Quantum Corrections to the Semiclassical Quantization of the SU(3) Shell Model[1]

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Abstract

We apply the canonical perturbation theory to the semi–quantal hamiltonian of the SU(3) shell model. Then, we use the Einstein–Brillowin–Keller quantization rule to obtain an analytical semi–quantal formula for the energy levels, which is the usual semi–classical one plus quantum corrections. Finally, a test on the numerical accuracy of the semiclassical approximation and of its quantum corrections is performed.

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In the last few years, there has been considerable renewed interest in the semi–classical approximation, due to the close connection to the problem of the so–called quantum chaos [1,2]. One important aspect is the semi–classical quantization formula of the energy levels for quasi–integrable systems [3,4].

It has recently been shown [5,6] that, for perturbed non–resonant harmonic oscillators, the algorithm of classical perturbation theory may also be used in the quantum–mechanical perturbation theory, with quantum corrections in powers of $\hbar$.

In this paper, on the contrary, we calculate the quantum corrections to the semi–classical quantization [3,4] of a many–body model related to nuclear physics. Its classical counterpart, obtained in the limit of the number of particles that goes to infinity, is represented by a non–integrable hamiltonian with two degrees of freedom [7,8,9,10]. The semi–classical quantization of this model has been studied in [7] and here we calculate the quantum corrections and then analyze their numerical accuracy.

The model is a three–level schematic nuclear shell model, whose hamiltonian is:

$$\hat{H} = \sum_{k=0}^{2} \epsilon_k \hat{G}_{kk} + \frac{V}{2} \sum_{k \neq l=0}^{2} \hat{G}_{kl}^2, \tag{1}$$

where

$$\hat{G}_{kl} = \sum_{m=1}^{M} \hat{a}_{km}^{+} \hat{a}_{lm} \tag{2}$$

are the generators of the SU(3) group. This model describes M identical particles in three, M–fold degenerate, single particle levels ϵ_i. There is a vanishing interaction for particles in the same level and an equal interaction V for particles in different levels. We assume $\epsilon_2 = -\epsilon_0 = \epsilon = 1$, $\epsilon_1 = 0$.

For the SU(3) model the semi–quantal hamiltonian [11] is defined as [8]:

$$H(p_1,p_2,q_1,q_2;M) =< q_1p_1,q_2p_2;M|\frac{\hat{H}}{M}|q_1p_1,q_2p_2;M>, \qquad (3)$$

where $|q_1p_1,q_2p_2;M>$ is the coherent state, given by:

$$|q_1p_1,q_2p_2;M>= \exp\left[z_1G_{01}+z_2G_{02}\right]|00>, \qquad (4)$$

with:

$$\frac{1}{\sqrt{2M}}(q_k+ip_k) = \frac{z_k}{\sqrt{1+z_1^*z_1+z_2^*z_2}}, \quad k=1,2 \qquad (5)$$

and $|00>=\Pi_{k=1}^{M}a_{0k}^{+}|0>$ is the ground state. Here $1/M$ plays the role of the Planck constant $\hbar$ [10].

As discussed in great detail in [10], the semi–quantal hamiltonian is:

$$H(p_1,p_2,q_1,q_2;M) = -1+\frac{1}{2}(p_1^2+q_1^2)+(p_2^2+q_2^2)+\frac{1}{4}\chi[1-\frac{1}{M}]\times$$

$$\times[(q_1^2+q_2^2)^2-(p_1^2+p_2^2)^2-(q_1^2-p_1^2)(q_2^2-p_2^2)-4q_1q_2p_1p_2-2(q_1^2+q_2^2-p_1^2-p_2^2)], \quad (6)$$

with $\chi = MV/\epsilon$. The phase space has been scaled to give $(q_1^2+q_2^2+p_1^2+p_2^2)\leq 2$. The classical hamiltonian can be obtained in the "thermodynamical" limit [10,12]:

$$H_{cl}(p_1,p_2,q_1,q_2) = \lim_{M\to\infty} H(p_1,p_2,q_1,q_2;M), \qquad (7)$$

and the semi–quantal hamiltonian is given by:

$$H(p_1,p_2,q_1,q_2;M) = H_{cl}(p_1,p_2,q_1,q_2)+H_{qc}(p_1,p_2,q_1,q_2;M), \qquad (8)$$

where H_{qc} is the hamiltonian of quantum corrections.

Through the canonical transformation in action–angle variables [11]:

$$q_k=\sqrt{2I_k}\cos(\theta_k), \quad p_k=\sqrt{2I_k}\sin(\theta_k), \quad k=1,2 \qquad (9)$$

the semi–quantal hamiltonian can be written:

$$H(I_1,I_2,\theta_1,\theta_2;M)=H_0(I_1,I_2)+\chi V(I_1,I_2,\theta_1,\theta_2;M), \qquad (10)$$

where:

$$H_0(I_1,I_2)=-1+I_1+2I_2, \qquad (11)$$

$$V(I_1,I_2,\theta_1,\theta_2;M)=[1-\frac{1}{M}](1-I_1-I_2)[I_1\cos(2\theta_1)+I_2\cos(2\theta_2)]+I_1I_2\cos(2\theta_2-2\theta_1). \qquad (12)$$

We applied a canonical transformation $(I_1,I_2,\theta_1,\theta_2)\to(\tilde{I}_1,\tilde{I}_2,\tilde{\theta}_1,\tilde{\theta}_2)$ in order to obtain a new hamiltonian that depends only on the new action variables up to the second order in a power series of χ:

$$\tilde{H}(\tilde{I}_1,\tilde{I}_2;M)=\tilde{H}_0(\tilde{I}_1,\tilde{I}_2)+\chi\tilde{H}_1(\tilde{I}_1,\tilde{I}_2;M)+\chi^2\tilde{H}_2(\tilde{I}_1,\tilde{I}_2;M). \qquad (13)$$

It is well known that the canonical perturbation theory presents many difficulties which are essentially related to the so–called small denominators. The resonance of the unperturbed frequencies $\omega_1=\frac{\partial H_0}{\partial I_1}=1,\omega_2=\frac{\partial H_0}{\partial I_2}=2$:

$$m\omega_1+n\omega_2=0, \qquad (14)$$

can lead to divergent expressions in the perturbative solution to the problem. This drawback occurs only if the integer numbers m and n are present as Fourier harmonics in the perturbation theory. We will show that the resonance condition (14) is not satisfied up to the second order in χ.

We assume that the generator S of the canonical transformation may be expanded as a power series in χ:

$$S(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M)=\tilde{I}_1\theta_1+\tilde{I}_2\theta_2+\chi S_1(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M)+\chi^2 S_2(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M). \qquad (15)$$

The generator S satisfies the equations:

$$I_k = \frac{\partial S}{\partial \theta_k} = \tilde{I}_k + \chi \frac{\partial S_1}{\partial \theta_k} + \chi^2 \frac{\partial S_2}{\partial \theta_k}, \tag{16}$$

$$\tilde{\theta}_k = \frac{\partial S}{\partial \tilde{I}_k} = \theta_k + \chi \frac{\partial S_1}{\partial \tilde{I}_k} + \chi^2 \frac{\partial S_2}{\partial \tilde{I}_k}, \tag{17}$$

with $k = 1, 2$. From the Hamilton–Jacobi equation:

$$H_0(\frac{\partial S}{\partial \theta_1}, \frac{\partial S}{\partial \theta_2}) + V(\frac{\partial S}{\partial \theta_1}, \frac{\partial S}{\partial \theta_2}, \theta_1, \theta_2; M) = \tilde{H}_0(\tilde{I}_1, \tilde{I}_2) + \tilde{H}_1(\tilde{I}_1, \tilde{I}_2; M) + \tilde{H}_2(\tilde{I}_1, \tilde{I}_2; M), \tag{18}$$

we have a number of differential equations obtained by equating the coefficients of the powers of χ:

$$\tilde{H}_0(\tilde{I}_1, \tilde{I}_2) = H_0(\tilde{I}_1, \tilde{I}_2) = -1 + \tilde{I}_1 + 2\tilde{I}_2, \tag{19}$$

$$\tilde{H}_1(\tilde{I}_1, \tilde{I}_2; M) = \left(\omega_1 \frac{\partial S_1}{\partial \theta_1} + \omega_2 \frac{\partial S_1}{\partial \theta_2} \right) + V(\tilde{I}_1, \tilde{I}_2, \theta_1, \theta_2; M), \tag{20}$$

$$\tilde{H}_2(\tilde{I}_1, \tilde{I}_2; M) = \left(\omega_1 \frac{\partial S_2}{\partial \theta_1} + \omega_2 \frac{\partial S_2}{\partial \theta_2} \right) + \left(\frac{\partial V}{\partial I_1} \frac{\partial S_1}{\partial \theta_1} + \frac{\partial V}{\partial I_2} \frac{\partial S_1}{\partial \theta_2} \right) \tag{21}$$

The unknown functions $\tilde{H}_1$, S_1, $\tilde{H}_2$ and S_2 may be determined by averaging the time variation of the unperturbed motion. At the first order in χ we obtain:

$$\tilde{H}_1(\tilde{I}_1, \tilde{I}_2; M) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} d\theta_1 d\theta_2 V(\tilde{I}_1, \tilde{I}_2, \theta_1, \theta_2; M) = 0, \tag{22}$$

and

$$S_1(\tilde{I}_1, \tilde{I}_2, \theta_1, \theta_2; M) = - \sum_{\{(m,n)\}} \frac{V_{mn}(\tilde{I}_1, \tilde{I}_2; M)}{(m\omega_1 + n\omega_2)} \sin{(m\theta_1 + n\theta_2)}, \tag{23}$$

where $\{(m,n)\} = \{(2,0),(0,2),(-2,2)\}$ are the Fourier harmonics of the perturbation potential V. The resonance condition is not satisfied, and we have:

$$S_1(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M) = -\frac{1}{2}[1-\frac{1}{M}][(1-\tilde{I}_1-\tilde{I}_2)(\tilde{I}_1\sin(2\theta_1)+$$

$$+\frac{1}{2}[1-\frac{1}{M}]\tilde{I}_2\sin(2\theta_2))] - \frac{1}{2}[1-\frac{1}{M}]\tilde{I}_1\tilde{I}_2\sin(2\theta_2-2\theta_1). \qquad (24)$$

At the second order in χ:

$$\tilde{H}_2(\tilde{I}_1,\tilde{I}_2;M) = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 \left(\frac{\partial V}{\partial I_1}\frac{\partial S_1}{\partial \theta_1} + \frac{\partial V}{\partial I_1}\frac{\partial S_1}{\partial \theta_2}\right)$$

$$= \frac{1}{4}[1-\frac{1}{M}](-1+\tilde{I}_1+2\tilde{I}_2)(2\tilde{I}_1-4\tilde{I}_1^2+\tilde{I}_2-\tilde{I}_1\tilde{I}_2-\tilde{I}_2^2) \qquad (25)$$

and:

$$S_2(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M) = -\sum_{\{(m,n)\}}\frac{W_{mn}(\tilde{I}_1,\tilde{I}_2;M)}{(m\omega_1+n\omega_2)}\sin(m\theta_1+n\theta_2), \qquad (26)$$

where $\{(m,n)\} = \{(2,0),(4,0),(2,-4),(4,-4),(2,-2),(0,4),(2,2)\}$ are the Fourier harmonics of the function W, given by:

$$W(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M) = \tilde{H}_2(\tilde{I}_1,\tilde{I}_2;M) - \left(\frac{\partial V}{\partial I_1}\frac{\partial S_1}{\partial \theta_1} + \frac{\partial V}{\partial I_2}\frac{\partial S_1}{\partial \theta_2}\right). \qquad (27)$$

In this case too, the resonance condition is not satisfied and we have:

$$S_2(\tilde{I}_1,\tilde{I}_2,\theta_1,\theta_2;M) = \frac{1}{8}[1-\frac{1}{M}][3\tilde{I}_1\tilde{I}_2(1-\tilde{I}_1-\tilde{I}_2)\sin(2\theta_1)+$$

$$+\tilde{I}_1(1-3\tilde{I}_1+2\tilde{I}_1^2-2\tilde{I}_2+3\tilde{I}_1\tilde{I}_2+\tilde{I}_2^2)\sin(4\theta_1)+$$

$$+3\tilde{I}_1\tilde{I}_2(\tilde{I}_1+\tilde{I}_2^2-1)\sin(2\theta_1-4\theta_2)+$$

$$+\tilde{I}_1\tilde{I}_2(\tilde{I}_2-\tilde{I}_1)\sin(4\theta_1-4\theta_2)+$$

$$+3\tilde{I}_1\tilde{I}_2(1-\tilde{I}_1-\tilde{I}_2)\sin(2\theta_1-2\theta_2)+$$
$$+\frac{1}{4}\tilde{I}_2(1-2\tilde{I}_1+\tilde{I}_1^2-3\tilde{I}_2+3\tilde{I}_1\tilde{I}_2+2\tilde{I}_2^2)\sin(4\theta_2)+$$
$$+3\tilde{I}_1\tilde{I}_2(\tilde{I}_1+\tilde{I}_2-1)\sin(2\theta_1+2\theta_2)] \quad (28)$$

In conclusion:

$$\tilde{H}(\tilde{I}_1,\tilde{I}_2;M)=-1+\tilde{I}_1+2\tilde{I}_2+\frac{\chi^2}{4}[1-\frac{1}{M}](-1+\tilde{I}_1+2\tilde{I}_2)(2\tilde{I}_1-4\tilde{I}_1^2+\tilde{I}_2-\tilde{I}_1\tilde{I}_2-\tilde{I}_2^2). \quad (29)$$

This approximate semi–quantal hamiltonian depends only on the actions. Thus, a semi–quantal quantization formula may be obtained by applying the Einstein–Brillowin–Keller rule [2,3]:

$$\tilde{I}_k=(n_k+\frac{1}{2})\frac{1}{M}, \quad k=1,2 \quad (30)$$

where $1/M$ plays the role of the Planck constant $\hbar$. In this way we have:

$$E_{n_1n_2}(M)=E^{sc}_{n_1n_2}(M)+E^{qc}_{n_1n_2}(M) \quad (31)$$

where:

$$E^{sc}_{n_1n_2}(M)=-1+(n_1+\frac{1}{2})\frac{1}{M}+2(n_2+\frac{1}{2})\frac{1}{M}+\frac{\chi^2}{4}[-1+(n_1+\frac{1}{2})\frac{1}{M}+2(n_2+\frac{1}{2})\frac{1}{M}]\times$$
$$\times[2(n_1+\frac{1}{2})\frac{1}{M}-4(n_1+\frac{1}{2})^2\frac{1}{M^2}+(n_2+\frac{1}{2})\frac{1}{M}-(n_1+\frac{1}{2})(n_2+\frac{1}{2})\frac{1}{M^2}-(n_2+\frac{1}{2})^2\frac{1}{M^2}], \quad (32)$$

is the semi–classical quantization formula, and

$$E^{qc}_{n_1n_2}(M)=-\frac{\chi^2}{4M}[-1+(n_1+\frac{1}{2})\frac{1}{M}+2(n_2+\frac{1}{2})\frac{1}{M}]\times$$
$$\times[2(n_1+\frac{1}{2})\frac{1}{M}-4(n_1+\frac{1}{2})^2\frac{1}{M^2}+(n_2+\frac{1}{2})\frac{1}{M}-(n_1+\frac{1}{2})(n_2+\frac{1}{2})\frac{1}{M^2}-(n_2+\frac{1}{2})^2\frac{1}{M^2}], \quad (33)$$

are the quantum corrections.

In order to test the accuracy of the semiclassical approximation and its quantum corrections, the eigenvalues of the hamiltonian (1) must be calculated. A natural basis can be written: $|bc>$, meaning b particles in the second level, c in the third and, of course, $M-b-c$ in the first level. In this way $|00>$ is the ground state with all the particles in the lowest level [7,8]. We can write the general basis state:

$$|bc>=\sqrt{\frac{1}{b!c!}}\hat{G}_{21}^{b}\hat{G}_{31}^{c}|00>, \tag{34}$$

where $\sqrt{\frac{1}{b!c!}}$ is the normalizing constant.

We can calculate the expectation values of $\frac{\hat{H}}{M}$ and, therefore, the eigenvalues and eigenstates of $\frac{\hat{H}}{M}$. In this way, the energy spectrum range is independent of the number of the particles:

$$<b^{'}c^{'}|\frac{\hat{H}}{M}|bc>=\frac{1}{M}(-M+b+2c)\delta_{bb'}\delta_{cc'}-\frac{\chi}{2M^{2}}Q_{b'c',bc}, \tag{35}$$

where:

$$\begin{aligned}Q_{b'c',bc}=&\sqrt{b(b-1)(M-b-c+1)(M-b-c+2)}\delta_{b-2,b'}\delta_{cc'}\\&+\sqrt{(b+1)(b+2)(M-b-c)(M-b-c-1)}\delta_{b+2,b'}\delta_{cc'}\\&+\sqrt{c(c-1)(M-b-c+1)(M-b-c+2)}\delta_{b,b'}\delta_{c-2,c'}\\&+\sqrt{(c+1)(c+2)(M-b-c)(M-b-c-1)}\delta_{b,b'}\delta_{c+2,c'}\\&+\sqrt{(b+1)(b+2)c(c-1)}\delta_{b+2,b'}\delta_{c-2,c'}\\&+\sqrt{b(b-1)(c+1)(c+2)}\delta_{b-2,b'}\delta_{c+2,c'}\end{aligned} \tag{36}$$

and $\chi = MV/\epsilon$. The expectation value $< \frac{\hat{H}}{M} >$ is real and symmetric. For a given number of particles M, we can set up the complete basis state, write down the matrix elements of $< \frac{\hat{H}}{M} >$ and then diagonalize $< \frac{H}{M} >$ to find its eigenvalues. $< \frac{H}{M} >$ connects only states with $\Delta b = -2, 0, 2$ and $\Delta c = -2, 0, 2$ which makes the problem easier. We group states with b,c even; b,c odd; b even and c odd; b odd and c even. This means that $< \frac{\hat{H}}{M} >$ becomes block diagonal containing 4 blocks which can be diagonalized separately. These matrices are referred to as ee, oo, oe and eo (for further details see also [17]).

Then we compare these "exact" levels to those obtained by the semi–quantal perturbation theory. A very good agreement is displayed (see Fig. 1).

In Table 1, we show the difference between the "exact" levels and those obtained by the semi–classical and semi–quantal perturbation theory. We observe that the algorithm provided by the semi–quantal perturbation theory gives better results than that of the ordinary semi–classical perturbation theory.

Obviously if $1/M$, no matter how small, is kept fixed, this semi–quantal approximation on the individual levels has the meaning of a perturbation theory in $1/M$ [5,6,13]. Therefore, the accuracy of the approximation decreases for higher levels [14]. To obtain a better agreement it is necessary, as is well known, to implement the classical limit $1/M \to 0$, $n_k \to \infty$ and, at the same time, to keep the action $\tilde{I}_k = (n_k + 1/2)/M$ constant [15,16].

Finally, we stress that, for systems with a finite number of Fourier harmonics, like the SU(3) model, rational frequencies do not give rise to the problem of small denominators up to a certain order of the canonical perturbation theory.

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Table Captions

Table 1: The differences for the first 10 levels, with $\chi = 0.75$ and $M = 100$, for the *eo* class. E^{ex} are the "exact" levels, E^{sc} are the semi–classical levels, and E^{sq} are the semi–quantal levels.

Figure Captions

Figure 1: Comparison between "exact" levels (left) and those obtained by the semi–quantal perturbation theory (right); with $\chi = 0.75$ and $M = 100$ for the *eo* class.

$\|E^{ex} - E^{sc}\|$	$\|E^{ex} - E^{sq}\|$
$1.3086796 \cdot 10^{-3}$	$1.1860132 \cdot 10^{-3}$
$1.6146898 \cdot 10^{-3}$	$1.3964772 \cdot 10^{-3}$
$2.7745962 \cdot 10^{-4}$	$2.2178888 \cdot 10^{-4}$
$1.4380813 \cdot 10^{-3}$	$1.1500716 \cdot 10^{-3}$
$1.5463829 \cdot 10^{-3}$	$1.3815761 \cdot 10^{-3}$
$1.0503531 \cdot 10^{-3}$	$7.1579218 \cdot 10^{-4}$
$1.9035935 \cdot 10^{-3}$	$1.6558170 \cdot 10^{-3}$
$4.4906139 \cdot 10^{-4}$	$3.5130978 \cdot 10^{-4}$
$6.0987473 \cdot 10^{-4}$	$2.4980307 \cdot 10^{-4}$
$1.8021464 \cdot 10^{-3}$	$1.4950633 \cdot 10^{-3}$

Table 1