DESCRIPTION OF ANHARMONICITIES IN A SOLVABLE MODEL BY THE GENERATOR COORDINATE METHOD

Maria Helena Caldeira and Célia A. de Sousa
Laboratório de Física, Universidade de Coimbra,
Coimbra, Portugal

1. INTRODUCTION

In real nuclei with well-defined vibrational levels, degenerate states appear which are interpreted as simultaneous excitation of two (or more) vibrational quanta.

The interpretation of the vibrational spectrum of these nuclei, in particular the ordering and splitting of quasi-degenerate two-phonon levels from a microscopic point of view, is a problem of considerable interest |1|.

In the harmonic approximation, two-phonon levels are degenerate in spherical nuclei. The degeneracy is removed by the anharmonic terms in the Hamiltonian.

By applying the ideas of ref. |2| to the soluble model of Moszkowsky, we shall demonstrate in the present work that the boson expansion technique based on the generator coordinate method (G.C.M.) enables us to construct on a microscopic basis the correct collective Hamiltonian including anharmonic terms. The advantage of using a soluble model for testing an approximation method lies, of course, in the perfect knowledge of the microscopic Hamiltonian, so that no lack of agreement between the approximate and the exact result may be attributed to an insufficient knowledge of the forces.

The Moszkowsky model has some features very similar to real nuclei. This is a consequence of the invariance of the model with respect to rotations around the z axes and of the existence of Hartree-Fock solutions which may be deformed or non-deformed according to the

value of the coupling constant. When the non-deformed solution is the stable one, the model presents two normal vibrational modes with angular momenta $m=\pm 1$. We shall see, for this model, that even at the transition point (i.e., the point which separates the region where the non-deformed solution is stable from the region where the deformed solution is stable, or in other words, the point for which the frequency of the collective oscillation becomes zero in the harmonic approximation) the inclusion of the anharmonic terms of lowest order (containing three and four boson operators) is sufficient to obtain a satisfactory description of the energy spectrum.

Having in mind the complication which would arise when applying the method proposed here to realistic situations, we thought that it might be useful to investigate possible simplifications.

A simplified version of our method, described in sec. 3, consists essentially in treating the collective kinetic energy in the harmonic approximation, and in considering only those anharmonic terms which arise from the expansion of the potential energy, for an appropriate definition of the collective variables.

2. BRIEF DESCRIPTION OF THE MOSZKOWSKY MODEL

The Moszkowsky model is a two-level model with two different kinds of particles, 2j of a type, a, and 2j of another type, b.

The Hamiltonian of the system may be written in the following form:

$$H = T_z(a) - T_z(b) + V(T_x^2 + T_y^2) \quad , \qquad \text{(ref. [3])}$$

where T_x, T_y and T_z are operators which obey the commutation relations of the angular momentum operators.

We define $|\Phi_o>$, the lowest energy state for V=0, as

$$T_+(b)|\Phi_o> = 0 ,$$
$$T_-(a)|\Phi_o> = 0 ,$$

where

$$T_+(\mu) = T_x(\mu)+iT_y(\mu)$$
$$T_-(\mu) = T_x(\mu)-iT_y(\mu) \quad .$$

with μ=a,b

We also define

$$T_z(a)|\Phi_o> = -j|\Phi_o>$$
$$T_z(b)|\Phi_o> = j|\Phi_o> .$$

We notice that

$$T_\eta = T_\eta(a)+T_\eta(b) ,$$

with η=x,y,z,+,-.

3. DESCRIPTION OF THE METHOD

Application to the Moszkowsky model

The method used in this work is the generator coordinate method (G.C.M.) with harmonic and Gaussian overlap approximations.

We have taken the generator wave function |4|

$$|\Phi(\alpha,\beta)> = e^{\alpha T_+(a)+\beta T_-(b)} |\Phi_o> , \qquad (3.1)$$

where the parameters α and β are the generator coordinates.

Then, we could construct the trial wave function:

$$|\Psi> = \int |\Phi(\alpha', \beta')> f(\alpha', \beta') \, d\alpha' d\beta' , \qquad (3.2)$$

where the weight function $f(\alpha', \beta')$ can be determined variationally.

It may be observed that the parameters α and β enter into the Moszkowsky model on very similar terms, i.e., if we replace β by α and β' by α', the overlap kernels remain

invariant.

In this model, these parameters play an analogous role to the coordinates α_μ^2 (μ = -2, -1, 0, 1, 2) which usually describe quadrupole deformations in spherical nuclei.

We expand the overlap kernel

$$I(\alpha',\beta',\alpha,\beta) = \langle\Phi(\alpha',\beta')|\Phi(\alpha,\beta)\rangle$$

up to fourth order and we make the Gaussian approximation simultaneously |2|. So it becomes

$$I(\alpha',\beta',\alpha,\beta) = e^{s(\alpha'\alpha+\beta'\beta)}\left[1+s^2F(\alpha'^{-2}\alpha^2+\beta'^{-2}\beta^2)\right] \quad (3.3)$$

It turns out that α and β are of the order of $1/\sqrt{s}$ and s^2F is of the order of s. The parameter s is related to the number of particles. Explicitly we have: $s = 2j$ and $s^2F = -j$.

By expanding the kernel up to fourth order

$$K(\alpha',\beta',\alpha,\beta) = \frac{\langle\Phi(\alpha',\beta')|H|\Phi(\alpha,\beta)\rangle}{\langle\Phi(\alpha',\beta')|\Phi(\alpha,\beta)\rangle},$$

where H is the Hamiltonian, we obtain

$$\begin{aligned} K(\alpha',\beta',\alpha,\beta) = {} & E_o+sA(\alpha'\alpha+\beta'\beta)+sB(\alpha'\beta'+\alpha\beta) \\ & +s^2C(\alpha'^{-2}\alpha^2+\beta'^{-2}\beta^2)+s^2D(\alpha\beta^2\beta'+\alpha^2\beta\alpha' \\ & +\alpha'^{-2}\beta'\alpha+\beta'^{-2}\alpha'\beta) \end{aligned} \quad (3.4)$$

where

$$A = 1 - \frac{V}{2} - jV \qquad D = \frac{V}{2}$$

$$B = jV \qquad E_o = j(V-2)$$

$$C = \frac{1}{2j}(V-1-2jV)$$

If we call E the energy eigenvalue associated with $f(\alpha',\beta')$, the Hill-Wheeler equation becomes, keeping terms up to order 1/s,

$$\int \{ sA(\alpha'\alpha+\beta'\beta)+sB(\alpha'\beta'+\alpha\beta)+s^2C(\alpha^2\alpha'^2+\beta^2\beta'^2)+s^2D(\alpha\beta^2\beta'$$

$$+\alpha^2\beta\alpha'+\alpha'^2\beta'\alpha+\beta'^2\alpha'\beta)+s^3AF(\alpha'\alpha+\beta'\beta)(\alpha^2\alpha'^2+\beta^2\beta'^2)$$

$$+ BF(\alpha'\beta'+\alpha\beta)(\alpha^2\alpha'^2+\beta^2\beta'^2)+(E_o-E)[1+s^2F(\alpha^2\alpha'^2+\beta^2\beta'^2)]\}$$

$$\exp\{s(\alpha'\alpha+\beta'\beta)\}f(\alpha',\beta')d\alpha'\,d\beta' = 0 \qquad (3.5)$$

Notice that as sA, sB, s^2D are of order s, the successive terms correspond to an expansion in powers of 1/s.

Following the method used by Jancovici and Schiff [5], which consists in introducing differential operators acting on functions of α and β

$$a = \frac{1}{\sqrt{s}}\frac{\partial}{\partial\alpha}\ ;\quad b = \frac{1}{\sqrt{s}}\frac{\partial}{\partial\beta}\ ;\quad a^+ = \sqrt{s}\,\alpha;\quad b^+ = \sqrt{s}\,\beta \qquad (3.6)$$

equation (3.5) is replaced by the differential equation

$$(\tilde{H}-E\tilde{N})\tilde{f}(\alpha,\beta) = 0 \qquad (3.7)$$

where $\tilde{H}$ and $\tilde{N}$ result from the replacement of the operators (3.6) in equation (3.5), so that

$$\tilde{H} = E_o[1+s^2F(a^{+2}a^2+b^{+2}b^2)]+A(a^+a+b^+b)+B(a^+b^++ab)$$

$$+ C(a^{+2}a^2+b^{+2}b^2) + D(a^+b^{+2}b+a^{+2}b^+a+a^+a^2b+b^+b^2a)$$

$$+ AF(b^+a^{+2}a^2b+a^{+3}a^3+b^{+3}b^3+a^+b^{+2}b^2a)+BF(a^{+2}ba^3+$$

$$+ b^{+2}b^3a+a^{+3}b^+a^2+b^{+3}a^+b^2) \qquad (3.8)$$

$$\hat{N} = 1+F(a^{+2}a^2+b^{+2}b^2)$$

and

$$\tilde{f}(\alpha,\beta) = \int e^{s(\alpha'\alpha+\beta'\beta)} f(\alpha',\beta')d\alpha'd\beta' \qquad (3.9)$$

We may observe that the equation (3.7) is not an equation of the conventional Schrödinger type, because of the appearance of the operator N. (See Appendix I).

We try to obtain an approximate solution of this equation by the variational method. An alternative could be to use perturbation theory, since anharmonic Hamiltonians cannot be diagonalized exactly. We consider the following standard canonical transformation

$$\left.\begin{aligned}\theta_1 &= xa-yb^+\\ \theta_2 &= xb-ya^+\end{aligned}\right\} \quad \text{with } x^2-y^2=1$$

We denote the vacuum of the operators θ_1 and θ_2 by $|\Psi(y)>$

$$\theta_1|\Psi(y)> = 0 \quad ,$$

$$\theta_2|\Psi(y)> = 0 \quad .$$

Now we construct the following basis which spans a subspace of the Hilbert space, which contains the vacuum state and states with one and two phonons, as required for our purpose,

$$|\Psi>,\ a|\Psi>,\ b|\Psi>,\ a^2|\Psi>,\ b^2|\Psi>,\ ab|\Psi> \ .$$

Then we try to diagonalize the Hamiltonian $\tilde{H}$ in this subspace keeping in mind the lack of orthonormality of the basis.

In this model, the diagonalization is greatly reduced, since there is only coupling between the vacuum state and the state $ab|\Psi>$.

So we can easily write the non-zero matrix elements of $\tilde{H}$. (See Appendix II).

The coupling between $|\Psi\rangle$ and $ab|\Psi\rangle$ which diagonalizes $\tilde{H}$ in the given subspace is easily found.

Finally, we have computed the minima of the energy eigenvalues (which are obviously functions of y).

The numerical results are shown in tables 1 (for 2V = -0.030) and 2 (for 2V = -0.036). The latter value 2V = -0.036, corresponds to the transition point where the RPA breaks down |4|.

TABLE 1

Energy levels near the transition point

2V=-0.030	n	m	Present approx.	Simplified method (sec. 4)	Exact
		2	-27.604	-27.589	-27.621
	2				
		0	-27.607	-27.564	-27.626
	1	1	-28.126	-28.088	-28.130
	0	0	-28.586	-28.564	-28.586

TABLE 2

Energy levels at the transition point

2V=-0.036	n	m	Present approx.	Simplified method (sec. 4)	Exact
		2	-28.042	-28.042	-28.130
	2				
		0	-28.090	-27.979	-28.164
	1	1	-28.504	-28.422	-28.536
	0	0	-28.814	-28.758	-28.821

4. SIMPLIFIED METHOD

The inclusion of anharmonic terms in the collective Hamiltonian is conceptually simple.

However, this may lead to quite a tedious piece of work. The classical analogy suggests that it might possibly be enough to expand the potential energy around the equilibrium point, that is to say, it should be enough to include anharmonic terms obtained from expanding the potential energy, around the equilibrium point, if the oscillations are adiabatic. The velocity of the collective motion will then be small and so it is enough to expand the Hamiltonian up to second order in velocity. In order to ensure the validity of this argument, it is important to define conveniently the coordinates because we might easily run into the undesirable situation in which we have non-adiabatic (large velocity), small amplitude oscillations instead of large amplitude, small velocity oscillations.

As we have said, with this method we want to provide a simplification of the method explained in the last section, by expanding only the part of the Hamiltonian that is easier to expand - the potential energy.

For this purpose, we have defined the generator coordinates so that in the harmonic approximation the two collective degrees of freedom of the Hamiltonian are separated. This is always possible.

At this point we used the family of wave functions

$$|\gamma\delta\rangle = \exp\{\gamma[T_+(a)+T_-(b)]+i\delta[T_+(a)-T_-(b)]\}|\Phi_o\rangle$$

which is equivalent to the family of wave functions we started with

$$|\Phi(\alpha,\beta)\rangle = e^{\alpha T_+(a)+\beta T_-(b)}|\Phi_o\rangle \qquad \text{(ref. |4|)}$$

It can be seen that the overlap integral is

$$\langle\gamma'\delta'|\gamma\delta\rangle = e^{4j(\gamma'\gamma+\delta'\delta)}[1-2j(\gamma'^2\gamma^2+\delta'^2\delta^2+2\gamma'\gamma\delta'\delta)]$$

so that the Jancovici-Schiff operators may be written as follows

$$a = \frac{1}{\sqrt{4j}} \frac{\partial}{\partial \gamma} , \qquad a^+ = \sqrt{4j}\, \gamma ,$$

$$b = \frac{1}{\sqrt{4j}} \frac{\partial}{\partial \delta} , \qquad b^+ = \sqrt{4j}\, \delta .$$

If we introduce the operators

$$Q_1 = \frac{a+a^+}{2\sqrt{4j}} , \qquad P_1 = -i(a-a^+)\sqrt{4j} ,$$

$$Q_2 = \frac{b+b^+}{2\sqrt{4j}} , \qquad P_2 = -i(b-b^+)\sqrt{4j} ,$$

this leads in the harmonic approximation to the Hamiltonian

$$H = E_o - A + 4j(A+B)\,(Q_1^2+Q_2^2) + \frac{1}{16j}(A-B)(P_1^2+P_2^2) .$$

Our choice of the generator coordinates is the correct one for considerations of adiabaticity, because in the appropriate scale for comparing P_i with Q_i we have $\langle P_i'^2 \rangle < \langle Q_i'^2 \rangle$, since

$$\langle P_1^2 \rangle = \langle P_2^2 \rangle = 4j(x-y)^2 ,$$

$$\langle Q_1^2 \rangle = \langle Q_2^2 \rangle = \frac{1}{16j}(x+y)^2 .$$

The appropriate scale is suggested by the Gaussian exponent and is given by

$$P_i' = \frac{P_i}{\sqrt{8j}} \quad \text{and} \quad Q_i' = \sqrt{8j}\, Q_i$$

Then, in the anharmonic situation it may be reasonable to expand only the potential energy (ref. |6|).

$$\frac{\langle\gamma\delta|H|\gamma\delta\rangle}{\langle\gamma\delta|\gamma\delta\rangle} = E_o+4j(A+B)(\gamma^2+\delta^2)+4jL(\gamma^4+\delta^4+2\gamma^2\delta^2)$$

where $L=V-1-4Vj$.

Finally, we may give the Hamiltonian the form

$$H = E_o-A + \frac{1}{16j}(A-B)(P_1^2+P_2^2)+4j(A+B)(Q_1^2+Q_2^2)$$

$$+ 4jL(Q_1^4+Q_2^4+2Q_1^2Q_2^2) .$$

To diagonalize the Hamiltonian, we used the same method as in the last section.

The subspace used is defined by the basis

$$|\Psi\rangle,\ Q_1|\Psi\rangle,\ Q_1Q_2|\Psi\rangle,\ (Q_1^2+Q_2^2)|\Psi\rangle .$$

Notice that this basis is equivalent to

$$|\Psi\rangle\ ,\ (Q_1\pm iQ_2)|\Psi\rangle,\ (Q_1\pm iQ_2)^2|\Psi\rangle,\ (Q_1^2+Q_2^2)|\Psi\rangle,$$

where $|\Psi\rangle$ is the vacuum of the operator A_i,

$$\left.\begin{aligned} A_i &= ixP_i + \frac{1}{2x}Q_i \\ A_i^+ &= -ixP_i + \frac{1}{2x}Q_i \end{aligned}\right\} \quad i=1,2$$

and is defined by

$$A_i|\Psi\rangle = 0\ , \qquad i = 1,2\ .$$

The minima, with respect to x, of the expectation values of the energy, obtained numerically, are also shown in tables I and II.

5. DISCUSSION

It may be seen by inspection of tables 1 and 2 that the anharmonic approximation considerably improves

the Hartree-Fock results of the ground-state energy even close to the transition point.

In the vibration region, the results we have obtained are in good agreement with the exact value.

The sequence of energy levels is correct. The value of the splitting is also in good agreement with the exact value, although at the transition point the results become slightly worse.

Although the simplified method considerably reduces calculational labor,it needs improvement, because it leads to worse results, since it does not reproduce the order of the two-phonon levels correctly.

However, the magnitude of the energies obtained by this method is quite good, even at the transition point.

So, we arrive at the conclusion that the splitting and order of the two-phonon levels is such a delicate effect that any type of rougher approximation may give rise to errors of the order of magnitude of the splittings between the two-phonon levels, so that such approximations should be taken with great caution.

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APPENDIX I

An equation of the conventional Schrödinger type holds for the Hamiltonian

$$\tilde{H}' = \tilde{N}^{-\frac{1}{2}} \tilde{H} \tilde{N}^{-\frac{1}{2}}$$

and for the wave functions

$$\tilde{f}'(\alpha,\beta) = \tilde{N}^{\frac{1}{2}} \tilde{f}(\alpha,\beta)$$

So we have the Schrödinger equation

$$(\tilde{H}'-E)\tilde{f}'(\alpha,\beta) = 0$$

instead of equation (3.7). Here

$$\tilde{H}' = E_o+A(a^+a+b^+b)+B(a^+b^++ab)+(C-2FA)(a^{+2}a^2$$

$$+b^{+2}b^2)+(D-FB)(a^{+2}ab^++a^+b^{+2}b+a^+a^2b+ab^+b^2)$$

where all the quantities have the same meaning as previously.

APPENDIX II

In this appendix we are going to write explicitly the non-zero matrix elements of $\tilde{H}$ and $\tilde{N}$.

For the collective Hamiltonian $\tilde{H}$ we have:

$$\langle\Psi|\tilde{H}|\Psi\rangle = E_o+4E_oFy^4+2Ay^2+2Bxy+16FAy^6$$

$$+ 8FB(x^2y^4+3xy^5)+4Cy^4+8Dxy^3$$

$$\langle\Psi|a^+\tilde{H}a|\Psi\rangle = E_oy^2+4E_oF(2y^6+x^2y^4)+A(3y^4+x^2y^2)+4Bx^3y$$

$$+ 4FA(10y^8+13x^2y^6+x^2y^4)+24FB(3xy^7+x^3y^5)$$

$$+4C(2y^6+x^2y^4)+4D(5xy^5+x^3y^3)$$

$$\langle\Psi|\tilde{H}ab|\Psi\rangle = E_oxy+12E_oFxy^5+4Axy^3+B(3x^2y^2+y^4)$$

$$+24FA(x^3y^5+3xy^7)+12FB(4x^2y^6+y^8)$$

$$+ 12Cxy^5+4D(5x^2y^4+y^6)$$

$$\langle\Psi|a^{+2}\tilde{H}a^{2}|\Psi\rangle = 2E_{o}y^{4}+4E_{o}F(7y^{8}+4x^{2}y^{6}+x^{4}y^{4})+4A(x^{2}y^{4}+2y^{6})$$
$$+ 12Bxy^{5}+4C(7y^{8}+4x^{2}y^{6}+x^{4}y^{4})+24D(3xy^{7}+x^{3}y^{5})$$
$$+ 24FA(7y^{10}+10x^{2}y^{8}+3x^{4}y^{6})+$$
$$+ 24FB(13xy^{9}+6x^{3}y^{7}+x^{5}y^{5})$$

$$\langle\Psi|a^{+}b^{+}\tilde{H}ab|\Psi\rangle = E_{o}(x^{2}y^{2}+y^{4})+4E_{o}F(3y^{8}+9x^{2}y^{6})+4A(y^{6}+2x^{2}y^{4})$$
$$+ 4B(x^{3}y^{3}+2xy^{5})+4C(3y^{8}+9x^{2}y^{6})+48D(xy^{7}+x^{3}y^{5})$$
$$+ 24FA(3y^{10}+14x^{2}y^{8}+3x^{4}y^{6})+96FB(2xy^{9}+3x^{3}y^{7}).$$

The corresponding elements of N are:

$$\langle\Psi|\tilde{N}|\Psi\rangle = 1 + 4Fy^{4}$$
$$\langle\Psi|a^{+}\tilde{N}a|\Psi\rangle = y^{2} + 4F(2y^{6}+x^{2}y^{4})$$
$$\langle\Psi|\tilde{N}ab|\Psi\rangle = xy + 12Fxy^{5}$$
$$\langle\Psi|a^{+2}\tilde{N}a^{2}|\Psi\rangle = 2y^{4}+4F(7y^{8}+x^{4}y^{4}+4x^{2}y^{6})$$
$$\langle\Psi|a^{+}b^{+}\tilde{N}ab|\Psi\rangle = x^{2}y^{2}+y^{4}+12F(y^{8}+3x^{2}y^{6}) \ .$$

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