$

$$\langle I,v-1,N+1 | A_\mu^+ | IvN \rangle = (I,v-1,N+1 | b_{2\mu}^+ | InV)\sqrt{(1-\frac{N}{L})(1-\frac{(N-v-3)}{2K})}$$

$$\langle I-1,v-1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I-1,v-1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1-\frac{N}{L})(1-\frac{(N-v-3)}{2K})(1-\frac{(2I-3)}{2R})}$$

$$\langle I-2,v-1,N+1 | A_\mu^+ | IvN \rangle \;=$$

$$= (I-2,v-1,N+1 | b_{2\mu}^+ | IvN)\sqrt{(1 - \frac{N}{L})(1 - \frac{(N-v-3)}{2K})(1-\frac{(2I-4)}{R})}$$

$$(17)$$

b. From (17) it is seen immediately that the boundaries of the phycical region in the whole boson space are determined by values of the constants K and L. On Figures la,b,c the boundaries of the physical regions are shown for the cases:

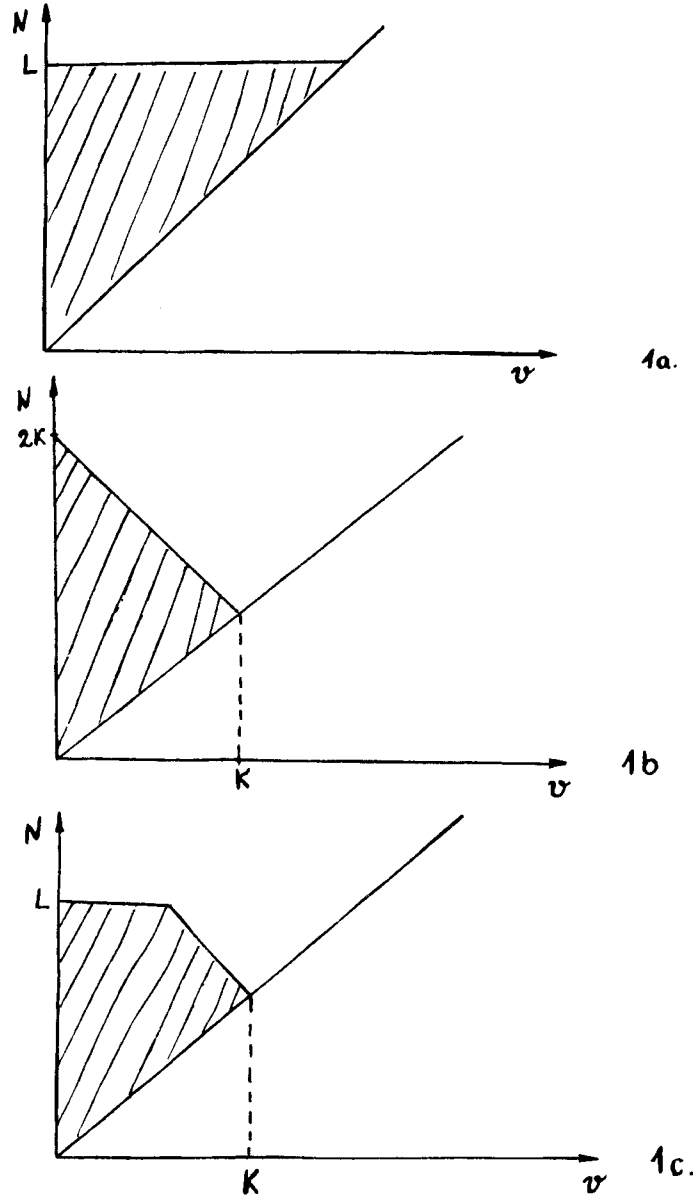$$\text{a) } L \leq K \qquad \text{b) } 2K \leq L \qquad \text{c) } K < L < 2K \qquad (18)$$

Fig. 1. The boundaries of the physical regions: a) $L \leq K$
b) $2K \leq L$ *c)* $K < L < 2K$.

The constants L, K and R are defined from condition

$$< 0 | (AA)_{IM} (A^+ A^+)_{IM} | 0 > = (0 | (b_2 b_2)_{IM} (B_2^+ B_2^+)_{IM} | 0)$$

$$= \frac{1}{F^{-2}(\frac{6}{R})} \times (0 | (b_2 b_2)_{IM} \frac{1}{F(\frac{I^2}{R}) \Phi(N,v)} (b_2 b_2)_{IM} | 0)$$

$$= \frac{1}{F^{-2}(\frac{6}{R})} \frac{2}{F(\frac{(I+1)I}{R}) \Phi(2,v)}$$

$$\Phi(2,0) = \frac{1}{(1-\frac{1}{L})(1+\frac{3}{2K})} \qquad \Phi(2,2) = \frac{1}{(1-\frac{1}{L})(1-\frac{1}{K})} \qquad (19)$$

III. A METHOD FOR CONSTRUCTION OF THE COLLECTIVE HAMILTONIAN

Since we have confined the consideration to the space of state vectors constructed from binar quadrupole fermion operators A_μ^+, then to construct the collective Hamiltonian by the method developed in sect. 3 we first must find out an approximate expression for the fermion Hamiltonian in terms of the operators A_μ, A_μ^+ and $[A_\mu, A_{\mu'}^+]$. To this end one can use the following prescription:

$$a^+ a \rightarrow g \ [A, A^+]$$

$$a^+ a^+ aa \rightarrow g_1 [A, A^+] \times [A, A^+] + g_2 A^+ A$$

$$a^+ a^+ a^+ a \rightarrow g_3 A^+ \times [A, A^+]$$

$$a^+ a^+ a^+ a^+ \rightarrow g_4 A^+ A^+. \qquad (20)$$

We obtain the coefficients g_K equating the matrix elements of both sides of the relations (20) taken between the states $|0>$, $A_\mu^+|0>$, $A_\mu^+ A_\mu^+|0>$. Then the equation (17) can be used for constructing the collective Hamiltonian.

IV. KINEMATICAL INTERACTION

From eq. (17) for the matrix elements of the fermion operators A_μ^+ , A_μ it is seen, that the fermion operator matrix elements are equal to that of the boson one, multiplied by a definite factor. This factor being dependent on K, L, R produces an additional effective interaction in the boson space, which is due to the Pauli principle for fermions. This interaction will be called kinematical interaction. Let us look now at the following Hamiltonian

$$H = C_1 \sum_\mu [A_\mu, A_\mu^+] + c_2 \sum A_\mu^+ A_\mu \qquad (21)$$

If we assume that $K = L = R = \infty$, then the kinematic interaction vanishes. In this case we neglect the Pauli principle and the Hamiltonian spectrums (21) is the one simply equidistant, i.e.,

$$E_N = 5c_1 + c_2 N \qquad (N = 0,1,2,...) .$$

If K, L, R are finite, from (17), (21) we get:

$$E_{N,v,I} = c_1 \{ 5(1 - \frac{6}{R}) - \frac{N}{L(K+1)} [6L + 6K + 7 + \frac{6}{R}(2LK - 2L - 4K - 3)]$$

$$+ \frac{6N^2}{L(K+1)}(1 + \frac{2}{R}(K + L)) - \frac{12N^3}{RL(K+1)} + \frac{(N(N+3)-v(v+3))}{2L(K+1)}(1 - \frac{6}{R})$$

$$- \frac{2I(I+1)}{RL(K+1)}(3N - K - L - 2) \}$$

$$+ c_2 \{ 5(1 - \frac{6}{R}) + N(1 - \frac{6}{R}) \frac{1}{L(K+1)}(LK - 4L - 5K - 5) -$$

$$- N^2(1 - \frac{6}{R}) \frac{(K+L-3)}{L(K+1)}(1 - \frac{6}{R})$$

$$- \frac{(N(N+3)-v(v+3))}{2L(K+1)}(1 - \frac{6}{R})N - \frac{2I(I+1)}{RL(K+1)}(KL + L - N(L+K) + N^2) \} .$$

$$(22)$$

It is clear that one can obtain characteristic spectra of the vibrational or rotational type depending on the choice of constants L, K and R. Thus, the energy deviation off its equidistancy can arise even from the existence of the kinematical interaction, that means from the action of the Pauli principle.

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