# Improved Semiclassics for the Excited States of Three Particles

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**Abstract**

We extend a previous proposal of improving the EBK semiclassical quantization rules to three-particle systems in states with zero total angular momentum. Semiclassical quantization is carried on in a modified potential, which can be interpreted as coming from supersymmetric Quantum Mechanics after the fermion-boson interaction is neglected. The standard EBK rules in this potential with no Maslov's indexes lead to the exact ground-state energy and to an improved description of the excited states. The method is tested in a model Hamiltonian with quartic and sextic anharmonicities. Approximate integrals of motion of the modified Hamiltonian are constructed by means of the Birkhoff-Gustavson reduction to normal forms. We expect the method to provide a good semiclassical description of the first excited states of strongly quantum few-particle systems.

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# 1 Introduction

Attempts to apply the rules of the old semiclassical Mechanics to the quantization of a 3B problem (the Helium atom) date back to Bohr and Kramers [1], and their failure was a great motivation towards a consequent formulation of Quantum Mechanics.

In modern terms, the conceptual difficulty in semiclassical quantizing a 3B system lies in the nonintegrability of the classical 3B problem [2]. Apart from this point, we now understand that quantum phenomena are not always governed by semiclassical Mechanics, and this concerns, in particular, the first energy levels of many small systems.

However, a great progress has been achieved in the last years in the understanding of semiclassical Mechanics [3,4] and in the development of methods for carrying on quantization in systems with a few degrees of freedom. Among these methods, one can mention, for example, the Fourier transform of classical trajectories [5] and the Birkhoff-Gustavson reduction to normal forms [6], which have been applied to molecular problems, or the trace formula which has been used in the quantization of hardly chaotic [7] and even ergodic [8] systems. Applications have been, however, restricted to systems with at most two degrees of freedom and one is tempted to apply these methods to 3B problems in real three dimensional space.

On the other hand, an interesting possibility of describing quantum effects by means of an effective classical potential is suggested by supersymmetric Quantum Mechanics [9]. Let us write the Hamiltonian for the interaction of a boson and a fermion:

$$H = \frac{1}{2}\left(p^2 + (\mathrm{d}W/\mathrm{d}x)^2\right) - \frac{\hbar}{2}\left(\mathrm{d}^2W/\mathrm{d}x^2\right)\sigma_3, \tag{1}$$

the mass of the particle is taken to be unity and $\sigma_3$ is the third Pauli matrix. The eigenvectors of $\sigma_3$ define the sectors in Hilbert space with zero and one fermion numbers. Bosonic Hamiltonians act in each of these sectors. They are respectively

$$H_\pm = \frac{1}{2}\left(p^2 + (\mathrm{d}W/\mathrm{d}x)^2\right) \pm \frac{\hbar}{2}\left(\mathrm{d}^2W/\mathrm{d}x^2\right), \tag{2}$$

and are shown to be isospectral with the exception of the ground state, which is contained only in the spectrum of one of the Hamiltonians, let us say of

$H_-$. The g. s. function is $\psi = \exp -W/\hbar$, and the g. s. energy is redefined to be zero.

Let us recall then the two basic properties of the "classical" potential

$$U = \frac{1}{2}(\mathrm{d}W/\mathrm{d}x)^2. \tag{3}$$

i) Its minimum is located at the point of maximal probability, i. e. of maximal $\psi^2$, and ii) The value of $U$ at its minimum, $U = 0$, coincides exactly with the g. s. energy. Quantum corrections do not change this "classical" result.

Then, one is tempted to semiclassically quantize the motion in $U$ in order to obtain the excited states. Note that the zero-length orbit shall be included and it corresponds to the ground state. In the one degree of freedom case, one arrives to the modified Bohr-Sommerfeld rule

$$\frac{1}{2\pi}\oint \mathrm{d}x\sqrt{2(E-U)} = n\hbar, \tag{4}$$

which has proven to be exact in a wide class of exactly solvable problems [10].

In the 3B case, we expect the analog of Eq. (4) to hold only approximately, although there are indications [11] that there is a class of problems in one dimension, which includes the Calogero problem [12], for which the improved quantization may be exact. In paper [11], we computed the small-oscillation frequencies around the "Bohr configuration" of the 3B system (i. e. the configuration of maximal probability, for which $U = 0$) and showed that they are more naturally related to the excitation energies of the quantum system than are the ordinary frequencies computed in the actual potential $V$. In papers [13], we went beyond the small-oscillation approximation and constructed approximate action variables in the 3B problem by applying successive canonical transformations which reduce the Hamiltonian to a sum of simple forms, i. e. the normal forms of Birkhoff and Gustavson [6]. The method was applied to a model triatomic molecule in one dimension which showed the interesting feature that the ordinary (in $V$) BG quantization breaks down for some particular value of the parameter entering the Hamiltonian.

In the present paper, we extend the above method to three identical particles in real 3D space. We restrict ourselves to states with total angular

momentum, $L = 0$, for which the Hamiltonian reduces to a scalar Hamiltonian with 3 degrees of freedom. It is worth stressing that the condition $L = 0$ is exact in the quantum sense. In other words, we start from the exact quantum $L = 0$ Hamiltonian in which we replace $V$ by $U$ and the momentum operators by classical magnitudes. After that, we apply the BG method to construct the approximate action variables of the problem, which are quantized by simply assigning to them integer multiples of the elementary quantum of action.

Besides giving the general quantization recipe, we apply it to a model problem in which the potential exhibits quartic and sextic anharmonicities. This may be seen as a model of a quantum system with a depth potential well as may be, for example, a $3\alpha$ model of $^{12}$C [14] or a trimer of heavy noble gas atoms [15]. We do not, however, choose the parameter of the Hamiltonian to fit the energies of any of these systems. Instead of that, we compare with the results of a numerical estimation of energy levels. Details are given below.

## 2 The BG Procedure in the Potential $U$

We start by recalling the restriction of the 3B Hamiltonian to states with total angular momentum $L = 0$:

$$\begin{aligned} H = & - \frac{\hbar^2}{2\mu_r}\frac{\partial^2}{\partial r^2} - \frac{\hbar^2}{2\mu_\rho}\frac{\partial^2}{\partial \rho^2} - \frac{\hbar^2}{2}(1-\gamma^2)\left(\frac{1}{\mu_r r^2} + \frac{1}{\mu_\rho \rho^2}\right)\frac{\partial^2}{\partial \gamma^2} \\ & - \frac{\hbar^2}{2(1-\gamma^2)}\left(\frac{1}{\mu_r r^2} + \frac{1}{\mu_\rho \rho^2}\right) + v. \end{aligned} \tag{5}$$

In Eq. (5), $\vec{r}$ and $\vec{\rho}$ are the Jacobi vectors

$$\vec{r} = \vec{r}_2 - \vec{r}_1, \tag{6}$$

$$\vec{\rho} = \vec{r}_3 - \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}, \tag{7}$$

and $\mu_r$, $\mu_\rho$ are the associated reduced masses,

$$\mu_r = \frac{m_1 m_2}{m_1 + m_2}, \tag{8}$$

$$\mu_\rho = \frac{m_3(m_1+m_2)}{m_1+m_2+m_3}. \tag{9}$$

The interaction potential, $v$, may contain two- or three-body forces, but it is supposed to be central such that total angular momentum is conserved. In states with $L=0$, the wave function is a function of scalar combinations of $\vec{r}$ and $\vec{\rho}$, i.e. of $r$, $\rho$ and $\gamma = \vec{r}.\vec{\rho}/r\rho$. We eliminated the first derivatives in the Hamiltonian by changing to the reduced wave function:

$$\chi = r\rho(1-\gamma^2)^{1/2}\psi. \tag{10}$$

such that $\chi^2$ is the probability density of 3B configurations.

The modified potential $U$ may be obtained from the Schrodinger equation

$$(H - E_{gs})\chi_{gs} = 0, \tag{11}$$

simply by writing the g.s. wave function in the form $\chi_{gs} = \exp -W/\hbar$ and neglecting the terms proportional to $\hbar$ in the representation of the potential in terms of $W$,

$$-\frac{\hbar^2}{2(1-\gamma^2)}\left(\frac{1}{\mu_r r^2}+\frac{1}{\mu_\rho \rho^2}\right) + v - E_{gs} = U - \hbar U_\hbar, \tag{12}$$

$$\begin{aligned} U(r,\rho,\gamma) &= \frac{1}{2\mu_r}\Big(\partial W/\partial r\Big)^2 + \frac{1}{2\mu_\rho}\Big(\partial W/\partial \rho\Big)^2 \\ &+ \frac{1}{2}\Big(1-\gamma^2\Big)\Big(1/(\mu_r r^2) + 1/(\mu_\rho \rho^2)\Big)\Big(\partial W/\partial\gamma\Big)^2, \end{aligned} \tag{13}$$

$$U_\hbar(r,\rho,\gamma) = \frac{1}{2\mu_r}\frac{\partial^2 W}{\partial r^2} + \frac{1}{2\mu_\rho}\frac{\partial^2 W}{\partial \rho^2} + \frac{1}{2}(1-\gamma^2)\left(\frac{1}{\mu_r r^2}+\frac{1}{\mu_\rho\rho^2}\right)\left(\frac{\partial^2 W}{\partial\gamma^2}\right). \tag{14}$$

We note that $U$ is again a nonnegative function. The conditions of minimum

$$\frac{\partial W}{\partial r} = \frac{\partial W}{\partial \rho} = \frac{\partial W}{\partial \gamma} = 0, \tag{15}$$

are equivalent to the requirements of maximal probability

$$\frac{\partial \chi_{gs}}{\partial r} = \frac{\partial \chi_{gs}}{\partial \rho} = \frac{\partial \chi_{gs}}{\partial \gamma} = 0, \tag{16}$$

Because of the fact that $\chi_{gs}$ has only one extremum (its maximum) Eqs. (16) have only one solution. Permutation symmetry implies that the configuration of minimum is an equilateral triangle, and thus the system (16) reduces to one equation to determine the side of the triangle. At its minimum

$$U(r_0, \rho_0, \gamma_0) = 0, \tag{17}$$

i.e. $E = E_{gs}$.

To obtain the excitation energies, we should start from the classical Hamiltonian,

$$H_{class} = \frac{1}{2} \sum_{\alpha} g_\alpha p_\alpha^2 + U, \tag{18}$$

where $\alpha = r, \rho, \gamma$, $\quad g_r = 1/\mu_r$, $g_\rho = 1/\mu_\rho$, $g_\gamma = (1-\gamma^2)(1/\mu_r r^2 + 1/\mu_\rho \rho^2)$, and impose quasiclassical quantization conditions on the classical bounded motion governed by the Hamiltonian (18). Due to the particular form of the potential $U$, which has an absolute minimum at the configuration of maximal probability, we find most convenient to expand $H_{class}$ around the minimum and then, by means of successive canonical transformations, to reduce the first terms of the series to simple forms from which the action variables of our problem are straightforwardly extracted. After truncation of the series, we are led to an integrable Hamiltonian which approximately describes the problem and which is suitable for semiclassical quantization. This is the so called BG procedure, let us briefly describe it.

Expanding $H_{class}$ around the minimum, we get

$$H_{class} = H_2(p,q) + H_3(p,q) + \ldots, \tag{19}$$

where the $H_\alpha$ are homogeneous polynomials of degree $\alpha$. The $q$'s are the normal coordinates of the small oscillations around the minimum, and the $p$'s are their conjugated momenta. In other words, $H_2$ takes the form

$$H_2 = \frac{\omega_0}{2}(p_0^2 + q_0^2) + \frac{\omega_1}{2}(p_1^2 + q_1^2) + \frac{\omega_1}{2}(p_2^2 + q_2^2). \tag{20}$$

Notice that there is a non degenerated mode of oscillation (the symmetric mode) and a two-fold degenerated mode (the mode with mixed symmetry) simply as a consequence of permutation symmetry.

The Birkhoff-Gustavson procedure [6] enables us to reduce the Hamiltonian (19) to the form

$$\Gamma = \sum_i \frac{\omega_i}{2}(P_i^2 + Q_i^2) + \Gamma_4(P,Q) + \Gamma_6(P,Q) + \cdots, \tag{21}$$

where the frequencies are the same as above and the $\Gamma_\alpha$ are homogeneous polynomials in the new variables $P_i$, $Q_i$. The $\Gamma_\alpha$ are required to commute with $\Gamma_2$, such that the action variables become trivial. Of course, we can not satisfy this requirement for all terms in the expansion because the original Hamiltonian is not integrable. However, by truncating the expansion we obtain an approximate classically integrable Hamiltonian.

The requirement of $\Gamma_\alpha$ to be reduced to normal forms may be concisely written in the following way

$$0 = D\Gamma_\alpha = \sum_j \omega_j \left( P_j \frac{\partial \Gamma_\alpha}{\partial Q_j} - Q_j \frac{\partial \Gamma_\alpha}{\partial P_j} \right). \tag{22}$$

The Hamiltonian $H_{class}$ is reduced to the form (21) by means of successive canonical transformations, each one designed to do the job for the polynomial of a given degree. The generating function of such transformation is the following

$$\begin{aligned} F^{(\alpha)} &= \sum_j P_j q_j + W_\alpha(P,q) \\ &= \sum_j P_j q_j + \sum f^{(\alpha)}_{\beta_1 \ldots \beta_n \gamma_1 \ldots \gamma_n} P_1^{\beta_1} \ldots P_n^{\beta_n} q_1^{\gamma_1} \ldots q_n^{\gamma_n}, \end{aligned} \tag{23}$$

where the second sum runs over indexes such that $\sum_j (\beta_j + \gamma_j) = \alpha$. It leads to the following relations

$$Q_i = \frac{\partial}{\partial P_i} F^{(\alpha)}(P,q) = q_i + \frac{\partial W_\alpha}{\partial P_i}, \tag{24}$$

$$p_i = \frac{\partial}{\partial q_i} F^{(\alpha)}(P,q) = P_i + \frac{\partial W_\alpha}{\partial q_i}, \tag{25}$$

$$H_{class}(p,q) = \Gamma(P,Q), \tag{26}$$

where in each step $p$, $q$ and $P$, $Q$ denote the old and new variables respectively.

Substituting (24) and (25) into (26) and expanding in powers of $P$ and $q$, we obtain the following system of recurrent relations for the $\Gamma_\beta$ and the function $W_\alpha$:

$$\Gamma_\beta(P,q) = H_\beta(P,q), \quad \beta < \alpha, \tag{27}$$

$$W_\alpha(P,q) = D^{-1}\left[\Gamma_\alpha(P,q) - H_\alpha(P,q)\right], \tag{28}$$

$$\Gamma_\beta(P,q) = H_\beta(P,q) + \text{terms of order } \beta \text{ in } \sum_{\beta/(\alpha-1)\leq\rho\leq\beta+2-\alpha} \left\{ H_\rho(P + \frac{\partial W^{(\alpha)}}{\partial q}, q) - \Gamma_\rho(P, q + \frac{\partial W^{(\alpha)}}{\partial P}) \right\}, \quad \beta > \alpha. \tag{29}$$

Note that in Eq. (28), the $\Gamma_\alpha$ is chosen such as to cancel all terms of $H_\alpha$ which are null vectors of $D$. In other words, if we write

$$H_\alpha = N_\alpha + R_\alpha, \tag{30}$$

where $DN_\alpha = 0$, but $DR_\alpha \neq 0$, then

$$\Gamma_\alpha = N_\alpha, \quad \text{and} \tag{31}$$

$$W_\alpha = -D^{-1} R_\alpha. \tag{32}$$

There is an efficient way for solving Eqs. (31) and (32). The point is that the operator $D$ is diagonalized when we change to the variables

$$\xi = \tfrac{1}{\sqrt{2}}(P + iq), \tag{33}$$

$$\eta = \tfrac{i}{\sqrt{2}}(P - iq), \tag{34}$$

i.e.

$$D = i \sum_j \omega_j (\xi_j \frac{\partial}{\partial \xi_j} - \eta_j \frac{\partial}{\partial \eta_j}). \tag{35}$$

Consequently, every monomial

$$\Phi_{ml} = \prod_j \xi_j^{m_j} \eta_j^{l_j}, \tag{36}$$

is an eigenvector of $D$ and $D^{-1}$ with eigenvalues $\lambda = i \sum_j \omega_j (m_j - l_j)$ and $\lambda^{-1}$ respectively.

After the application of the BG procedure through a given order, we obtain a truncated expansion of the form (21). Under the assumption that $\omega_0$ and $\omega_1$ are no commensurate, it is easy to see that the variables $P_0$ and $Q_0$ will enter the $\Gamma_\alpha$ only in the combination $(P_0^2 + Q_0^2)/2$, which after quantization becomes $\hbar$ times the number of quanta in the symmetric mode

$$J_0 = \frac{1}{2}(P_0^2 + Q_0^2) \to n_0 \hbar. \tag{37}$$

The argument is the following. No commensurability implies that the term proportional to $\omega_0$ in (22) shall be zero by itself, and this in turn implies that $\Gamma_\alpha$ is a function of $\frac{1}{2}(P_0^2 + Q_0^2)$. On the other hand, degeneracy of the mixed-symmetry mode leads to the fact that the $\Gamma_\alpha$ will not only depend on the combinations $\frac{1}{2}(P_i^2 + Q_i^2)$ , $i$= 1, 2, but also on some combinations between the $i$= 1 and $i$= 2 variables. It can be seen, however, that the total number of quanta in the mixed-symmetry mode

$$J_1 = \frac{1}{2}(P_1^2 + Q_1^2) + \frac{1}{2}(P_2^2 + Q_2^2), \tag{38}$$

is an action variable of the problem and, thus, it may be quantized according to the rule

$$J_1 \to n_1 \hbar. \tag{39}$$

For the quantization of the remaining degree of freedom, one shall apply the Bohr - Sommerfeld rule (4), where the momentum variable is obtained from the equation $\Gamma = E$ as a function of $E$, $J_0$, $J_1$ and the remaining angular coordinate.

Let us see how the method works in an example.

# 3 A Model with Quartic and Sextic Two- and Three-Body Potentials

We consider the central interaction of three spin-less particles described by the potential

$$
\begin{aligned}
V &= -\frac{1}{2(1-\gamma^2)}\left(\frac{1}{\mu_r r^2}+\frac{1}{\mu_\rho \rho^2}\right)+v \\
&= -\frac{1}{(1-\gamma^2)}\left(\frac{1}{r^2}+\frac{3}{4\rho^2}\right)+9(r^2+4\rho^2/3)(1-7\lambda/3) \\
&+ 6\lambda\left[\frac{9}{4}(r^2+4\rho^2/3)^2+4r^2\rho^2(1-\gamma^2)\right] \\
&+ \lambda^2\left[\frac{81}{16}(r^2+4\rho^2/3)^3+21r^2\rho^2(1-\gamma^2)(r^2+4\rho^2/3)\right]. \qquad (40)
\end{aligned}
$$

We use units in which $\hbar$ and the mass of the particles are set to one, so that $\mu_r = 1/2$, $\mu_\rho = 2/3$.

Besides the term coming from the elimination of first derivatives in the Hamiltonian and the harmonic terms, the potential $V$ contains quartic and sextic anharmonicities which respect permutation invariance. It may be thought of as an approximation to a deep well, intended to describe the first energy levels above the bottom of the well. The most interesting property of $V$ is that the g.s. energy and wave function may be explicitly written

$$
\begin{aligned}
E_{gs} &= 18, \\
\psi_{gs} &= \exp-\Big\{r_{12}^2+r_{23}^2+r_{31}^2 \\
&+ \lambda(r_{12}^2r_{23}^2+r_{23}^2r_{31}^2+r_{31}^2r_{12}^2)\Big\}, \qquad (41)
\end{aligned}
$$

so that, instead of computing numerically $\psi_{gs}$ and obtaining an expansion like (19) by fitting coefficients, we may write an explicit expression for $U$

$$
U = V + \frac{2}{1-\gamma^2}\left(\frac{1}{r^2}+\frac{3}{4\rho^2}\right) - 12, \qquad (42)
$$

which is our starting point in the application of the BG procedure.

The minimum of $U$ is , of course, $U = 0$. It is reached in configurations corresponding to equilateral triangles

$$\gamma = 0, \quad \rho^2 = 3r^2/4. \tag{43}$$

In these configurations, we obtain the following equation for the equlibrium distance, $r_0$

$$0 = -1 + 3r_0^2 + 6\lambda r_0^4, \tag{44}$$

i.e.

$$r_0^2 = \frac{1}{4\lambda}\Big( -1 + \sqrt{1 + 8\lambda/3}\Big). \tag{45}$$

We will expand around the equilibrium configuration

$$\begin{aligned} r &= r_0 + x, \\ \rho &= \frac{\sqrt{3}}{2}(r_0 + y), \\ \gamma &= z, \end{aligned} \tag{46}$$

and change to the normal mode coordinates $p, q$

$$\begin{aligned} x &= q_1/\sqrt{\omega_0} + q_2/\sqrt{\omega_1}, \\ p_x &= \frac{1}{2}(\sqrt{\omega_0}p_1 + \sqrt{\omega_1}p_2), \\ y &= q_1/\sqrt{\omega_0} - q_2/\sqrt{\omega_1}, \\ p_y &= \frac{1}{2}(\sqrt{\omega_0}p_1 - \sqrt{\omega_1}p_2), \\ z &= q_3/\sqrt{1 - \frac{3}{2}\lambda r_0^4}, \\ p_z &= \sqrt{1 - \frac{3}{2}\lambda r_0^4}\; p_3, \end{aligned} \tag{47}$$

where $\omega_0$, $\omega_1$ are the small-oscillation frequencies

$$\omega_0 = \frac{4}{r_0^2}(1 + 6\lambda r_0^4), \tag{48}$$

$$\omega_1 = \frac{4}{r_0^2}(1 - \frac{3}{2}\lambda r_0^4). \tag{49}$$

Substitution of (46 - 49) into the modified Hamiltonian (18) leads to the series (19), in which $H_2$ takes the form (20) and the $H_\alpha$ with $\alpha > 2$ are given by

$$H_\alpha = \sum_{i+j+k+l=\alpha} h_{ijkl}\ p_3^i q_1^j q_2^k q_3^l, \tag{50}$$

where there are only a few nonzero $h_{ijkl}$. Explicit expressions for the $H_\alpha$ at $\lambda = .2$ are given in Appendix 1. They were obtained (as well as the rest of the algebraic calculations in this paper) on a computer with the help of Mathematica.

We apply the transformations (27 - 29) on the Hamiltonian (19) to obtain the normal form (21) through sixth order ($\alpha \leq 6$). We introduce explicitly the conserved quantities (37 - 38) according to

$$\begin{aligned} P_1 &= \sqrt{2J_0}\cos(\theta_0), \quad Q_1 = \sqrt{2J_0}\sin(\theta_0), \\ P_2 &= \sqrt{J_1 - J}\cos(\theta_1 - \theta), \quad Q_2 = \sqrt{J_1 - J}\sin(\theta_1 - \theta), \\ P_3 &= \sqrt{J_1 + J}\cos(\theta_1 + \theta), \quad Q_3 = \sqrt{J_1 + J}\sin(\theta_1 + \theta). \end{aligned} \tag{51}$$

The result for $\Gamma$, Eq. (21), is as follows

$$\Gamma_2 = \omega_0 J_0 + \omega_1 J_1, \tag{52}$$

$$\begin{aligned} \Gamma_4 &= \gamma_1^{(4)} J_1^2 + \gamma_2^{(4)} J^2 + \gamma_3^{(4)} J_1 J_0 + \gamma_4^{(4)} J_0^2 \\ &+ \gamma_2^{(4)}(J_1^2 - J^2)\cos(4\theta), \end{aligned} \tag{53}$$

$$
\begin{aligned}
\Gamma_6 &= -\gamma_1^{(6)} J_1^3 + \gamma_2^{(6)}(J_1^2 J - J^3) - \gamma_3^{(6)} J_1 J^2 - \gamma_4^{(6)} J_1^2 J_0 \\
&+ \gamma_5^{(6)} J^2 J_0 - \gamma_6^{(6)} J_1 J_0^2 - \gamma_7^{(6)} J_0^3 \\
&+ \Big[ -\gamma_3^{(6)} J_1^3 - \gamma_2^{(6)} J_1^2 J + \gamma_3^{(6)} J_1 J^2 + \gamma_2^{(6)} J^3 \\
&+ \gamma_5^{(6)} J_1^2 J_0 - \gamma_5^{(6)} J^2 J_0 \Big] \cos(4\theta). \qquad (54)
\end{aligned}
$$

The explicit values of the coefficients at $\lambda = 0.1$, 0.2 and 0.5 are also given in Appendix 1.

We shall quantize the classical motion described by $\Gamma$, Eqs. (21, 52 - 54). As mentioned above, two quantization rules are trivial

$$J_0 = n_0, \quad J_1 = n_1. \qquad (55)$$

Substituting them into the truncated expression

$$\Gamma = \Gamma_2 + \Gamma_4 + \Gamma_6, \qquad (56)$$

we obtain $\Gamma$ as a function of the generalized canonical variables $J$, $\theta$, and of the parameters $n_0$, $n_1$. The remaining degree of freedom is quantized with the help of a one-dimensional Bohr-Sommerfeld rule.

With the purpose of comparison, we numerically computed the eigenvalues of the Hamiltonian (5, 40) using a basis of 120 functions of the unperturbed Hamiltonian ($\lambda = 0$). We present in Appendix 2 some details needed in this calculation. The results for the first 19 excited states are shown in the last column of Tables 1 - 3, corresponding respectively to $\lambda = 0.1$, 0.2 and 0.5. As will be seen below, these levels are related to states with less than four excitation quanta, i.e. $n_0 + n_1 \leq 3$. The obtained values of energies will be taken as the "exact energies". Some remarks concerning this point will be given below.

Let us consider step by step the different contributions to $\Gamma$.

In the harmonic approximation, $\Gamma = \Gamma_2$, the energy is given by

$$E_2 = n_0\omega_0 + n_1\omega_1, \qquad (57)$$

i.e. harmonic oscillators of frequencies $\omega_0$ and $\omega_1$. The values coming from (57) are shown in the first energy entry of Tables 1 - 3. One may see that

the corresponding spectrum may differ considerably from the free spectrum ($\lambda = 0$, the energies are given by $12N$, where $N$ is the total number of quanta). One may see also that, even at $\lambda = 0.1$, anharmonicities become very strong (15 %) for the higher levels, so that corrections shall be included.

Through fourth order, we get

$$\Gamma = E_2 + f_4 + \Delta\Gamma_4, \tag{58}$$

where

$$\begin{aligned} f_4 &= \gamma_1^{(4)} n_1^2 + \gamma_3^{(4)} n_1 n_0 + \gamma_4^{(4)} n_0^2, & (59) \\ \Delta\Gamma_4 &= \gamma_2^{(4)} n_1^2 \cos(4\theta) + \gamma_2^{(4)} J^2 \Big(1 - \cos(4\theta)\Big). & (60) \end{aligned}$$

Consequently, the energy is given by

$$E_4 = E_2 + f_4 + \epsilon_4, \tag{61}$$

where $\epsilon_4$ shall be found from the Bohr-Sommerfeld condition

$$n = \frac{1}{2\pi} \oint J \mathrm{d}\theta = \frac{1}{\pi} \int_{\theta_i}^{\theta_f} \sqrt{\frac{\epsilon_4 - \gamma_2^{(4)} n_1^2 \cos(4\theta)}{\gamma_2^{(4)}(1 - \cos(4\theta))}} \mathrm{d}\theta. \tag{62}$$

The $\theta_i, \theta_f$ are the turning points for the clasical motion in $\theta$. The dependence of $\Delta\Gamma_4$ on $\theta$ is essentially $\cos(4\theta)$, so that

$$0 \leq \theta_i \leq \pi/4 \leq \theta_f \leq \pi/2. \tag{63}$$

The value $\pi/4$ is reached at $n = 0$, in which case $\epsilon_4 = -\gamma_2^{(4)} n_1^2$. Note also that, in general, the allowed interval for $J$ is $-n_1 \leq J \leq n_1$, thus

$$\frac{1}{2\pi} \oint J \mathrm{d}\theta \leq \frac{1}{2\pi} \times 2n_1 \times \pi/2 = n_1/2, \tag{64}$$

and corrections will not completely break the degeneracy of the harmonic approximation.

The results of this approximation are shown in the $E_4$ column of Tables 1 - 3. Some remarks are needed. The maximum relative errors are 4 %, 5.4 % and

6.6 % at $\lambda = 0.1$, 0.2 and 0.5 respectively. As a rule, the higher the level, the bigger the relative error. However, one can verify that states corresponding to excitations of the symmetric mode ($n_0$) are better described by this scheme than states corresponding to excitations of the mixed-symmetry mode ($n_1$). Note also that the energy values, $E$, do not show exact doublet degeneracy in many cases. This is an indication that the numerical estimate is not accurate enough to observe the degeneracy. Anyway, we will take them as the "exact" energies.

Next, we include the sixth order correction

$$\Gamma = E_2 + f_4 + f_6 + \Delta\Gamma_6, \tag{65}$$

where

$$\begin{aligned} f_6 &= -\gamma_1^{(6)} n_1^3 - \gamma_4^{(6)} n_1^2 n_0 - \gamma_6^{(6)} n_1 n_0^2 - \gamma_7^{(6)} n_0^3, && (66) \\ \Delta\Gamma_6 &= A n_1^2 \cos(4\theta) + \left[ A J^2 + \gamma_2^{(6)} (n_1^2 - J^2) J \right] (1 - \cos(4\theta)), && (67) \\ A &= \gamma_2^{(4)} - \gamma_3^{(6)} n_1 + \gamma_5^{(6)} n_0. && (68) \end{aligned}$$

It may be easily verified that, with the exception of $n_1 = 0$ states for which $\Delta\Gamma_6 = 0$, the minimum of $\Delta\Gamma_6$ is reached at the point

$$\theta_{min} = \pi/4, \quad J_{min} = -\frac{n_1^2 \gamma_2^{(6)}}{A + \sqrt{A^2 + 3(\gamma_2^{(6)} n_1)^2}}, \tag{69}$$

so that the cycle in the phase space $(J, \theta)$ will be a loop around this point. The energy in this approximation is given by

$$E_6 = E_2 + f_4 + f_6 + \epsilon_6, \tag{70}$$

where $\epsilon_6$ is obtained from the quantization rule

$$\frac{1}{2\pi} \oint J(\epsilon_6, \theta) \mathrm{d}\theta = n, \tag{71}$$

in which $J(\epsilon_6, \theta)$ is the solution of the equation $\Delta\Gamma_6 = \epsilon_6$ that generates a loop around the point of minimum. Note that, when $n = 0$, $\epsilon_6 = \Delta\Gamma_6(J_{min}, \theta_{min})$.

In the $E_6$ column of Tab. 1, we have included the energy of $n = 0$ states. We see again that the "breathing states" ($n_0 \neq 0, n_1 = 0$) are best described. One can verify also that the inclusion of the sixth order term does not necessarily lead to an improvement of the fourth order approximation. One shall remember that the BG series for the energy is only asymptotical, so that its terms should be included with care or resummed up with the help of Pade approximants. We have not enough terms to make a Pade analysis, so that in Tables 2 and 3, we show $E_6$ only if it is the best fit to the energy.

The maximum relative error of the best fit is thus 6.6 % reached in a state with three excitation quanta at $\lambda = 0.5$. Note that the actual energy in three-quanta states may be 30 % larger than the free value at $\lambda = 0.1$ and twice larger than the free value at $\lambda = 0.5$, so that our results are essentially nonperturbative in $\lambda$.

# 4 Conclusions

We have extended to three-particle systems in three dimensions and in states with zero total angular momentum a semiclassical quantization recipe which, in one dimension, has shown to improve the ordinary quasiclassics.

To semiclassically quantize a 3B problem, we need approximate action variables. In the present paper, they were obtained by expanding in series the improved Hamiltonian around the configuration of minimum and, after that, reducing the series through a given order to normal forms with the help of canonical transformations (the BG procedure). The action variables of the truncated normal form are easily identified, so that quantization becomes trivial.

There are two sources of errors which can be immediatly stated. One is the series expansion of a Hamiltonian like (5) containing inverse powers of coordinates and $1 - \gamma$. The second is the handling of an asymptotical series.

We intended to give an "empirical" answer to the question about to what extent semiclassics in $U$ is the same as Quantum Mechanics in the unmodified potential. Comparison in a model example leads to energy values with maximum relative errors of 6.6 % in states with three excitation quanta and very strong anharmonicities ($\lambda = 0.5$). A conceptual answer to this question is, however, still lacking.

Our results may be continued further on in many directions. One may, for

example, avoid series expanding $H$ by using a different quantization scheme like Gutzwiller's trace formula. Anharmonicities in the potential will exactly be taken into account in this way. We believe that the leading term of the trace formula will play the same rol as the modified BS rule, so that there will not be necessary to include corrections. On the other hand, one may, for example, further study the classical motion in $U$ in order to decide whether there are some connections with the probability distributions of excited states or with the quantum scattering properties of the unmodified potential.

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## Appendix 1

The following are explicit expressions for the $H_\alpha$, equations (50), at $\lambda = .2$ and $\alpha \leq 6$:

$$H_3 = -6.2137p_3^2q_1 - 2.1724q_1^3 - 9.4789q_1q_2^2 - 7.2796q_1q_3^2, \tag{72}$$

$$\begin{aligned} H_4 = \;& 4.4304p_3^2q_1^2 + 1.8375q_1^4 + 5.0361p_3^2q_2^2 + 11.797q_1^2q_2^2 \\ + \;& 2.3052q_2^4 - 6.7148p_3^2q_3^2 + 4.1153q_1^2q_3^2 + 5.4926q_2^2q_3^2 \\ + \;& 7.0870q_3^4, \end{aligned} \tag{73}$$

$$\begin{aligned} H_5 = \;& -2.8079p_3^2q_1^3 - .96661q_1^5 - 9.5755p_3^2q_1q_2^2 - 11.103q_1^3q_2^2 \\ - \;& 6.3104q_1q_2^4 + 6.3836p_3^2q_1q_3^2 - 3.1780q_1^3q_3^2 - 9.2993q_1q_2^2q_3^2 \\ - \;& 6.7375q_1q_3^4, \end{aligned} \tag{74}$$

$$\begin{aligned} H_6 = \;& 1.6684p_3^2q_1^4 + .54307q_1^6 + 11.379p_3^2q_1^2q_2^2 + 9.2459q_1^4q_2^2 \\ + \;& 2.1558p_3^2q_2^4 + 10.510q_1^2q_2^4 + .79763q_2^6 - 4.5516p_3^2q_1^2q_3^2 \\ + \;& 1.7180q_1^4q_3^2 - 5.1738p_3^2q_2^2q_3^2 + 12.060q_1^2q_2^2q_3^2 + 2.2559q_2^4q_3^2 \\ + \;& 4.8039q_1^2q_3^4 + 5.4606q_2^2q_3^4 + 7.2808q_3^6. \end{aligned} \tag{75}$$

After the application of the BG procedure, this Hamiltonian is reduced to the form (52 - 54), where

$$\Gamma_2 = 14.859J_0 + 13.072J_1, \tag{76}$$

$$\begin{aligned} \Gamma_4 = \;& 1.0582J_1^2 + .097612J^2 + 2.5634J_1J_0 \\ & +1.5652J_0^2 + .097612(J_1^2 - J^2)\cos(4\theta), \end{aligned} \tag{77}$$

$$
\begin{aligned}
\Gamma_6 = \quad & -.11203J_1^3 + .051729J_1^2J - .023966J_1J^2 - .051729J^3 \\
- \quad & .22517J_1^2J_0 + .093076J^2J_0 - .63376J_1J_0^2 - .17098J_0^3 \\
+ \quad & \Big[ -.023966J_1^3 - .051729J_1^2J + .023966J_1J^2 + .051729J^3 \\
+ \quad & \qquad .093076J_1^2J_0 - .093076J^2J_0 \Big] \cos(4\theta). \qquad (78)
\end{aligned}
$$

Similar expressions are obtained at any other value of $\lambda$. We show the results at $\lambda = 0.1$ and 0.5.

$\lambda = 0.1$

$$\Gamma_2 = 13.506J_0 + 12.565J_1, \qquad (79)$$

$$
\begin{aligned}
\Gamma_4 = & .57926J_1^2 + .049300J^2 + 1.4925J_1J_0 \\
& +.94737J_0^2 + .049300(J_1^2 - J^2)\cos(4\theta), \qquad (80)
\end{aligned}
$$

$$
\begin{aligned}
\Gamma_6 = \quad & -.036742J_1^3 + .025424J_1^2J - .0065956J_1J^2 - .025424J^3 \\
- \quad & .077015J_1^2J_0 + .051735J^2J_0 - .29419J_1J_0^2 - .078761J_0^3 \\
+ \quad & \Big[ -.0065956J_1^3 - .025424J_1^2J + .0065956J_1J^2 + .025424J^3 \\
+ \quad & \qquad .051735J_1^2J_0 - .051735J^2J_0 \Big] \cos(4\theta). \qquad (81)
\end{aligned}
$$

$\lambda = 0.5$

$$\Gamma_2 = 18.330J_0 + 14.374J_1, \qquad (82)$$

$$
\begin{aligned}
\Gamma_4 = & 2.1853J_1^2 + .24042J^2 + 4.5488J_1J_0 \\
& +2.5714J_0^2 + .24042(J_1^2 - J^2)\cos(4\theta), \qquad (83)
\end{aligned}
$$

$$
\begin{aligned}
\Gamma_6 = \quad & -.40938J_1^3 + .13646J_1^2J - .12560J_1J^2 - .13646J^3 \\
- \quad & .31755J_1^2J_0 + .20015J^2J_0 - 1.0593J_1J_0^2 - .21376J_0^3 \\
+ \quad & \Big[ -.12560J_1^3 - .13646J_1^2J + .12560J_1J^2 + .13646J^3 \\
+ \quad & \qquad .20015J_1^2J_0 - .20015J^2J_0 \Big] \cos(4\theta). \qquad (84)
\end{aligned}
$$

**Appendix 2**

After a trivial change of variables, the Hamiltonian (5) may be written in the following form (the g. s. energy is shifted to zero):

$$\begin{aligned} H = & -\partial^2/\partial x^2 - \partial^2/\partial y^2 - (1/x^2 + 1/y^2)(1-z^2)\partial^2/\partial z^2 - 18 \\ - & (1-z^2)^{-1}(1/x^2 + 1/y^2) + 9(x^2+y^2) \\ + & 6\lambda\Big\{ -\tfrac{7}{2}(x^2+y^2) + \tfrac{9}{4}(x^2+y^2)^2 + 3x^2y^2(1-z^2)\Big\} \\ + & \lambda^2\Big\{\tfrac{81}{16}(x^2+y^2)^3 + \tfrac{63}{4}x^2y^2(1-z^2)(x^2+y^2)\Big\}. \end{aligned} \tag{85}$$

We numerically computed the energy levels of this Hamiltonian by writting it in matrix form. In quality of basis functions we used the eigenfunctions of the unperturbed Hamiltonian

$$H_0 = H_{\{\lambda=0\}}. \tag{86}$$

The eigenfunctions of $H_0$ are given by

$$|n_x> \ |n_y> \ |n_z>, \tag{87}$$

where $|n_z>$ satisfies the equation

$$\left[(1-z^2)\frac{\partial^2}{\partial z^2} + \frac{1}{1-z^2}\right]|n_z> = -n_z(n_z+1)|n_z>, \tag{88}$$

i.e.

$$|n_z> = (1-z^2)^{1/2}P_{n_z}(z), \tag{89}$$

where $P_{n_z}$ are the Legendre polynomials. On the other hand, $|n_x>$ and $|n_y>$ are solutions of the same equation, which for $|n_x>$ takes the form

$$\left[-\frac{\partial^2}{\partial x^2} + 9x^2 + \frac{n_z(n_z+1)}{x^2}\right]|n_x> = 6(n_z + 2n_x + 3/2)|n_x> . \tag{90}$$

It means that $|n_x>$ and $|n_y>$ are expressed in terms of radial oscillator functions. The eigenvalues of $H_0$ are, evidently,

$$12(n_x + n_y + n_z), \tag{91}$$

and the matrix elements of the perturbation are computed from the following basic quantities

$$\begin{aligned} < n'_x, n'_y, n'_z | x^2 | n_x, n_y, n_z > &= \delta_{n'_y n_y} \delta_{n'_z n_z} \frac{1}{3} \Big\{ \\ &- (n'_x + 1)^{1/2} (n'_x + n'_z + 3/2)^{1/2} \delta_{n_x, n'_x + 1} \\ &+ (2n'_x + n'_z + 3/2) \delta_{n_x n'_x} \\ &- (n'_x)^{1/2} (n'_x + n'_z + 1/2)^{1/2} \delta_{n_x, n'_x - 1} \Big\}, \end{aligned} \tag{92}$$

$$\begin{aligned} < n'_x, n'_y, n'_z | z^2 | n_x, n_y, n_z > &= \delta_{n'_x n_x} \delta_{n'_y n_y} \frac{1}{\sqrt{(2n'_z + 1)(2n_z + 1)}} \\ &\Big\{ \frac{(n_z + 2)(n_z + 1)}{2n_z + 3} \delta_{n'_z, n_z + 2} \\ &+ \left[ \frac{n_z^2}{2n_z - 1} + \frac{(n_z + 1)^2}{2n_z + 3} \right] \delta_{n_z n'_z} \\ &+ \frac{(n_z - 1) n_z}{2n_z - 1} \delta_{n'_z, n_z - 2} \Big\}. \end{aligned} \tag{93}$$

To compute the eigenvalues of $H$, we used the 120 functions of $H_0$ which quantum numbers fulfil the requirement

$$n_x + n_y + n_z \leq 7. \tag{94}$$

Note that we did not constructed explicitly basis functions with defined symmetry properties. This may be a reason for the numerical estimate not showing exact degeneracy in some cases.

- Tab. 1 Comparison between the improved BG estimates of energy levels ($E_2$, $E_4$ and $E_6$) and the energy values, $E$, obtained from a direct numerical diagonalization of the quantum Hamiltonian. The parameter $\lambda$ is equal to 0.1.

| $n_0$ | $n_1$ | $n$ | $E_2$ | $E_4$ | $E_6$ | $E$ |
|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 12.56 | 13.09 | 13.08 | 13.29 |
| | | | | | | 13.29 |
| 1 | 0 | 0 | 13.51 | 14.45 | 14.37 | 14.38 |
| 0 | 2 | 0 | 25.13 | 27.25 | 26.91 | 27.46 |
| | | | | | | 27.59 |
| 0 | 2 | 1 | 25.13 | 27.64 | | 27.83 |
| 1 | 1 | 0 | 26.07 | 29.04 | 28.50 | 28.93 |
| | | | | | | 28.93 |
| 2 | 0 | 0 | 27.01 | 30.80 | 30.17 | 30.15 |
| 0 | 3 | 0 | 37.69 | 42.46 | 41.27 | 42.49 |
| | | | | | | 42.69 |
| 0 | 3 | 1 | 37.69 | 43.25 | | 42.96 |
| | | | | | | 43.18 |
| 1 | 2 | 0 | 38.64 | 44.69 | 43.22 | 44.24 |
| | | | | | | 44.42 |
| 1 | 2 | 1 | 38.64 | 45.08 | | 44.82 |
| 2 | 1 | 0 | 39.58 | 46.88 | 44.78 | 45.73 |
| | | | | | | 45.76 |
| 3 | 0 | 0 | 40.51 | 49.04 | 46.92 | 47.17 |

- Tab. 2 Same as in Tab. 1 for $\lambda = 0.2$.

| $n_0$ | $n_1$ | $n$ | $E_2$ | $E_4$ | $E_6$ | $E$ |
|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 13.07 | 14.03 | | 14.32 |
| | | | | | | 14.32 |
| 1 | 0 | 0 | 14.86 | 16.42 | 16.25 | 16.27 |
| 0 | 2 | 0 | 26.14 | 29.99 | | 30.12 |
| | | | | | | 30.35 |
| 0 | 2 | 1 | 26.14 | 30.55 | | 30.73 |
| 1 | 1 | 0 | 27.93 | 33.02 | | 32.67 |
| | | | | | | 32.67 |
| 2 | 0 | 0 | 29.72 | 35.98 | 34.60 | 34.75 |
| 0 | 3 | 0 | 39.22 | 47.86 | | 47.31 |
| | | | | | | 47.67 |
| 0 | 3 | 1 | 39.22 | 49.42 | | 48.08 |
| | | | | | | 48.44 |
| 1 | 2 | 0 | 41.00 | 51.54 | | 50.28 |
| | | | | | | 50.59 |
| 1 | 2 | 1 | 41.00 | 52.10 | | 51.22 |
| 2 | 1 | 0 | 42.79 | 55.14 | 50.77 | 52.80 |
| | | | | | | 52.83 |
| 3 | 0 | 0 | 44.58 | 58.66 | 54.05 | 55.15 |

• Tab. 3 Same as in Tab. 1 for $\lambda = 0.5$.

| $n_0$ | $n_1$ | $n$ | $E_2$ | $E_4$ | $E_6$ | $E$ |
|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 14.37 | 16.34 | | 16.73 |
| | | | | | | 16.74 |
| 1 | 0 | 0 | 18.33 | 20.90 | 20.69 | 20.71 |
| 0 | 2 | 0 | 28.75 | 36.53 | | 36.20 |
| | | | | | | 36.69 |
| 0 | 2 | 1 | 28.75 | 38.45 | | 37.34 |
| 1 | 1 | 0 | 32.70 | 41.77 | | 41.19 |
| | | | | | | 41.22 |
| 2 | 0 | 0 | 36.66 | 46.95 | 45.24 | 45.19 |
| 0 | 3 | 0 | 43.12 | 60.63 | | 58.65 |
| | | | | | | 59.45 |
| 0 | 3 | 1 | 43.12 | 64.67 | | 60.20 |
| | | | | | | 60.96 |
| 1 | 2 | 0 | 47.08 | 66.53 | | 65.35 |
| | | | | | | 66.08 |
| 1 | 2 | 1 | 47.08 | 68.45 | | 67.55 |
| 2 | 1 | 0 | 51.03 | 72.36 | | 71.83 |
| | | | | | | 71.88 |
| 3 | 0 | 0 | 54.99 | 78.13 | | 78.79 |

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