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APPLICATION OF THE BOGOLYUBOV TRANSFORMATION TO ANHARMONIC OSCILLATORS

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Abstract. We discuss the application of the Bogolyubov transformation to anharmonic oscillators and show that an iterative procedure recently proposed to eliminate part of the off-diagonal terms in the transformed Hamiltonian operator is unnecessary. If one transforms the whole operator instead of a part of it, then the final result is obtained directly.

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Recently R. Jáuregui and J. Récamier [1] treated anharmonic oscillators of the form $H = \frac{p^2}{2m} + A_1x + A_2x^2 + A_3x^3 + A_4x^4$ by means of a procedure consisting of several steps. The method is based on the fact that the operators 1, a, $a^\dagger$, $a^\dagger a$, a^2, a^{+2}, a and $a^\dagger$ being respectively the annihilation and creation operators, span a six-dimensional Lie algebra. First, one splits H into two disjoint parts: $H_0^{(0)}$ which belongs to the algebra and the remainder $H_1^{(0)}$. Then one modifies $H_0^{(0)}$ by means of the Bogolyubov transformation $a(1) = t_2(1)a + t_1(1)a^\dagger + t_3(1)$, and $a^\dagger(1) = t_1(1)^*a + t_2(1)^*a^\dagger + t_3(1)^*$ choosing t_1, t_2 and t_3 in such a way that the coefficients of $a(1)$, $a^\dagger(1)$, $a(1)^2$, and $a^\dagger(1)^2$ vanish. When this same transformation is applied to the remainder $H_1^{(0)}$, the removed operators reappear with different coefficients. One then splits the resulting Hamiltonian operator into two parts $H_0^{(1)}$ and $H_1^{(1)}$ as before, and tries a second Bogolyubov transformation which removes the operators $a(2)$, $a^\dagger(2)$, $a(2)^2$, and $a^\dagger(2)^2$ from $H_0^{(1)}$. This procedure is repeated until a Bogolyubov transformation reduces to the identity transformation. In this way one obtains a convenient reference operator for perturbation or variation calculations even if the iteration does not converge [1].

It is our purpose to show that when the iterative procedure is convergent one easily obtains the result straightforward by transforming the whole Hamiltonian operator instead of only that part which belongs to the Lie algebra. To facilitate the discussion we consider the quartic anharmonic oscillator

$$H = \frac{1}{2}(p^2 + x^2) + \lambda x^4 \tag{1}$$

where $[x, p] = i$. The coordinate and momentum operators are related to the boson operators by

$$x = \frac{1}{\sqrt{2}}(a + a^\dagger) , \qquad p = \frac{i}{\sqrt{2}}(a^\dagger - a) . \tag{2}$$

We define new boson operators b and $b^\dagger$ by means of the Bogolyubov transformation

$$a = t_1 b + t_2 b^\dagger , \qquad a^\dagger = t_2 b + t_1 b^\dagger , \tag{3}$$

where t_1 and t_2 are real. It follows from $[a, a^\dagger] = [b, b^\dagger] = 1$ that $t_1^2 - t_2^2 = 1$ so that there is only one independent parameter. If we substitute (2) and (3) into (1) we obtain

$$H = \sum_{k=0}^{4} \sum_{j=0}^{k} G_{j,k-j}(t_1)(b^\dagger)^j b^{k-j} \tag{4}$$

where

$$\begin{aligned} G_{00} &= \frac{1}{2}(t_1^2 + t_2^2) + \frac{3\lambda}{4}(t_1 + t_2)^4 , & G_{11} &= t_1^2 + t_2^2 + 3\lambda(t_1 + t_2)^4 , \\ G_{20} = G_{02} &= t_1 t_2 + \frac{3\lambda}{2}(t_1 + t_2)^4 , & G_{22} &= \frac{3\lambda}{2}(t_1 + t_2)^4 , \\ G_{31} &= \lambda(t_1 + t_2)^4 , & G_{04} = G_{40} &= \frac{\lambda}{4}(t_1 + t_2)^4 . \end{aligned} \tag{5}$$

On setting t_1 so that $G_{02} = 0$ we obtain the same Hamiltonian operator that comes out of the iterative procedure proposed by R. Jáuregui and J. Récamier [1] because such an operator does not contain neither b^2 nor $(b^\dagger)^2$. More precisely we have

$$\begin{aligned} H &= H_{\mathrm{D}} + H_{\mathrm{ND}} , \qquad H_{\mathrm{D}} = G_{00} + G_{11} b^\dagger b + G_{22}(b^\dagger)^2 b^2 , \\ H_{\mathrm{ND}} &= \sum_{k=3}^{4} \sum_{j=0}^{k} G_{j,k-j}(t_1)(b^\dagger)^j b^{k-j} - G_{22}(b^\dagger)^2 b^2 , \end{aligned} \tag{6}$$

so that the eigenvalues E_n^{D} of H_{D} should equal the indicated $E_{(np)}^{(k,n)}$ by R. Jáuregui and J. Récamier [1] in the limit $k \to \infty$.

Before proceeding forward with the comparison we rewrite the Bogolyubov transformation in a more convenient way. If instead of (2) and (3) one writes

$$x = \sqrt{\frac{\sigma}{2}}(b + b^\dagger) , \qquad p = \frac{i}{\sqrt{2\sigma}}(b^\dagger - b) , \tag{7}$$

then the coefficients G_{jk} become

$$G_{00} = \frac{1}{4}\left(\sigma + \frac{1}{\sigma}\right) + \frac{3\lambda}{4}\sigma^2 , \qquad G_{11} = \frac{1}{2}\left(\sigma + \frac{1}{\sigma}\right) + 3\lambda\sigma^2 ,$$
$$G_{20} = G_{02} = \frac{1}{4}\left(\sigma - \frac{1}{\sigma}\right) , \qquad G_{22} = \frac{3\lambda}{2}\sigma^2 , \tag{8}$$
$$G_{31} = G_{13} = \lambda\sigma^2 , \qquad G_{40} = G_{04} = \frac{\lambda}{4}\sigma^2 .$$

The scaling parameter σ is related to the Bogolyubov parameters by

$$t_1 = \frac{1}{2}\left(\sqrt{\sigma} + \frac{1}{\sqrt{\sigma}}\right) , \qquad t_2 = \frac{1}{2}\left(\sqrt{\sigma} - \frac{1}{\sqrt{\sigma}}\right) . \tag{9}$$

The coefficients G_{02} and G_{20} vanish when the scaling parameter is a solution of

$$6\lambda\sigma^3 + \sigma^2 - 1 = 0 . \tag{10}$$

For instance, when $\lambda = 1$ we have the exact result $\sigma = \frac{1}{2}$, $E_0^{\rm D} = \frac{13}{16} = 0.8125$ and $E_1^{\rm D} = \frac{45}{16} = 2.8125$ which does not completely agree with the results reported by R. Jáuregui and J. Récamier [1] because they stopped the procedure after the first iteration.

R. Jáuregui and J. Récamier found that the iterative Bogolyubov transformations do not always converge. Divergence may occur because either the iterative algorithm is inappropriate or a solution does not exist. In the case of the double-well potential they have concluded that the method converges provided the coordinate origin coincides with the deepest minimum. Here we show that divergence in the mentioned case is entirely due already to the iterative algorithm because a solution have existed when the origin is located on the maximum of the barrier. For simplicity we consider the symmetric example $H = p^2 + \lambda\left(x^2 - \frac{1}{2\lambda}\right)^2$. On arguing as before we conclude that the coefficients of b^2 and $(b^\dagger)^2$ vanish when $3\lambda\sigma^3 - \sigma^2 - 1 = 0$. This equation has a real positive solution for all values of λ. For instance, when $\lambda = 0.3$ we obtain $\sigma = 1.565$ and $E_0^{\rm D} = 0.9214$. This energy value is smaller, and therefore more accurate by virtue of the variational theorem than the one reported by R. Jáuregui and J. Récamier [1]. The value of the scaling parameter just obtained is not the best one for the corresponding to the minimum of $E_n^{\rm D}$. Direct comparison of the minima of $E_n^{\rm D}$ in Table 1 with the $E_{(np)}$ values reported by R. Jáuregui and J. Récamier [1] clearly shows that the Bogolyubov parameters produced by the iterative method are far from being optimum. Furthermore, the condition that the coefficients of b^2 and $(b^\dagger)^2$ vanish produces parameters that are independent of the quantum number and therefore this approach disagrees with the variational method except for the ground state.

We have shown how to obtain the limit of the iterative Bogolyubov transformations directly by transforming the whole Hammiltonian operator instead of only the part belonging to the Lie algebra. For simplicity we have restricted our discussion to parity

Table 1. Approximate eigenvalues E_n^{D} of the double-well oscillator $H = p^2 + \lambda\left(x^2 - \frac{1}{2\lambda}\right)^2$

n	σ	E_n^{D}
0	1.565	0.9214
1	1.161	1.900
2	0.9249	3.726
3	0.7990	6.008
4	0.7178	8.625

invariant anharmonic oscillators because in that case there is only one relevant parameter. If the potential energy function is not parity invariant one needs at least two parameters to remove the oprators b, $b^\dagger$, b^2 and $(b^\dagger)^2$. These parameters are a coordinate scaling and a translation of the coordinate origin. The resulting equations are somewhat more complicated than those derived here but they can be easily solved numerically [2]. Furthermore, it follows from the results above that for many purposes the Bogolyubov transformation and the scaling method [2] yield exactly the same result but the latter is remarkably simpler and more practical than the former.

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