Quantum anharmonic oscillator in the Heisenberg picture and multiple scale techniques

G. Auberson and M. Capdequi Peyranère

Laboratoire de Physique Mathématique et Théorique, CNRS UMR 5825, Université Montpellier II, F-34095 Montpellier Cedex 5, PM 0136, France

Multiple scale techniques are well known in classical mechanics to give perturbation series free from resonant terms. When applied to the quantum anharmonic oscillator, these techniques lead to interesting features concerning the solution of the Heisenberg equations of motion and the Hamiltonian spectrum.

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I. INTRODUCTION

Multiple scale techniques (MST) originated in Poincaré works have been developed by many authors, mainly in solving (partial) differential equations related to physical problems in celestial mechanics or in fluid dynamics. All of these methods have a common mathematical purpose: to avoid resonances or secularities appearing in the usual or conventional perturbative theory. From a more physical point of view, one can see the MST as adaptable methods that feel the underlying physical phenomena in order to fit them. In other words, the usual perturbative theory tends to impose its choices while MST are flexible and compose with the real medium.

In this work, we apply one of the various MST to the quantum anharmonic oscillator. Such studies have been initiated by Bender and Bettencourt (B&B) in two recent papers [1,2]. They have found that the nonresonance condition leads to a "mass renormalization" of the oscillator and—as a by-product—to the energy-level differences of the quantum oscillator. This pioneering work was limited to the first nontrivial order in MST perturbation of the coupling constant of the anharmonicity. The aim of the present paper is to extend this early study in several directions. First, we introduce an alternative framework, which turns out to be more convenient than the B&B one for performing higher-order calculations. Second, it turns out that we are able to obtain the energy levels themselves at these perturbative orders. In the third point, we show that the diagonalization of the Hamiltonian is rather easy once the free Hamiltonian has been recast in an appropriate form. Finally, this approach leads to a natural and elegant method to find perturbatively the eigenvalues of the full Hamiltonian, far away from the original MST concept.

The paper is organized as follows. In the first section, although the classical anharmonic oscillator is studied in detail in many textbooks [3,4], we sketch some relevant points in order to further clarify the differences and the analogies between the classical and the quantum cases. In the second section we explain our framework and we work out the two first orders in MST perturbation, that includes the full solution of the Heisenberg equations and the energy levels. The third section is devoted to general arguments showing that the method is compelled to work at any order, due to its connection with a certain unitary transformation which diagonalizes the Hamiltonian of the anharmonic oscillator. We

postpone to an Appendix some explicit results: the solutions of the Heisenberg equations of motion and the energy levels of the full Hamiltonian, up to the order 6 included.

II. THE CLASSICAL CASE

The classical anharmonic oscillator (CAO) is probably one of the most popular examples where the conventional and MST perturbative theories lead to obvious differences. Often, one speaks of the Duffing equation instead, although this equation is nothing but the equation of motion of the CAO. To be precise, the Duffing equation is a second-order nonlinear equation in the time variable, the solution of which being the position of the CAO. Starting from the CAO Lagrangian (in units where the mass parameter is one)

$$L(q,\dot{q}) = \dot{q}^2/2 - \omega^2 q^2/2 - gq^4,$$

one readily gets from the Euler-Lagrange equation

$$(e): \ddot{q} + \omega^2 q + 4gq^3 = 0.$$

The usual formal perturbation expansion reads

$$q(t) = \sum_{n=0}^{\infty} g^n q_n(t),$$

[with some initial conditions, say $q(0) = Q$ and $\dot{q}(0) = 0$], and the first equations one obtains from (e) are

$$(e_0): \ddot{q}_0 + \omega^2 q_0 = 0,$$

$$(e_1): \ddot{q}_1 + \omega^2 q_1 = -4q_0^3.$$

Then the frequency of the solution of the homogeneous part of (e_1) coincides with the frequency of $q_0(t) = Q \cos \omega t$, which generates a resonance in the solution $q_1(t)$ of the full equation (e_1)

$$q_1(t) = \frac{Q^3}{8\omega^2} (\cos 3\omega t - \cos \omega t - 12\omega t \sin \omega t).$$

Hence $q_1(t)$ is unbounded and the truncated expansion $q_0(t) + gq_1(t)$ cannot be an acceptable approximation of $q(t)$ for times t larger than $\omega/Q^2 g$, however small g may be. The flaw is even worse at the higher orders. It is obvious on

this simple example that the perturbative solution develops spurious behavior which is absent in the exact solution. Indeed, it is well known that the exact solution is bounded and periodic.

The main idea of MST for dealing with this problem is the introduction of new variables, independent and appropriate, and we refer to textbooks for an extensive review of the various possibilities. Here we concentrate on the anharmonic oscillator. Some methods take into account *ab initio* that the circular functions play a major role. For instance, in the Poincaré method, one looks for sine and cosine solutions whose argument is still ωt but where ω is now an arbitrary function of the coupling constant, actually $\omega = \Sigma g^n \omega_n$. Then one has to find the ω_n's, order by order, to discard the resonance. We do not insist on the application of these methods to the CAO because we believe they are not suitable for the quantum case. Another class of MST seems to be of a larger use, since there is no "prerequisite" in these methods. The MST we will use, also called the derivative expansion method, belongs to this class: it promotes the time variable to be a function of the coupling constant, namely, $t_n = g^n t$. Actually, the method is not so rough and one first extends the function depending on t to an "extended" function depending on all the variables t_n $(n = 0, 1, 2, \dots)$ assumed to be independent [5]. So, one introduces a position function $Q(T, g)$ depending on the collection $T = \{t_0, t_1, t_2, \dots,\}$ of independent variables t_n. This function is considered as an extension of the true position in the Lagrange formalism, which is recovered by restricting Q to the section $t_n = g^n t$ of the T space: $q(t, g) = Q(T, g)|_{t_n = g^n t}$.

Then, forgetting temporarily any reference to the coupling constant in these t_n variables, one expands in power of g the position function Q

$$Q(T, g) = \sum_{n=0}^{\infty} g^n Q_n(T).$$

One obtains from (e) the following set of equations, limited here at the three first orders:

$$D_0^2 Q_0(T) + \omega^2 Q_0(T) = 0,$$

$$D_0^2 Q_1(T) + \omega^2 Q_1(T) = -2 D_0 D_1 Q_0(T) - 4 Q_0^3(T),$$

$$D_0^2 Q_2(T) + \omega^2 Q_2(T) = -(D_1^2 + 2 D_0 D_2) Q_0(T)$$
$$- 2 D_0 D_1 Q_1(T) - 12 Q_0^2(T) Q_1(T),$$

using $d/dt = \Sigma_n g^n D_n$, $D_n = \partial/\partial t_n$.

The basic principle of the method now consists of adjusting the t_1 dependence of $Q(T)$ so as to eliminate the secularity in the second equation, next the t_2 dependence of $Q(T)$ so as to eliminate the secularity in the third equation, and so on. We shall not work out the derivation here (it can be found for example in Refs. [3] or [4]) and we merely give the solution up to the second order in g in its final form, for further classical versus quantum discussions

$$q(t, g) = \frac{a}{2} \left[\exp(-i(\Omega t + b)) + \frac{\lambda}{8} \left(1 - \frac{21\lambda}{8} \right) \exp(-3i(\Omega t + b)) + \frac{\lambda^2}{64} \exp(-5i(\Omega t + b)) \right] + \text{C.C.},$$

where

$$\Omega = \omega \left(1 + \frac{3\lambda}{2} - \frac{15\lambda^2}{16} \right), \lambda = \frac{g a^2}{\omega^2} \qquad (1)$$

and a and b are two real integration constants fixed by the initial conditions (here unspecified).

Since the (perturbative) energy is conserved, it can be computed most easily by choosing $t = -b/\Omega$ or $t = (\pi/2 - b)/\Omega$ in $q(t, g)$

$$E_c = \frac{a^2 \omega^2}{2} \left(1 + \frac{9\lambda}{4} + \frac{25\lambda^2}{64} \right) + O(\lambda^3). \qquad (2)$$

We conclude this section with a few comments. As far as we know, all the multiple scale techniques dealing with the secularities of the classical anharmonic oscillator are successful. However this is not a general feature, and some methods are not suitable for certain problems. Moreover, it is absolutely not our purpose to discuss on a rigorous basis the mathematical aspects of the secular or nonsecular perturbative expansions.

III. THE QUANTUM CASE: DERIVATION

The quantum anharmonic oscillator (QAO) has been studied in the paper of B&B through the Heisenberg equation of motions for the relevant operators and we will follow this method. The main difference between the work of B&B and ours is that we will use the creation and annihilation operators to manage the problem of removing the secularities. At first sight the gain in doing this choice is not obvious and perhaps not essential. Moreover one can detect in the B&B paper an indication pointing to this direction. Let us look at the couple of Eqs. (21) in their work [1], which can be written as

$$D_1 Y = -CX - XC \quad \text{and} \quad D_1 X = CY + YC,$$

where X and Y are t_1 dependent, self-adjoint operators while C is a constant, self-adjoint operator. The authors proceed with some arguments "suggesting" the form of the solution, with the help of Weyl ordered products and Euler polynomials to deal with these equations. Of course, it seems difficult, or at least hazardous, to generalize at high orders a "suggestive" method, which could be seen as a reminiscence of the Poincaré method, but we have more convincing arguments to leave this path. First, using $Z = X + iY$, the previous couple of equations reduces to the single equation

$$D_1 Z(t_1) = -i[Z(t_1) C + C Z(t_1)]$$

whose solution is $Z(t_1) = \exp(-iCt_1) Z(0) \exp(-iCt_1)$, as it is easy to check. The operator $Z(t_1)$ is closely related to the

creation/annihilation operators. Once derived the expression of the creation/annihilation operators, it is not necessary, in order to proceed further, to write down the position operator. Indeed, almost all the informations, the "mass renormalization" effect and the difference of energy levels, are already contained in the argument of the exponentials. Second, the Heisenberg equations in terms of creation/annihilation operators are first-order differential equations in place of the second-order one for the position operator, which simplifies noticeably the whole procedure. To be honest, one has the disadvantage to carry both creator and annihilator, but this is not a serious complication. Last, there appears also a large variation between the B&B works and ours in the status of the initial conditions: we do not use these conditions as in the classical case, which is the way taken by B&B. This point will become obvious throughout our study.

We start with the QAO Hamiltonian H written in terms of the momentum p and position q operators in convenient units ($\hbar = \omega = 1$): $H = p^2/2 + q^2/2 + gq^4$, where g is assumed to be a "small" (positive) coupling constant. Within the Heisenberg picture, the dynamics is governed by the equations

$$\dot{q} = i[H,q], \quad \dot{p} = i[H,p],$$

supplemented by the canonical commutation relation $[q,p] = i$, valid at all times. The Heisenberg equations give: $\dot{q} = p$ and $\dot{p} = -q - 4gq^3$. Writing as usual $q = (a + a^\dagger)/\sqrt{2}$ and $p = -i(a - a^\dagger)/\sqrt{2}$, the Hamiltonian becomes

$$H(a,a^\dagger,g) = 1/2 + a^\dagger a + g(a + a^\dagger)^4/4 \tag{3}$$

together with

$$[a(t,g), \ a(t,g)] = 1, \quad \forall t, \tag{4}$$

where, to avoid possible confusion later on, we have kept track of the variables t and g.

The Heisenberg equation for the annihilator

$$\dot{a}(t,g) = i[H(a(t,g),a^\dagger(t,g),g),a(t,g)],$$

reads, in our case

$$\dot{a}(t,g) = -i[a(t,g) + g(a(t,g) + a^\dagger(t,g))^3]. \tag{5}$$

Since the Hamiltonian is conserved, its formal solution is

$$a(t,g) = \exp[iH(a(0),a^\dagger(0),g)t]a(0)$$
$$\times \exp[-iH(a(0),a^\dagger(0),g)t],$$

with $a(0) \equiv a(0,g)$.

We now turn on the formal series of the multitime perturbative expansion, similar to that used in the classical case. First one introduces an operator valued function $A(T,g)$ depending on the collection T of independent variables t_j. This function is considered as an extension of the true annihilation operator in the Heisenberg picture, which is recovered through the restriction

$$a(t,g) = A(T,g)\big|_{t_j = g^j t}. \tag{6}$$

Then the time derivative becomes

$$\dot{a}(t,g) = \sum_{n \geq 0} g^n D_n A(T,g)\big|_{t_j = g^j t}.$$

Second, $A(T,g)$ is expanded as

$$A(T,g) = \sum_{n \geq 0} g^n A_n(T). \tag{7}$$

As for the initial conditions to be associated with the equation of motion (5), one notices that

$$a(0,g) = \sum_{n \geq 0} g^n A_n(0). \tag{8}$$

This forces us to choose between two possible starting viewpoints either (a): $a(0,g)$ is taken as independent of g, which implies

$$A_n(0) = 0, \forall n \geq 1, \tag{9}$$

or (b): the previous condition is not imposed, in which case the initial values of $a(t,g)$ must be considered as a function of g.

It turns out that both approaches lead to consistent multitime expansions. In fact, the choice (a) was (implicitly) adopted by B&B. However, these authors did not extend their analysis beyond the first order. In this paper, we rather follow the procedure (b), which we found much more convenient, and in a sense, more natural.

The equation of motion for $a(t,g)$ gives us the following infinite system for the $A_n(T)$'s:

$$D_0 A_n + iA_n = -\sum_{m=0}^{n-1} D_{n-m}A_m - i \sum_{\substack{m,r,s,>,0 \\ m+r+s=n-1}} Q_m Q_r Q_s$$

$$(n = 0,1,2, \ldots) \tag{10}$$

where $Q_n = A_n + A_n^\dagger$, or explicitly

$$D_0 A_0 + iA_0 = 0, \tag{10a}$$

$$D_0 A_1 + iA_1 = -D_1 A_0 - iQ_0^3, \tag{10b}$$

$$D_0 A_2 + iA_2 = -(D_2 A_0 + D_1 A_1)$$
$$- i(Q_0^2 Q_1 + Q_0 Q_1 Q_0 + Q_1 Q_0^2), \tag{10c}$$

etc.

A simple check shows us that **any** formal solution of Eq. (10) generates via Eqs. (6) and (7) a formal solution $a(t,g)$ of Eq. (5). In particular, this implies that, for such a solution, $[A(T,g),A^\dagger(T,g)]\big|_{t_j = g^j t}$ is independent of t. Of course, this does no mean yet that $[A(T,g),A^\dagger(T,g)]$ is independent of T, allowing us to impose

$$[A(T,g),A^\dagger(T,g)] = 1 \quad \forall T, \tag{11}$$

in order to insure the canonical commutation relation (4). However, one can look for **those** solutions of Eq. (10) which are subjected to the stronger condition (11), if such solutions do exist indeed, i.e., if no inconsistencies or obstructions arise in their iterative construction. Together with Eq. (7), this entails

$$[A_0(T), A_0^\dagger(T)] = 1$$
$$\forall T$$
$$\sum_{m=0}^{n} [A_m(T), A_{n-m}^\dagger(T)] = 0, \quad n \geq 1. \tag{12}$$

We are now ready to construct step by step the resonance-free solution of the problem. To zeroth order, Eq. (10a) and the first Eq. (12) yield

$$A_0(T) = A_{01}(T_1) \exp(-it_0) \tag{13}$$

with

$$[A_{01}(T_1), A_{01}^\dagger(T_1)] = 1, \quad \forall T_1, \tag{14}$$

and the notation $T_k = \{t_k, t_{k+1}, \ldots, \}, (k = 1, 2, \ldots)$.

Then, one can proceed to the first order step by inserting Eq. (13) into Eq. (10b)

$$D_0 A_1 + i A_1 = -[D_1 A_{01} + i(A_{01}^2 A_{01}^\dagger + A_{01} A_{01}^\dagger A_{01}$$
$$+ A_{01}^\dagger A_{01}^2)] \exp(-it_0) - i[A_{01}^3 \exp(-3it_0)$$
$$+ A_{01}^{\dagger 3} \exp(+3it_0) + (A_{01}^{\dagger 2} A_{01} + A_{01}^\dagger A_{01} A_{01}^\dagger$$
$$+ A_{01} A_{01}^{\dagger 2}) \exp(+it_0)]. \tag{15}$$

Before integrating this equation, one has to get rid of the first resonant term on the right-hand side, which would produce a contribution growing linearly with $t_0(=t)$. This leads to the condition

$$D_1 A_{01} = -i(A_{01}^2 A_{01}^\dagger + A_{01} A_{01}^\dagger A_{01} + A_{01}^\dagger A_{01}^2), \tag{16}$$

which will fix the t_1 dependence of A_{01}.

To do that, let us first introduce the self-adjoint operator $N(T) = A_0^\dagger(T) A_0(T)$. Thanks to Eq. (13) and its creator version, $N(T)$ is only T_1 dependent: $N(T) = A_{01}^\dagger(T_1) A_{01}(T_1)$. Moreover as a consequence of Eq. (14), $A_{01}(T_1) N(T_1) = [N(T_1) + 1] A_{01}(T_1)$. Last, from Eq. (16), one observes that $D_1 N(T_1) = 0$. Thus, N is also independent of t_1 and Eq. (16) can be now written in the tractable form

$$D_1 A_{01} = -3i A_{01}(T_1) N(T_2),$$

which produces

$$A_{01}(T_1) = A_{02}(T_2) \exp[-3iN(T_2)t_1].$$

This allows us to write down the first-order annihilation operator

$$A_0(T) = A_{02}(T_2) \exp[-i(t_0 + 3N(T_2)t_1)]. \tag{17}$$

At the same time, Eq. (14) becomes

$$[A_{02}(T_2), A_{02}^\dagger(T_2)] = 1, \forall T_2. \tag{18}$$

One can now come back to the form of Eq. (15) exempted of secularity to obtain its general solution

$$A_1(T) = A_{01}^3(T_1) \exp(-3it_0)/2 - A_{01}^{\dagger 3}(T_1) \exp(+3it_0)/4$$
$$- 3N(T_2) A_{01}^\dagger(T_1) \exp(+it_0)/2 + C_1(T_1) \exp(-it_0), \tag{19}$$

where the operator $C_1(T_1)$ is an integration "constant." The latter must be so adjusted, if possible, as to insure that the second Eq. (12)

$$[A_0(T), A_1^\dagger(T)] + [A_1(T), A_0^\dagger(T)] = 0, \tag{20}$$

be fulfilled at all times T. Here, it turns out that Eq. (20) is satisfied by taking simply $C_1(T_1) = 0$. One ends up with

$$A_1(T) = A_0^3(T)/2 - A_0^{\dagger 3}(T)/4 - 3N(T_2) A_0^\dagger(T)/2 \tag{21}$$

and the first-order step is complete.

Before going further, some comments are in order. First, writing the position operator $q_0 + g q_1$, one notes that the coefficients of $\exp(\pm it_0)$ in q_0 get corrections coming from q_1. It means, in the position formalism, the scheme used by B&B, that one would have to take into account the solutions of the homogeneous second-order differential equation. Second, it appears in Eq. (21) that any power of $\exp(+it_0)$ [respectively, $\exp(-it_0)$] is multiplied by the same power of $A_{01}^\dagger(T_1)$ [respectively, $A_{01}(T_1)$]. Such a correspondance, which is specific to our way of managing the initial conditions, will be a guide throughout our study. Last, the solution of the homogeneous equation in the classical case is different. This variation with the quantum case is due to the different status of the initial conditions.

Clearly, one can go iteratively through the higher-order steps by similar (although rapidly tedious) calculations as long as the integration "constants" analogous to $C_1(T_1)$ can be properly adjusted. As in the first-order step, we gather in Eq. (10c) the terms containing $\exp(-it_0)$, since $\exp(-it_0)$ is again (and always) solution of the homogeneous equation. Because $D_1 A_1(T)$ does not provide such a term, we just have to take into account the nonderivative part of the right-hand side of Eq. (10c). Through an intensive use of the relation $A_{01}(T_1) N(T_2) = [N(T_2) + 1] A_{01}(T_1)$, this expression can be reduced to $-3A_{02}(T_2)[17N^2(T_2) + 7] \exp[-it_0 - 3iN(T_2)t_1]/4$, and the nonresonance condition coming from the second order reads

$$D_2 A_{02}(T_2) = 3i A_{02}(T_2)[17N^2(T_2) + 7]/4.$$

This equation shows that $N(T_2)$ is in fact independent of t_2, too, [i.e. $N(T_2) = A_{03}^\dagger(T_3) A_{03}(T_3)$] and we find through integration

$$A_{02}(T_2) = A_{03}(T_3) \exp[+3i(17N^2(T_3) + 7)t_2/4], \tag{22}$$

whereas Eq. (18) becomes

$$[A_{03}(T_3),A_{03}^\dagger(T_3)]=1, \quad \forall T_3. \tag{23}$$

Collecting Eqs. (7), (17), and (22), we see that the nonresonance conditions, up to the second order, imply that the first-order term of the expansion of the annihilation operator is, in the variable t

$$a_0(t,g)=a_0(0,g)\{\exp[-it(1+3gN-3g^2(17N^2+7)/4)]$$
$$+O(g^3)\}, \tag{24}$$

which exhibits a large difference with the classical case: 17 is a prime number, difficult to link with the other prime number 5 coming in the CAO frequency (1). We will discuss later on this CAO/QAO (apparent) discrepancy. Nevertheless, the result, Eq. (24), is in perfect agreement with the perturbative expression of the energy levels of the QAO, as calculated by standard methods:

$$E_n(g)=1/2+n+3g(1+2n+2n^2)/4-g^2(1+2n)(21+17n$$
$$+17n^2)/8+O(g^3). \tag{25}$$

Indeed, a straightforward argument based on the formal expression of $a(t,g)$ in the Heisenberg picture shows us that the frequency appearing in Eq. (24) for $N=n$ should coincide with $E_n(g)-E_{n-1}(g)$. This is readily checked.

Turning back on the second-order Eq. (10c) cleared from its resonant terms, we obtain its general solution

$$A_2(T)=-15A_0^3(N-1)/4+3A_0^5/16+3(23N^2+7)A_0^\dagger/8$$
$$+21(N-1)A_0^{\dagger 3}/16-A_0^{\dagger 5}/8+C_2(T_1)\exp(-it_0),$$
$$\tag{26}$$

where A_0 and N stand for $A_0(T)$ and $N(T_3)$. In contrast with $C_1(T_1)$ in Eq. (19), the operator $C_2(T_1)$ cannot be taken as vanishing, because the second condition (12),

$$[A_0(T),A_2^\dagger(T)]+[A_1(T),A_1^\dagger(T)]+[A_2(T),A_0^\dagger(T)]=0,$$

would not be fulfilled. Imposing this and using Eqs. (12), (17), (18), and (26), one finds instead an appropriate expression for the solution of the homogeneous version of Eq. (10c), namely,

$$C_2(T_1)\exp(-it_0)=-9A_0(T)(1-3N^2)/32. \tag{27}$$

Let us notice that the (operator) coefficients of $\exp(\pm it_0)$ which appear in the zeroth-order solution get corrections from the first and second orders, and the coefficients of $\exp(\pm 3it_0)$ which appear at the first order get also corrections coming from the second order. Such a behavior still holds at the third order, as we have checked.

So far, the perturbative expression of the energy levels of the QAO (which was not our main goal) did not show up in full within our MST procedure. Yet, it can be found (without appealing to other perturbative methods) by inserting $a(t,g)$ as given by Eqs. (6), (21), (26), and (27) in the Hamiltonian

(3). Obviously, we are waiting for an expansion in powers of g polynomially dependent on A_0 and $A_0^\dagger$, up to the second order in g

$$H=H_0+gH_1+g^2H_2+O(g^3).$$

The result is that the H_j's are a function of $N=A_0^\dagger A_0$, not of A_0 and $A_0^\dagger$ separately

$$H=1/2+N+3g(1+2N+2N^2)/4-g^2(1+2N)(21+17N$$
$$+17N^2)/8+O(g^3). \tag{28}$$

This feature, which technically appears as an accident due to many cancellations, is in fact easy to understand. One observes, at each step, the $t_0,\ t_1,\ t_2,\ldots$ dependences of $A_0(T)$ arise from the exponentials only. Since the t dependence must eventually disappear from the conserved quantity H, a proper balance between $A_0(T)$ and $A_0^\dagger(T)$ is expected in each of the monomials H_j, namely, as many creators as annihilators. Then, whatever the number and the order of the A_0's and $A_0^\dagger$'s in those polynomials, the commutation relation (12) allows us to cast the H_j's in the form of polynomials in $N=A_0^\dagger A_0$. Furthermore, anticipating a result to be proved in the next section, $N(T)$ is not only independent of $t_0,\ t_1,$ and t_2 but in fact of T altogether: $N=A_0^\dagger(0)A_0(0)$. On account of the Heisenberg algebra (12) (taken at $T=0$) this implies that the spectrum of N is the set of non-negative integers, and the expression (28) for H is in complete agreement with Eq. (25) indeed.

Finally, we have to explain the apparent discrepancy noticed earlier between the classical and quantum results. Let us write the classical energy (2) for $\omega=1$: $E_c=a^2/2+3ga^4/8+O(g^2)$. Now for large n the quantum energy (25) reduces to: $E_q=n+3gn^2/2+O(g^2)$. Then the natural correspondance is $a^2/2\rightarrow n$ plus a quantum correction so adjusted as to insure $E_c=E_q+O(g^2)$. One finds $a^2/2\rightarrow n-3gn^2$ which, inserted in the classical frequency (1) gives $\Omega=1+3gn-51g^2n^2/4$, in agreement with the large n quantum frequency from Eq. (24), derived within the MST scheme.

IV. THE QUANTUM CASE: GENERAL DISCUSSION

In the previous section, in particular on Eqs. (21), (26), and (27), one observes that the construction is made with two elementary bricks $A_0(T)$ and $A_0^\dagger(T)$, where $A_0(T)$ is the first term in the MST expansion of the annihilation operator. We have also pointed out the simple connection between the operator N and the Hamiltonian. More precisely, the first perturbative results exhibit the following features:

(1) $N=A_0^\dagger(T)A_0(T)$ is independent of $t_0, t_1, t_2, \ldots$, i.e., of T.

(2) The "nonhomogeneous" parts of $A_n(T)$ depend on T through the basic operators $A_0(T)$ and $A_0^\dagger(T)$. The same is true for the "homogeneous" parts $C_n(T_1)\exp(-it_0)$ which, after determination of $C_n(T_1)$, can be recast in the form of functions of $A_0(T)$ and $A_0^\dagger(T)$ only.

(3) The operators H and N commute.

If these features persist at all orders, then (putting aside

any consideration of convergence) one should obtain in the limit

$$A(T,g)=A_0(T)+\sum_{n=1}^{\infty} g^n F_n[A_0(T),A_0^{\dagger}(T)], \quad (29)$$

where

$$A_0(T)=A_0\exp\left[-i\left(t_0+\sum_{n=1}^{\infty} f_n(N)t_n\right)\right] \quad (30)$$

together with $[A_0,A_0^{\dagger}]=1$, and where the F_n's are some polynomial functions of A_0 and $A_0^{\dagger}$ while the f_n's are some polynomial functions of N. We will show below that the resonance-free solutions of the perturbative multitime equations of motion do exist indeed, and have the general forms (29) and (30). This means, in particular, that no obstructions are encountered in determining the integration "constants" $C_n(T_1)$ and giving them the appropriate form. Equations (29) and (30) then yield

$$a(t,g)=a_0(t,g)+\sum_{n=1}^{\infty} g^n F_n(a_0(t,g),a_0^{\dagger}(t,g)), \quad (31)$$

where

$$a_0(t,g)=A_0\exp\left[-i\left(1+\sum_{n=1}^{\infty} g^n f_n(N)\right)t\right] \quad (32)$$

and $N=A_0^{\dagger}A_0$ is a constant operator.

Actually, these facts result from the full equivalence between the iterative process described in the previous section and the perturbative determination of an unitary transformation which brings the Hamiltonian to a diagonal form.

In order to prove this equivalence, let us consider the spectral decomposition of the Hamiltonian

$$H(a_0,a_0^{\dagger},g)\equiv 1/2+a_0^{\dagger}a_0+g(a_0+a_0^{\dagger})^4/4$$

$$=\sum_{n=0}^{\infty} E_n(g)|n,g\rangle\langle n,g|,$$

where $\{|n,g\rangle\}$ is the orthonormal basis made of the "perturbed" eigenvalues of H (for future convenience, a is written here as a_0). We also introduce the "unperturbed," orthonormal Fock basis $\{|n\rangle\}$ induced by the operators a_0 and $a_0^{\dagger}$, together with the unitary transformation which maps the former onto the latter

$$|n\rangle=U(g)|n,g\rangle (n=0,1,2,\dots).$$

The unitary operator $U(g)$ is determined up to a N-dependent, arbitrary, right phase factor, where $N=a_0^{\dagger}a_0$.

Then if we define H_d as $H_d(a_0,a_0^{\dagger},g)=U^{\dagger}(g)H(a_0,a_0^{\dagger},g)U(g)$, we have

$$H_d(a_0,a_0^{\dagger},g)=H(a(g),a^{\dagger}(g),g), \quad (33)$$

where we denote by $a(g)$ the annihilation operator transformed by $U(g)$

$$a(g)=U^{\dagger}(g)a_0U(g). \quad (34)$$

We also have

$$H_d(a_0,a_0^{\dagger},g)=\sum_{n=0}^{\infty} E_n(g)|n\rangle\langle n|.$$

In other words, the unitary transformations (34) of the dynamical variables is that one which diagonalizes the Hamiltonian in the $\{|n\rangle\}$ basis. The perturbative form of Eqs. (33) and (34) are

$$a(g)=a_0+\sum_{n=1}^{\infty} g^n a_n \quad (35)$$

and

$$H_d(a_0,a_0^{\dagger},g)=\sum_{n=0}^{\infty} g^k H_k=\frac{1}{2}+a_0^{\dagger}a_0+\sum_{n=1}^{\infty} g^k H_k, \quad (36)$$

where the explicit expressions of the H_k's in terms of the a_n's are obtained by substituing the perturbative form (35) in $H[a(g),a^{\dagger}(g),g]$, and expanding. For the QAO Hamiltonian we are interested in, those H_k's are

$$H_k=\sum_{n=0}^{k} a_m^{\dagger}a_{k-m}+\sum_{\substack{m,r,s,\ell\geqslant 0 \\ m+r+s+\ell=k-1}} q_m q_r q_s q_l/4,$$

$$(k=1,2,\dots),$$

where $q_m=a_m+a_m^{\dagger}$.

The operators a_n $(n=1,2,3,\dots)$ in Eq. (35) are determined recursively as polynomial functions of a_0 and $a_0^{\dagger}$ by requiring the following.

(i) $U(g)$ be unitary indeed, or equivalently (due to the Von Neumann theorem [6]) that the commutator of the variables $a(g)$ and $a^{\dagger}(g)$ be canonical: $[a(g),a^{\dagger}(g)]=1$, $\forall g$, i.e.,

$$\sum_{m=0}^{n} [a_m,a_{n-m}^{\dagger}]=\delta_{n,0},(n=0,1,2\cdots). \quad (37)$$

(ii) H_d be diagonal indeed in the $\{|n\rangle\}$ basis or, equivalently, that $[H_d,N]=0,\forall g$, i.e.,

$$[H_k,N]=0,(k=1,2,3,\dots). \quad (38)$$

Equations (38) imply that all the H_k's are functions of the operator $N=a_0^{\dagger}a_0$ only. In particular these operators H_k commute between themselves.

Evidently, Eqs. (37) and (38) *must* admit solution for $\{a_n\}$, due to the mere existence of the unitary operator $U(g)$ and its formal perturbative expansion. However, there is no uniqueness property because of the phase freedom in the mapping $U(g)$. In our case of QAO with standard quartic interaction, the "minimal" solution $\{a_n\}$ is such that each a_n

is a polynomial of degree $2n+1$ in a_0 and $a_0^\dagger$ with rational coefficients, and monomials of odd degrees only

$$a_n = \sum_{\substack{2k+\ell=2n+1 \\ 1 \leqslant l_{odd} \leqslant 2n+1}} (x_{n,k,l} a_0^l N^k + y_{n,k,l} N^k a_0^{\dagger l}).$$

Let us now define the T-dependent operators $a_n(T)$ by

$$a_n(T) = \exp\left(i \sum_{k=0}^{\infty} H_k t_k\right) a_n \exp\left(-i \sum_{k=0}^{\infty} H_k t_k\right),$$

$$(n = 0,1,2, \dots) \qquad (39)$$

where $t_k = g^k t$. We claim that these operators obey exactly the canonical commutation relations (12) and the differential Eqs. (10) which serve previously to determine the $A_n(T)$'s.

Because of Eq. (37), this is immediate for the relations (12). As for Eqs. (10), one first derives from Eq. (39)

$$D_{n-m} a_m(T) = i \exp\left(i \sum_{k=0}^{\infty} H_k t_k\right)[H_{n-m}(\{a_r\}), a_m]$$

$$\times \exp\left(-i \sum_{k=0}^{\infty} H_k t_k\right)$$

which, summing up, yields

$$\sum_{m=0}^{n} D_{n-m} a_m(T) = i \sum_{m=0}^{n} [H_{n-m}(\{a_r(T)\}), a_m(T)],$$

$$(40)$$

where the commutativity of the H_k's has been used twice. On the other hand, using Eq. (7) together with Eqs. (33) and (36) to express $H(A(T,g), A^\dagger(T,g), g)$ in terms of the function H_k, one readily finds that Eqs. (10) read as well

$$\sum_{m=0}^{n} D_{n-m} A_m(T) = i \sum_{m=0}^{n} [H_{n-m}(\{A_r(T)\}), A_m(T)],$$

$$(41)$$

identical to Eq. (40). This is actually true not only for the QAO but for a general interaction.

Therefore, $\{A_n(T)\}$ can be identified as one of the solutions $\{a_n(T)\}$, which establishes the equivalence of the two schemes, and hence the consistence of the multitime method we used, together with the general validity of the assertions (1) to (3) put forward at the beginning of this section.

It is possible now to comment on the "mass renormalization" introduced by B&B. Since H_d is a pure function of N, $H_d = H(N)$, Eq. (39) for $a_0(T)|_{t_j = g^j t} = A_0(T)|_{t_j = g^j t} = a_0(t,g)$ reads

$$a_0(t,g) = \exp(+iH(N)t) a_0 \exp(-iH(N)t),$$

or, by using $a_0 N = (N+1) a_0$

$$a_0(t,g) = a_0 \exp[-i(H(N) - H(N-1))t].$$

Together with Eq. (28), this gives

$$a_0(t,g) = a_0 \exp[-it(1 + 3gN - 3g^2(7 + 17N^2)/4) + O(g^3)].$$

The "renormalization" phenomenon can be pinned down to the fact that $H(N) - H(N-1)$ is the trivial identity operator at the zeroth order, and becomes a true operator for higher orders.

As mentioned at the beginning, and apparent in Eqs. (29) and (30), the solution $A(T,g)$ constructed there corresponds to initial conditions depending on A_0 *and* g. If one insists in having the perturbative solution with prescribed g-independent initial condition: $A(0,g) = a$, with $[a,a^\dagger] = 1$, this is easily achieved by a few additional manipulations. Indeed, it is sufficient to invert order by order the relation

$$a = A_0 + \sum_{n=1}^{\infty} g^n F_n(A_0, A_0^\dagger)$$

(which is straightforward in spite of the noncommutative algebra) to get

$$A_0 = a + \sum_{n=1}^{\infty} g^n G_n(a, a^\dagger)$$

and to reinsert this expression for A_0 in Eqs. (29) and (30), as well as in $N = A_0^\dagger A_0$, truncated at the relevant order. Then, of course, the expression of $A(T,g)$ in terms of a and $a^\dagger$ has no longer the "simple" structure that it exhibits in terms of A_0 and $A_0^\dagger$.

To conclude this section, we wish to stress again that the arguments presented here are quite general, not specific of the QAO. If one considers a Hamiltonian which is the sum of a harmonic oscillator one and a "potential" represented by a self-adjoint operator function of the position and the momentum, such an analysis can be repeated. Actually, the equivalence between MST and unitary transformation diagonalizing the Hamiltonian is likely to be a rather general feature. In particular, the previous discussion can be extended in a rather straigthforward way to systems with more than one degree of freedom.

Furthermore, the equivalence between the multitime approach and the perturbative construction of the relevant unitary transformation must have a classical counterpart. In the classical framework, multitime expansions should appear as essentially equivalent to the construction of appropriate canonical transformations, following the Poincaré–Von Zeipel method [7], or some of its disguises. As a matter of fact, one can find an indication of such a connection in the literature [4,8]. This aspect of the question, which we have not touched upon in the present paper, might deserve a further study.

V. CONCLUSION

In this paper, we have used the anharmonic oscillator in the Heisenberg picture as a model for investigating the practicability of the derivative expansion method, of common use in classical physics, within the quantum framework. This method turns out to be successful in providing us with the perturbative expansion of the time-dependent dynamical variables together with the energy levels, which we have

derived explicitly up to the second order. We also have proved that this MST is equivalent to the perturbative construction of an unitary transformation diagonalizing the full Hamiltonian, leading to a step-by-step algorithm for the calculation of the previous quantities at any order, and thereby strengthening the status of the multiple scale techniques in quantum mechanics.

APPENDIX

We give below, up to order 6 the following.

(i) The coefficients a_n of the expansion (35) of the annihilator $a(g)$ in terms of $N = a_0^\dagger a_0$.

(ii) The coefficients $E_k(n)$ of the expansion of the energy levels

$$E_n(g) = \frac{1}{2} + n + \sum_{n=1}^{\infty} g^k E_k(n).$$

Both have been computed by applying the algorithm described in Sec. IV [Eqs. (37) and (38)].

(i) To be simpler, a and $a^\dagger$ stand for a_0 and $a_0^\dagger$:

$$a_1 = (2a^3 - a^{\dagger 3} - 6Na^\dagger)/4,$$

$$a_2 = (-9a + 120a^3 + 6a^5 - 120a^3N + 27aN^2 + 84a^\dagger - 42a^{\dagger 3} - 4a^{\dagger 5} + 42Na^{\dagger 3} + 276N^2a^\dagger)/32,$$

$$a_3 = (6092a^3 + 756a^5 + 8a^7 - 8844a^3N + 4422a^3N^2 - 378a^5N + 1278aN - 1062aN^3 - 1708a^{\dagger 3} - 464a^{\dagger 5} - 6a^{\dagger 7} - 9282Na^\dagger + 2406Na^{\dagger 3} + 232Na^{\dagger 5} - 1203N^2a^{\dagger 3} - 9042N^3a^\dagger)/128,$$

$$a_4 = (-200\,645a + 1\,546\,416a^3 + 380\,868a^5 + 9264a^7 + 40a^9 - 2\,975\,280a^3N + 2\,143\,296a^3N^2 - 714\,432a^3N^3 - 322\,896a^5N + 80\,724a^5N^2 - 3088a^7N - 500\,298aN^2 + 162\,755aN^4 + 506\,760a^\dagger - 358\,200a^{\dagger 3} - 221\,832a^{\dagger 5} - 6696a^{\dagger 7} - 32a^{\dagger 9} + 673\,392Na^{\dagger 3} + 186\,464Na^{\dagger 5} + 2232Na^{\dagger 7} + 3\,040\,992N^2a^\dagger - 472\,788N^2a^{\dagger 3} - 46\,616N^2a^{\dagger 5} + 157\,596N^3a^{\dagger 3} + 1\,365\,240N^4a^\dagger)/2048,$$

$$a_5 = (116\,798\,776a^3 + 51\,228\,696a^5 + 2\,189\,520a^7 + 20\,832a^9 + 48a^{11} - 266\,946\,576a^3N + 255\,315\,936a^3N^2 - 121\,842\,648a^3N^3 + 30\,460\,662a^3N^4 - 58\,614\,828a^5N + 24\,750\,360a^5N^2 - 4\,125\,060a^5N^3 - 1\,300\,128a^7N + 216\,688a^7N^2 - 5208a^9N + 52\,602\,092aN + 41\,073\,824aN^3 - 6\,417\,388aN^5 - 21\,539\,684a^{\dagger 3} - 28\,787\,584a^{\dagger 5} - 1\,542\,096a^{\dagger 7} - 16\,320a^{\dagger 9} - 40a^{\dagger 11} - 121\,625\,250Na^\dagger + 50\,282\,976Na^{\dagger 3} + 32\,551\,232Na^{\dagger 5} + 912\,600Na^{\dagger 7} + 4080Na^{\dagger 9} - 47\,389\,884N^2a^{\dagger 3} - 13\,618\,080N^2a^{\dagger 5} - 152\,100N^2a^{\dagger 7} - 219\,914\,676N^3a^\dagger + 22\,248\,396N^3a^{\dagger 3} + 2\,269\,680N^3a^{\dagger 5} - 5\,562\,099N^4a^{\dagger 3} - 55\,675\,938N^5a^\dagger)/8192,$$

$$a_6 = (-2\,649\,077\,789a + 19\,854\,323\,040a^3 + 14\,799\,326\,898a^5 + 1\,000\,498\,176a^7 + 15\,874\,840a^9 + 78\,720a^{11} + 112a^{13} - 15\,744a^{11}N - 52\,410\,470\,592a^3N + 59\,605\,775\,856a^3N^2 - 37\,821\,182\,832a^3N^3 + 13\,464\,443\,160a^3N^4 - 2\,692\,888\,632a^3N^5 - 20\,808\,622\,800a^5N + 11\,852\,140\,500a^5N^2 - 3\,324\,992\,400a^5N^3 + 415\,624\,050a^5N^4 - 817\,924\,896a^7N + 242\,212\,752a^7N^2 - 26\,912\,528a^7N^3 - 7\,253\,184a^9N + 906\,648a^9N^2 - 16\,271\,788\,323aN^2 - 6\,097\,875\,991aN^4 + 521\,267\,535aN^6 + 4\,255\,953\,324a^\dagger - 2\,581\,523\,304a^{\dagger 3} - 8\,101\,045\,372a^{\dagger 5} - 691\,648\,560a^{\dagger 7} - 12\,242\,240a^{\dagger 9} - 64\,720a^{\dagger 11} - 96a^{\dagger 13} + 12\,944Na^{\dagger 11} + 7\,571\,823\,000Na^{\dagger 3} + 11\,245\,609\,120Na^{\dagger 5} + 562\,441\,728Na^{\dagger 7} + 5\,584\,128Na^{\dagger 9} + 35\,458\,238\,196N^2a^\dagger - 9\,129\,805\,056N^2a^{\dagger 3} - 6\,326\,409\,960N^2a^{\dagger 5} - 165\,946\,104N^2a^{\dagger 7} - 698\,016N^2a^{\dagger 9} + 5\,783\,860\,872N^3a^{\dagger 3} + 1\,757\,503\,840N^3a^{\dagger 5} + 18\,438\,456N^3a^{\dagger 7} + 29\,695\,249\,188N^4a^\dagger - 2\,055\,444\,390N^4a^{\dagger 3} - 219\,687\,980N^4a^{\dagger 5} + 411\,088\,878N^5a^{\dagger 3} + 4\,768\,483\,548N^6a^\dagger)/65\,536.$$

(ii)

$$E_1(n) = 3(1 + 2n + 2n^2)/4,$$

$$E_2(n) = -(1 + 2n)(21 + 17n + 17n^2)/8,$$

$$E_3(n) = 3(111 + 347n + 472n^2 + 250n^3 + 125n^4)/16,$$

$$E_4(n) = -(1 + 2n)(30\,885 + 49\,927n + 60\,616n^2 + 21\,378n^3 + 10\,689n^4)/128,$$

$$E_5(n) = 3(305\,577 + 1\,189\,893n + 2\,060\,462n^2 + 1\,857\,870n^3 + 1\,220\,765n^4 + 350\,196n^5 + 116\,732n^6)/256,$$

$$E_6(n) = -(1 + 2n)(65\,518\,401 + 146\,338\,895n + 21\,317\,2430n^2 + 139\,931\,868n^3 + 85\,627\,929n^4 + 18\,794\,394n^5 + 6\,264\,798n^6)/1024.$$

Several number theoretic properties of the $E_k(n)$'s are worth pointing out. First, all the coefficients c_{kp} of n^p in $E_k(n)$ are rational and positive, and the signs of the $E_k(n)$'s alternate, as it should be. Perhaps different are the following observations: whereas the denominator in the expression of $E_k(n)$ is a power of 2, the numerator is always a multiple of 3 (for integer n). This peculiarity was already noticed by Bender and Wu [9] for the ground state ($n=0$). It thus turns out to hold for the excited levels too. Also, the sum of the numerators of the coefficients c_{kp} in each $E_k(n)$ is a multiple of 5. Finally, if one expresses the $E_k(n)$'s in terms of the variable $m = n + \frac{1}{2}$, one observes that they are even polynomials with positive coefficients (multiplied by $-m$ if k is even). More than that, all the zeroes of these polynomials are pure imaginary. This means that all the zeroes of $E_k(n)$ lie on the line $n = -\frac{1}{2} + iy$.

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