COMMENTS

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Comment on "Iterative Bogoliubov transformations and anharmonic oscillators"

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We discuss a recently proposed method [R. Jáuregui and J. Récamier, Phys. Rev. A **46**, 2240 (1992)] based on the application of iterative Bogoliubov transformations to anharmonic oscillators and show that, if the algorithm converges, one easily obtains the final result directly in one step. We prove that the Bogoliubov transformation can be written in terms of scaling and translation parameters and present exact results for the coefficients of the Bogoliubov transformation for some selected examples.

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Recently Jáuregui and Récamier [1] treated anharmonic oscillators of the form $H=p^2/(2m)+A_1x+A_2x^2+A_3x^3+A_4x^4$ 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, and $(a^\dagger)^2$ (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 Bogoliubov 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 Bogoliubov 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 as many times as necessary and, if it converges, the Bogoliubov transformation reduces to the identity transformation and one obtains a Hamiltonian operator free from the operators a, $a^\dagger$, a^2, and $(a^\dagger)^2$. If the iterative Bogoliubov transformations do not converge, Jáuregui and Récamier [1] choose the parameters of an intermediate step before the instability region is reached. In any case, they use the final Hamiltonian operator in further perturbation or variation calculations to improve the accuracy of the results [1].

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

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

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

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

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

$$a=t_1b+t_2b^\dagger,\quad a^\dagger=t_2b+t_1b^\dagger , \tag{3}$$

in which 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

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

where

$$\begin{aligned}
&G_{00}=\tfrac{1}{2}(t_1^2+t_2^2)+\frac{3\lambda}{4}(t_1+t_2)^4 ,\\
&G_{11}=t_1^2+t_2^2+3\lambda(t_1+t_2)^4 ,\\
&G_{20}=G_{02}=t_1t_2+\frac{3\lambda}{2}(t_1+t_2)^4 ,\\
&G_{22}=\frac{3\lambda}{2}(t_1+t_2)^4 ,\\
&G_{13}=G_{31}=\lambda(t_1+t_2)^4,\quad G_{04}=G_{40}=\frac{\lambda}{4}(t_1+t_2)^4 .
\end{aligned} \tag{5}$$

On setting t_1 so that $G_{02}=0$, we obtain an operator that does not contain b^2 or $(b^\dagger)^2$. More precisely, we have

$$\begin{aligned}
&H=H_{\rm D}+H_{\rm ND},\quad H_{\rm D}=G_{00}+G_{11}b^\dagger b+G_{22}(b^\dagger)^2b^2 ,\\
&H_{\rm ND}=\sum_{\substack{k=-2\\(k\neq 0)}}^{2}G_{2+k\,2-k}(b^\dagger)^{2+k}b^{2-k} ,
\end{aligned} \tag{6}$$

and the eigenvalues $E_n^{\rm D}$ of $H_{\rm D}$ would equal those indicated $E_{(\rm np)}^{(k,n)}$ by Jáuregui and Récamier [1] when $k\to\infty$ if the iterative algorithm were convergent (np denotes nonperturbative and ND denotes nondiagonal).

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

$$x=\left[\frac{\sigma}{2}\right]^{1/2}(b+b^\dagger),\quad p=\frac{i}{\sqrt{2\sigma}}(b^\dagger-b)\ , \tag{7}$$

then the coefficients G_{jk} become

$$\begin{aligned}
G_{00}&=\frac{1}{4}\left[\sigma+\frac{1}{\sigma}\right]+\frac{3\lambda}{4}\sigma^2\ ,\\
G_{11}&=\frac{1}{2}\left[\sigma+\frac{1}{\sigma}\right]+3\lambda\sigma^2\ ,\\
G_{20}=G_{02}&=\frac{1}{4}\left[\sigma-\frac{1}{\sigma}\right]+\frac{3\lambda}{2}\sigma^2\ ,\\
G_{22}=\frac{3\lambda}{2}\sigma^2,\quad G_{31}&=G_{13}=\lambda\sigma^2,\quad G_{40}=G_{04}=\frac{\lambda}{4}\sigma^2\ .
\end{aligned} \tag{8}$$

The scaling parameter σ is related to the Bogoliubov coefficients by

$$t_1=\frac{1}{2}\left[\sqrt{\sigma}+\frac{1}{\sqrt{\sigma}}\right],\quad t_2=\frac{1}{2}\left[\sqrt{\sigma}-\frac{1}{\sqrt{\sigma}}\right], \tag{9}$$

and the Hamiltonian coefficients G_{02} and G_{20} vanish when σ is a solution of

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

It is not difficult to verify that this equation has a real positive root for every $\lambda>0$. For instance, when $\lambda=1$ we have $\sigma=\frac{1}{2}$, $E_0^{\rm D}=\frac{13}{16}=0.8125$, and $E_1^{\rm D}=\frac{45}{16}=2.8125$, which completely agree with the nonperturbative energies obtained earlier by Récamier and Jáuregui [2]. Furthermore, our exact values for the ground-state Hamiltonian coefficients $G_{00}=\frac{13}{16}$, $G_{11}=2$, $G_{22}=\frac{3}{8}$, $G_{13}=\frac{1}{4}$ are in total agreement with the converged results shown in Figs. 1 and 2 of Ref. [2]. Therefore, it is clear that if the iterative Bogoliubov transformations converge, the final parameters are given by the simple expressions shown above.

Jáuregui and Récamier find that the iterative Bogoliubov transformations do not always converge. Divergence may occur because either there is no transformation that eliminates the nondiagonal terms or because the algorithm is unstable in such cases. The latter situation is found in all the examples studied. For instance, Jáuregui and Récamier [1] conclude that the method converges for the double-well potential provided that at the starting point the coordinate origin coincides with the deepest minimum. Here we prove that a solution already exists for the symmetric example $H=p^2+\lambda[x^2-1/(2\lambda)]^2$ when the origin is located at the maximum of the barrier. 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 root for every $\lambda>0$. 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 those obtained by Jáuregui and Récamier [1] with as many as five basis functions and $k=0$, 1, and 8.

TABLE I. Approximate eigenvalues $E_n^{\rm D}$ of the double-well oscillator $H=p^2+\lambda[x^2-1/(2\lambda)]^2$ with $\lambda=1$.

n	σ	$E_n^{\rm D}$
0	0.8241	0.9540
1	0.6596	3.166
2	0.5508	6.370
3	0.4869	10.18
4	0.4441	14.45

The value of the scaling parameter obtained by the method above is not the best one for excited states. One expects the optimum value of this parameter to depend on the quantum number. For example, in Table I we show that the minimum of $E_n^{\rm D}$ gives acceptable results for $\lambda=1$. In other words, the scaling method provides a simpler way of deriving expressions for the Bogoliubov coefficients according to the variational theorem for a given state.

Summarizing, we have shown how to obtain the limit of the iterative Bogoliubov transformations directly by transforming the whole Hamiltonian operator instead of only the part belonging to the Lie algebra. For simplicity, we have restricted our discussion to parity-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 operators b, $b^\dagger$, b^2, and $(b^\dagger)^2$. These parameters are a dilatation (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 [3]. Furthermore, it follows from the results above that for many purposes the Bogoliubov transformation and the scaling method [3] yield exactly the same result but the latter is remarkably simpler and more practical than the former.

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