Quartic, sextic, and octic anharmonic oscillators: Precise energies of ground state and excited states by an iterative method based on the generalized Bloch equation

Holger Meißner* and E. Otto Steinborn†
Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany
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Recently, we proposed an iteration method for solving the eigenvalue problem of the time-independent Schrödinger equation [H. Meißner and E. O. Steinborn, Int. J. Quantum Chem. **61**, 777 (1997)]. This method, which is based on the generalized Bloch equation, calculates iteratively certain matrix elements of the wave operator which are the wave-function expansion coefficients (WECs). It is valid for boson as well as fermion systems. In this article we show that the WEC-iteration method, together with a renormalization technique, allows us to calculate energy eigenvalues for the ground state and excited states of the quartic, sextic, and octic anharmonic oscillator with very high accuracy. In order to overcome slow convergence in the iteration scheme we use a renormalization technique introduced by F. Vinette and J. Čížek [J. Math. Phys. (N.Y.) **32**, 3392 (1991)] and show that this method is equivalent to the renormalization scheme based on the Bogoliubov transformation [N. N. Bogoliubov, Izv. Akad. Nauk SSSR, Ser. Fiz. **11**, 77 (1947)] which is frequently used for the treatment of anharmonic oscillators in second quantization. [S1050-2947(97)02608-5]

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I. INTRODUCTION

A quantum-mechanical system is determined by its wave function, and the calculation of this wave function is a fundamental problem. In the case of stationary nonrelativistic systems one has to solve the time-independent Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{1.1}$$

where $\hat{H}$ is the appropriate Hamiltonian of the system and $|\psi\rangle$ its eigenfunction with corresponding eigenvalue E.

As is well known, an eigenfunction $|\psi\rangle$ can be expanded in terms of a complete orthonormal basis set $\{\phi_\eta\}_{\eta=1}^{\infty}$ (see, for instance, Chap. 2 of Ref. [1]),

$$|\psi\rangle = \sum_{\eta=1}^{\infty} a_\eta |\phi_\eta\rangle. \tag{1.2}$$

Then, the Schrödinger equation (1.1) can be considered to be solved if so many expansion coefficients a_η can be determined that one obtains a sufficiently accurate approximation to the exact wave function (1.2).

For that purpose, we use an iteration method, which we introduced in [2,3], for the calculation of the wave-function expansion coefficients (WECs) a_η of Eq. (1.2). This WEC-iteration method was originally designed to calculate the correlation energies [4–8] of atoms and molecules.

In the present paper, we use our formalism for the calculation of the energies of the ground and excited states of the anharmonic oscillators defined by the Hamiltonians

$$\hat{H}^{(m)}(\beta) = \hat{p}^2 + \hat{x}^2 + \beta\hat{x}^{2m}. \tag{1.3}$$

Here, $m=2,3,4$ corresponds to the quartic, sextic, and octic anharmonic oscillator, respectively, and $\beta \in [0,\infty)$.

Anharmonic oscillators are frequently used to test new approximation techniques since the calculation of the eigenvalues and eigenfunctions leads to challenging mathematical problems. For instance, Bender and Wu [9–11] showed that for the ground state of the quartic, sextic, and octic anharmonic oscillator the Rayleigh-Schrödinger perturbation series for an energy eigenvalue diverges strongly for every $\beta \neq 0$. The anharmonic oscillators are also used to test other computational approaches which are actually designed for the treatment of many-fermion systems, such as the coupled cluster approximation [5,6]. However, in this case some problems also occur [12,13] (see also [14–16]). Therefore, it turns out that the anharmonic oscillators defined by Eq. (1.3) are well suited to test the power as well as the shortcomings of approximation techniques.

For this purpose, we first present in Sec. II an overview of the nonlinear iterative method [2,3] which is based on the concept of the wave operator and the generalized Bloch equation. In Sec. III, a renormalization technique introduced by Vinette and Čížek [17], which is based on Symanzik scaling (Sec. II.2 of Ref. [18]), is applied to the ground state and first excited states of the quartic, sextic, and octic anharmonic oscillator. This renormalization technique is compared with the Bogoliubov transformation [19]. The results of the calculations which were performed with the help of MAPLE V (release 3) [20–22], are presented in Sec. IV.

II. METHOD

In this section we give a short overview of the method which we recently introduced [2,3], emphasizing some different aspects.

For the determination of the coefficients a_η in Eq. (1.2) we introduce a finite-dimensional reference space $\mathcal{P}$, which together with its orthogonal complement $\mathcal{Q}$ spans the space of basis functions. This reference space should consist of

*Electronic address: Holger.Meissner@chemie.uni-regensburg.de
†Electronic address: Otto.Steinborn@chemie.uni-regensburg.de

those basis functions whose expansion coefficients a_η in the wave function $|\psi\rangle$ have an appreciable absolute value.

A. Reference states

Some eigenstates $|\psi_a\rangle$ of the Hamiltonian $\hat{H}$, with

$$\hat{H}|\psi_a\rangle = E_a|\psi_a\rangle, \quad a \in I_p \tag{2.1}$$

are split into their main part $|\psi_a^0\rangle$ belonging to $\mathcal{P}$ and the remainder belonging to $\mathcal{Q}$ (see p. 202 of Ref. [24])

$$|\psi_a\rangle = |\psi_a^0\rangle + \sum_{\lambda \in I_q} C_\lambda^a |\phi_\lambda\rangle, \tag{2.2}$$

$$|\psi_a^0\rangle = \sum_{\alpha \in I_p} g_\alpha^a |\phi_\alpha\rangle, \quad a \in I_p . \tag{2.3}$$

Here, I_p and I_q denote the set of indices of the basis functions belonging to $\mathcal{P}$ and $\mathcal{Q}$, respectively. For each $|\psi_a\rangle$, the task is the determination of the state $|\psi_a^0\rangle$ belonging to the reference space and of the remainder of the expansion, $\Sigma_{\lambda \in I_q} C_\lambda^a |\phi_\lambda\rangle$. According to Eq. (2.3), the reference states can be represented by linear combinations of the basis functions building up the n-dimensional reference space $\mathcal{P}$ [24, p. 202]. In the following text, we use intermediate normalization of the exact wave functions $|\psi_a\rangle$:

$$\langle \psi_a^0|\psi_a\rangle = \langle \psi_a^0|\psi_a^0\rangle = 1, \quad a \in I_p . \tag{2.4}$$

B. Equation of motion

Instead of using the Schrödinger equation (2.1) for the determination of the reference states as linear combinations of the basis functions of $\mathcal{P}$ and for the determination of the coefficients C_λ^a of the basis function of $\mathcal{Q}$, we will use an *effective Hamiltonian* (see p. 238 of Ref. [23] and p. 207 of Ref. [24]) for the calculation of the reference states and the *generalized Bloch equation* [23–29] for the calculation of the C_λ^a. This leads to a formal separation of the two sets of coefficients $\{g_\alpha^a | a, \alpha \in I_p\}$ and $\{C_\lambda^a | a \in I_p, \lambda \in I_q\}$.

The effective Hamiltonian $\hat{H}^{\text{eff}}$, which is not necessarily Hermitian, is defined by

$$\hat{P}\hat{H}\hat{\Omega}\hat{P}|\psi_a^0\rangle = \hat{H}^{\text{eff}}|\psi_a^0\rangle = E_a|\psi_a^0\rangle. \tag{2.5}$$

Here, we use the so-called *wave operator* $\hat{\Omega}$ which transforms in an unambiguous way all states of the reference space $\{\psi_a^0\}_{a=1}^n$, which are linear independent but in general not orthogonal, into the corresponding exact eigenstates $\{\psi_a\}_{a=1}^n$ (see p. 202 of Ref. [24], and Refs. [30–32]),

$$|\psi_a\rangle = \hat{\Omega}|\psi_a^0\rangle, \quad a \in I_p \tag{2.6}$$

and the projection operator $\hat{P}$ according to

$$\hat{P}|\psi_a\rangle = |\psi_a^0\rangle = \sum_{\alpha \in I_p} g_\alpha^a |\phi_\alpha\rangle. \tag{2.7}$$

In general, for nonorthogonal reference functions $\{\psi_a^0\}_{a=1}^n$ we can express the projection operator $\hat{P}$ as (see p. 203 of Ref. [24])

$$\hat{P} = \sum_{a \in I_p} |\psi_a^0\rangle\langle\Psi_a^0|, \quad \langle\Psi_b^0|\psi_a^0\rangle = \delta_{ab} . \tag{2.8}$$

Here, $\{\Psi_a^0\}_{a=1}^n$ is a corresponding dual basis (see p. 6 of Ref. [33]). For the orthogonal case the $\{\Psi_a^0\}_{a=1}^n$ reduce to $\{\psi_a^0\}_{a=1}^n$.

In contrast to former considerations [2,3,24] we use a different representation of the generalized Bloch equation [23,34]:

$$\hat{U}\,\hat{H}\,\hat{U} = \hat{H}\,\hat{U}, \quad \hat{U} = \hat{\Omega}\hat{P}. \tag{2.9}$$

In [2,3] we use a special representation of the generalized Bloch equation where the Hamiltonian $\hat{H}$ is partitioned into an unperturbed part, $\hat{H}_0$, and a perturbation $\hat{V}$. However, the expressions of the following Secs. II C–II E correspond to the expressions in [2,3] if we use an Epstein-Nesbet partitioning of the Hamiltonian $\hat{H}$ where $(\hat{H}_0)_{\mu,\nu} = H_{\mu,\nu}\delta_{\mu,\nu}$ [35–37].

C. Basis set

Now, we use the following basis set for the entire space: In the reference space $\mathcal{P}$ the basis set is chosen to be the linearly independent reference states $\{\psi_a^0\}_{a=1}^n$, and in the remaining space $\mathcal{Q}$—the orthogonal complement of $\mathcal{P}$—the basis set will be the basis functions $|\phi_\lambda\rangle, \lambda \in I_q$, which do not occur in the linear combinations of $\{\psi_a^0\}_{a=1}^n$. In terms of this new basis the eigenstate $|\psi_a\rangle$ can be written as

$$|\psi_a\rangle = \sum_{b \in I_p} C_b^a |\psi_b^0\rangle + \sum_{\lambda \in I_q} C_\lambda^a |\phi_\lambda\rangle, \quad a \in I_p . \tag{2.10}$$

This implies

$$C_b^a = \delta_{ab}, \quad C_\lambda^a = \langle \phi_\lambda|\hat{\Omega}|\psi_a^0\rangle, \quad a,b \in I_p, \quad \lambda \in I_q . \tag{2.11}$$

Therefore, we have accomplished a formal separation of the two sets of coefficients $\{g_\alpha^a | a, \alpha \in I_p\}$ and $\{C_\lambda^a | a \in I_p, \lambda \in I_q\}$. In the sequel, we will call the matrix elements (2.11) of the wave operator $\hat{\Omega}$ the *wave-function expansion coefficients* (WECs).

To determine the reference space, we choose a basis function $|\phi_\alpha\rangle$ which represents the most significant contribution to the wave function $|\psi_a\rangle$. In addition to $|\phi_\alpha\rangle$, all other basis functions $|\phi_\eta\rangle, \eta \neq \alpha$, are included in the reference space $\mathcal{P}$ if they fulfill

$$\left|\frac{H_{\eta\alpha}}{\mathcal{E}_\alpha - \mathcal{E}_\eta}\right| \geq \theta, \quad 0 < \theta \leq 1, \quad \eta \neq \alpha \tag{2.12}$$

where

$$\mathcal{E}_\alpha = \langle \phi_\alpha|\hat{H}|\phi_\alpha\rangle, \quad H_{\alpha\beta} = \langle \phi_\alpha|\hat{H}|\phi_\beta\rangle. \tag{2.13}$$

Of course, the dimension of the reference space depends on the size of the parameter θ.

D. Effective Hamiltonian

The reference states in $\mathcal{P}$ will be determined by using the effective Hamiltonian according to Eq. (2.5) and by utilizing the orthonormality of the basis functions $\{\phi_\alpha\}_{\alpha=1}^{n}$ and the corresponding projection operator $\hat{P}=\Sigma_{\alpha\in I_p}|\phi_\alpha\rangle\langle\phi_\alpha|$. From the eigenvalue equation for the effective Hamiltonian Eq. (2.5), we obtain by sorting out a coefficient g_α^a the following nonlinear equations for the unknown coefficients $\{g_\alpha^a|a,\alpha\in I_p\}$ of the reference states:

$$g_\alpha^a=-\frac{1}{2A_\alpha^a}\{B_\alpha^a\pm\sqrt{[B_\alpha^a]^2-4A_\alpha^a\Gamma_\alpha^a}\},\quad a,\alpha\in I_p. \tag{2.14}$$

Here

$$A_\alpha^a=\sum_{\beta\in I_p} g_\beta^{a*}H_{\beta\alpha}, \tag{2.15}$$

$$B_\alpha^a=\sum_{\substack{\beta,\gamma\in I_p\\ \gamma\neq\alpha}} H_{\beta\gamma}\rho_{\gamma\beta}^{aa}+\sum_{\beta\in I_p} g_\beta^{a*}\Delta_\beta^a-H_{\alpha\alpha}, \tag{2.16}$$

$$\Gamma_\alpha^a=-\sum_{\beta\in I_{p\setminus\alpha}} H_{\alpha\beta}g_\beta^a-\Delta_\alpha^a, \tag{2.17}$$

$$\rho_{\alpha\beta}^{ab}=g_\alpha^a\,g_\beta^{b*},\quad a,b,\alpha,\beta\in I_p, \tag{2.18}$$

$$\Delta_\alpha^a=\sum_{\lambda\in I_q} H_{\alpha\lambda}C_\lambda^a,\quad H_{\eta\zeta}=\langle\phi_\eta|\hat{H}|\phi_\zeta\rangle \tag{2.19}$$

with $a,\alpha\in I_p$, $\eta,\zeta\in I_p\cup I_q$.

The coefficients $\{\vec{g}^a\}_{a\in I_p}$, which are written here in vector notation, have to be normalized such that $\langle\psi_a^0|\psi_a^0\rangle=1$ according to Eq. (2.4). Possible initial values for the coefficients g_α^a of the reference states are

$$g_\alpha^a(0)=\delta_{a\alpha},\quad a,\alpha\in I_p. \tag{2.20}$$

The sign in front of the square root in Eq. (2.14) is to be chosen such that one obtains the initial values (2.20) in the limit $H_{\mu\nu}\to 0$, $\mu\neq\nu$. With respect to Epstein-Nesbet partitioning of the Hamiltonian this corresponds to the limit $\hat{V}\to 0$ which leads to the unperturbed case $\hat{H}_0$.

Hence, the reference state $|\psi_a^0\rangle$, determined by the coefficients g_α^a, is also indirectly determined by the coefficients C_λ^a in Eq. (2.10). Therefore, we have to solve the equations for the g_α^a simultaneously with the equations for the C_λ^a [2,3].

E. Generalized Bloch equation

The contribution of the basis functions in $\mathcal{Q}$ to the wave function $|\psi_a\rangle$ will be determined via the generalized Bloch equation (2.9). The matrix form of the generalized Bloch equation leads to nonlinear equations for the WECs, $\{C_\lambda^a|a\in I_p,\lambda\in I_q\}$, a formal quadratic equation in C_λ^a, which can be solved for $H_{a\lambda}\neq 0$ yielding [3]

$$C_\lambda^a=\frac{1}{2H_{a\lambda}}\{\Lambda_\lambda^a-\sigma[\{\Lambda_\lambda^a\}^2+4H_{a\lambda}(H_{\lambda a}+\Gamma_{\lambda a})]^{1/2}\}, \tag{2.21}$$

where σ is the sign of $\Lambda_\lambda^a=D_\lambda^a-\Delta_\lambda^a$. If the matrix element $H_{a\lambda}$ vanishes, we obtain instead

$$C_\lambda^a=\frac{-\Gamma_{\lambda a}}{D_\lambda^a-\Delta_{a\lambda}}. \tag{2.22}$$

In Eqs. (2.21) and (2.22), we use the abbreviations

$$\Delta_{a\lambda}=\sum_{\mu\in I_{q\setminus\lambda}} H_{a\mu}C_\mu^a+\sum_{b\in I_{p\setminus a}} H_{b\lambda}C_\lambda^b, \tag{2.23}$$

$$\Gamma_{\lambda a}=\sum_{\mu\in I_{q\setminus\lambda}} H_{\lambda\mu}\,C_\mu^a-\sum_{b\in I_{p\setminus a}} H_{ba}C_\lambda^b-\sum_{\substack{b\in I_{p\setminus a}\\ \mu\in I_{q\setminus\lambda}}} C_\lambda^b H_{b\mu}C_\mu^a, \tag{2.24}$$

$$H_{\lambda\mu}=\langle\phi_\lambda|\hat{H}|\phi_\mu\rangle,\quad H_{a\mu}=\langle\psi_a^0|\hat{H}|\phi_\mu\rangle \tag{2.25}$$

$$H_{ba}=\langle\psi_b^0|\hat{H}|\psi_a^0\rangle,\quad D_\lambda^a=\mathcal{E}_\lambda-\mathcal{E}_a \tag{2.26}$$

$$\mathcal{E}_\lambda=\langle\phi_\lambda|\hat{H}|\phi_\lambda\rangle,\quad \mathcal{E}_a=\langle\psi_a^0|\hat{H}|\psi_a^0\rangle \tag{2.27}$$

with $a,b\in I_p$ and $\mu,\lambda\in I_q$. For the case of a nonorthogonal basis spanning the reference space, we refer to [3].

In Eq. (2.21) we used the negative sign in front of the square root, which gives the correct limit zero for the quantity $H_{a\lambda}C_\lambda^a$. As already mentioned at the end of Sec. II B, we obtain the same representation of the WECs by using the Epstein-Nesbet partitioning of the Hamiltonian. Then, this choice of the sign corresponds to the limit $H_{\mu\nu}\to 0$, $\mu\neq\nu$, of the perturbation in the case of Epstein-Nesbet partitioning which leads to the unperturbed case $\hat{H}_0$.

Instead of using $\sigma=\mathrm{sgn}(\Lambda_\lambda^a)$ we can also use $\tilde{\sigma}=\mathrm{sgn}(D_\lambda^a)$ in Eq. (2.21) because this leads to the same result for the limit $H_{\mu\nu}\to 0$. The sign of D_λ^a, i.e., $\tilde{\sigma}$ is independent of the WECs whereas σ depends on the WECs which can be important for iteration procedures.

For an iteration procedure one has to choose initial values for the WECs. This can be done by setting all coefficients on the right-hand side of Eqs. (2.21) and (2.22) equal to zero.

Here, it should be stressed that this representation of the WEC-iteration method does not depend on a special basis set or a set of eigenfunctions of an unperturbed Hamiltonian, respectively. Of course, the basis set should be chosen in such a way that the iteration procedure converges sufficiently fast to the correct solution.

III. RENORMALIZATION

In another article [3] it was shown that the iteration scheme for the ground state and for excited states of the quartic anharmonic oscillator does not converge sufficiently fast for large coupling constants. These convergence problems can be overcome by renormalization. We also use these renormalization techniques in the present investigation.

For that purpose, we consider the unitary scaling transformation $\hat{U}(\gamma),\gamma>0$ (Symanzik scaling), of the canonically

conjugate operators $\hat{x}$ and $\hat{p}$ according to (see p. 85 of Ref. [18], and Appendix C of Ref. [38])

$$\hat{U}(\gamma)\hat{x}\hat{U}^{-1}(\gamma)=\gamma\hat{x}, \tag{3.1}$$

$$\hat{U}(\gamma)\hat{p}\hat{U}^{-1}(\gamma)=\gamma^{-1}\hat{p}. \tag{3.2}$$

For a function $f(x)$, we have

$$\hat{U}(\gamma)f(x)=\gamma^{1/2}f(\gamma x). \tag{3.3}$$

The unitary transformation according to Eq. (3.3) ensures that the normalization of the function $f(x)$ does not change by scaling. Since a unitary transformation leaves the eigenvalues of a Schrödinger equation and the domain of the Hamiltonian, respectively, invariant we can apply scaling according to Eqs. (3.1) and (3.2) to the anharmonic oscillators [see [18] and Eq. (3.3) of Ref. [39]]

$$\hat{H}^{(m)}(\alpha,\beta)=\hat{p}^2+\alpha\hat{x}^2+\beta\hat{x}^{2m}, \tag{3.4}$$

where $m=2,3,4,\ldots$, and $\alpha>0$, $\beta>0$. To simplify the unitary transformation in the case of the anharmonic oscillators one can choose $\gamma=\tau^{1/2}$ [see p. 85 of Ref. [18], and Eqs. (3.1), (3.2) of Ref. [39]]. Using this unitary transformation, the transformed Hamiltonian of Eq. (3.4) will be written according to Eq. (3.2) and Eq. (3.3) as follows [Eq. (3.4) of Ref. [39]]

$$\hat{H}^{(m)}(\alpha,\beta;\tau)=\tau^{-1}\{\hat{p}^2+\alpha\tau^2\hat{x}^2+\beta\tau^{m+1}\hat{x}^{2m}\}. \tag{3.5}$$

Hence, the eigenvalue $E^{(m)}(\alpha,\beta)$ satisfies [see p. 112 of Ref. [18], and Eq. (3.5) of Ref. [39]]:

$$E^{(m)}(\alpha,\beta)=\tau^{-1}E^{(m)}(\alpha\tau^2,\beta\tau^{m+1}). \tag{3.6}$$

For the Hamiltonian of the anharmonic oscillators according to Eq. (1.3) we have to choose $\alpha=1$ yielding

$$\begin{aligned}\hat{H}^{(m)}(\beta;\tau)&=\hat{U}(\gamma)\hat{H}^{(m)}(\beta)\hat{U}^{-1}(\gamma)\\&=\tau^{-1}\{\hat{p}^2+\hat{x}^2+\beta\tau^{m+1}\hat{x}^{2m}-(1-\tau^2)\hat{x}^2\}.\end{aligned} \tag{3.7}$$

Here, $\tau>0$ is an unspecified scaling parameter which can be optimized to speed up convergence.

The renormalization scheme introduced by Vinette and Čížek [17] is based on Symanzik scaling [18]. Vinette and Čížek used this renormalization for calculations of upper and lower bounds for the ground-state energy of the anharmonic oscillators, Eq. (3.7), $m=2,3,4$, by using Löwdin's inner projection technique [29,40–46]. The scaling parameter τ was optimized by the use of a variational condition [Eq. (10) of Ref. [17]] with respect to the ground state (see also [47,48], Sec. 10 of [49], and Sec. 4 of [39]). Since we also want to calculate excited states, we generalized this condition to excited states by writing [2,3]

$$\frac{d}{d\tau}\left\{\frac{\langle\phi_n|\hat{H}^{(m)}(\beta;\tau)|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}\right\}=0. \tag{3.8}$$

Here, $|\phi_n\rangle$ is the nth eigenstate function of the unperturbed Hamiltonian $\hat{p}^2+\hat{x}^2$ with eigenvalue $E_n^0=1+2n$.

The variational condition (3.8) looks like the Rayleigh-Ritz variational condition if we apply the unitary scaling transformation $\hat{U}^{-1}(\gamma)$ on the basis function $|\phi_n\rangle$ instead of applying it on the Hamiltonian according to Eq. (3.7). However, this variational condition is not used to determine the wave function or the energy expectation value, respectively. It is only used to determine the unspecified scaling parameter τ in the Hamiltonian (3.7).

Of course, the procedure discussed above is not the only possible renormalization scheme. Numerous other renormalization techniques are described in the literature (see, for instance, [39] and references therein).

The variational condition (3.8) leads to a simple nonlinear relationship between the coupling constant β and the scaling parameter τ (Sec. 5.5 of Ref. [2])

$$B_m^n\tau^{m+1}\beta=1-\tau^2. \tag{3.9}$$

Here, we introduce the coefficients

$$B_m^n=\frac{m}{E_n^0}\langle\phi_n|\hat{x}^{2m}|\phi_n\rangle, \tag{3.10}$$

$$n=0,1,2,\ldots,\quad m=2,3,4,\ldots.$$

For the special cases $m=2,3,4$ we obtain the following expressions for B_m^n:

$$B_2^n=\frac{3}{E_n^0}[1+2n(n+1)], \tag{3.11}$$

$$B_3^n=\frac{15}{4E_n^0}(4n^3+6n^2+8n+3), \tag{3.12}$$

$$B_4^n=\frac{35}{2E_n^0}(2n^4+4n^3+10n^2+8n+3). \tag{3.13}$$

Setting $n=0$ in Eqs. (3.11)–(3.13) reproduces the results of Vinette and Čížek [Eq. (19) of Ref. [17]].

As in the renormalization scheme of Vinette and Čížek, we introduce a renormalized coupling constant [Eq. (23) of Ref. [17]]

$$\kappa=1-\tau^2. \tag{3.14}$$

Consequently, the original coupling constant β can be expressed in terms of the renormalized coupling constant κ [Eq. (5.5-13) of Ref. [2]]:

$$\beta=\frac{1}{B_m^n}\frac{\kappa}{(1-\kappa)^{(m+1)/2}},\quad m=2,3,4,\ldots. \tag{3.15}$$

Setting $n=0$ again yields the result of Vinette and Čížek [see Eq. (3.19) of Ref. [50]]. Thus, our renormalization scheme also maps $\beta\in[0,\infty)$ onto $\kappa\in[0,1)$ in such a way that $\beta=0$ corresponds to $\kappa=0$ and $\beta\to\infty$ to $\kappa\to1$.

By inserting Eqs. (3.9) and (3.14) into the Hamiltonian $\hat{H}^{(m)}$ (3.7), we obtain the renormalized Hamiltonian [see Eq. (9) of Ref. [17], and Eq. (4.10) of Ref. [39]]

TABLE I. Ground-state energies $E_0^{(2)}$ of the quartic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 200 basis functions and an accuracy of 70 decimal digits. The number k counts the iteration steps.

β	k	$E_0^{(2)}$
0.2	348	1.118 292 654 367 039 153 430 813 153 839 657 185 422 764 786 992 141 711 513 128 134 25
	349	1.118 292 654 367 039 153 430 813 153 839 657 185 422 764 786 992 141 711 513 128 134 29
	350	1.118 292 654 367 039 153 430 813 153 839 657 185 422 764 786 992 141 711 513 128 134 31
0.6	598	1.275 983 566 342 557 058 905 046 395 979 658 762 338 020 597 274 232 815 718 379 866 34
	599	1.275 983 566 342 557 058 905 046 395 979 658 762 338 020 597 274 232 815 718 379 815 14
	600	1.275 983 566 342 557 058 905 046 395 979 658 762 338 020 597 274 232 815 718 379 779 65
1.0	698	1.392 351 641 530 291 855 657 507 876 609 934 184 600 066 711 220 834 088 906 367 605 40
	699	1.392 351 641 530 291 855 657 507 876 609 934 184 600 066 711 220 834 088 906 366 133 94
	700	1.392 351 641 530 291 855 657 507 876 609 934 184 600 066 711 220 834 088 906 364 780 85
2.0	998	1.607 541 302 468 547 538 708 171 929 473 248 382 081 047 203 719 075 902 642 037 261 34
	999	1.607 541 302 468 547 538 708 171 929 473 248 382 081 047 203 719 075 902 642 037 261 25
	1000	1.607 541 302 468 547 538 708 171 929 473 248 382 081 047 203 719 075 902 642 037 261 17
4.0	1098	1.903 136 945 459 000 022 293 850 722 201 023 931 817 313 964 690 420 813 149 118 275 76
	1099	1.903 136 945 459 000 022 293 850 722 201 023 931 817 313 964 690 420 813 149 118 275 20
	1100	1.903 136 945 459 000 022 293 850 722 201 023 931 817 313 964 690 420 813 149 118 274 66
100.0	1398	4.999 417 545 137 587 829 294 632 037 349 652 718 625 507 385 776 536 826 258 596 229 78
	1399	4.999 417 545 137 587 829 294 632 037 349 652 718 625 507 385 776 536 826 258 596 229 96
	1400	4.999 417 545 137 587 829 294 632 037 349 652 718 625 507 385 776 536 826 258 596 230 12
400.0	1398	7.861 862 678 275 891 411 185 809 125 451 972 779 865 901 912 293 522 767 172 178 436 11
	1399	7.861 862 678 275 891 411 185 809 125 451 972 779 865 901 912 293 522 767 172 178 437 38
	1400	7.861 862 678 275 891 411 185 809 125 451 972 779 865 901 912 293 522 767 172 178 438 59
2000.0	1398	13.388 441 701 008 061 939 006 176 902 807 286 522 960 989 885 174 356 660 397 442 449 98
	1399	13.388 441 701 008 061 939 006 176 902 807 286 522 960 989 885 174 356 660 397 442 454 00
	1400	13.388 441 701 008 061 939 006 176 902 807 286 522 960 989 885 174 356 660 397 442 457 82
16 000.0	1498	26.733 815 088 189 002 423 231 037 392 721 473 617 618 290 515 353 621 795 417 542 530 07
	1499	26.733 815 088 189 002 423 231 037 392 721 473 617 618 290 515 353 621 795 417 542 530 12
	1500	26.733 815 088 189 002 423 231 037 392 721 473 617 618 290 515 353 621 795 417 542 530 16
40 000.0	1498	36.274 458 133 736 835 470 376 382 678 474 479 639 356 476 312 937 909 717 948 962 048 26
	1499	36.274 458 133 736 835 470 376 382 678 474 479 639 356 476 312 937 909 717 948 962 048 33
	1500	36.274 458 133 736 835 470 376 382 678 474 479 639 356 476 312 937 909 717 948 962 048 39

$$\hat{\mathcal{H}}^{(n,m)}(\kappa)=(1-\kappa)^{1/2}\hat{H}^{(m)}[\beta(\kappa);(1-\kappa)^{1/2}]$$
$$=\hat{p}^2+\hat{x}^2+\frac{\kappa}{B_m^n}\{\hat{x}^{2m}-B_m^n\hat{x}^2\}. \tag{3.16}$$

Hence, the renormalization scheme of Vinette and Čížek [17,39,50], which only applies to the ground state ($n=0$), as well as our generalization for excited states [2], transforms the perturbation operator $\hat{x}^{2m}$ into a double-minimum potential.

The renormalized Hamiltonian $\hat{\mathcal{H}}^{(n,m)}(\kappa)$ (3.16) fulfills the time-independent Schrödinger equation

$$\hat{\mathcal{H}}^{(n,m)}(\kappa)\Psi^{(n,m)}(x)=E_R^{(n,m)}(\kappa)\Psi^{(n,m)}(x). \tag{3.17}$$

The renormalized energy eigenvalue $E_R^{(n,m)}$ is related to the energy eigenvalue of $\hat{H}^{(m)}(\beta;\tau)$ according to

$$E_R^{(n,m)}(\kappa)=(1-\kappa)^{1/2}E^{(n,m)}(\beta). \tag{3.18}$$

In this context, we can consider the infinite coupling limit [see Eq. (4.19) of Ref. [39]]

$$k_m^n=\lim_{\beta\to\infty}\frac{E^{(n,m)}(\beta)}{\beta^{1/(m+1)}}=[B_m^n]^{1/(m+1)}E_R^{(n,m)}(1),\quad m=2,3,4 \tag{3.19}$$

which corresponds to the nth energy eigenvalue of the Hamiltonian $\hat{\mathbf{H}}_0^{(m)}=\hat{p}^2+\hat{x}^{2m}$ whose eigenvalues and eigenfunctions are not known in closed form.

TABLE II. Ground-state energies $E_0^{(2)}$ of the quartic anharmonic oscillator for different coupling constants β using the approach according to Eq. (4.18): $E_0^{(2)}$(app), compared with the results $E_0^{(2)}$(WEC) of Table I where $\Delta = E_0^{(2)}(\text{app}) - E_0^{(2)}(\text{WEC})$.

β	$E_0^{(2)}$ (app)	$E_0^{(2)}$ (WEC)	Δ
0.2	1.118 284	1.118 292	−0.000 008
0.6	1.275 946	1.275 983	−0.000 037
1.0	1.392 302	1.392 351	−0.000 049
2.0	1.607 496	1.607 541	−0.000 045
4.0	1.903 126	1.903 136	−0.000 010
100.0	4.999 905	4.999 417	0.000 488
400.0	7.862 742	7.861 862	0.000 880
2000.0	13.390 029	13.388 441	0.011 588
16 000.0	26.737 056	26.733 815	0.003 241
40 000.0	36.278 871	36.274 458	0.004 413

Alternatively, we now consider the renormalization scheme based on the well-known Bogoliubov transformation [19]. For that purpose, the Hamiltonians of the anharmonic oscillators have to be reformulated in second quantization:

$$\hat{H}^{(m)}(\beta) = \hat{\mathbf{1}} + 2\hat{a}^\dagger\hat{a} + \frac{\beta}{2^m}(\hat{a}+\hat{a}^\dagger)^{2m}, \quad m = 2,3,4, \ldots . \tag{3.20}$$

Here, $\hat{a}^\dagger$ and $\hat{a}$ are the usual creation and annihilation operators for the harmonic oscillator (see p. 165 of Ref. [51]).

In the literature [12,13,52], the most general linear Bogoliubov transformation is usually written as follows [Eqs. (2.1) and (2.5) of Ref. [12]]:

$$\hat{b} = u\hat{a} + v\hat{a}^\dagger + w, \tag{3.21}$$

$$\hat{b}^\dagger = u^*\hat{a}^\dagger + v^*\hat{a} + w^*. \tag{3.22}$$

Here, u,v, and w are complex numbers. In the following we restrict ourselves to $w=0$.

The transformations given above have to obey the same commutation relations as $\hat{a}^\dagger$ and $\hat{a}$: $[\hat{b},\hat{b}^\dagger]=1$, $[\hat{b},\hat{b}]=0$, $[\hat{b}^\dagger,\hat{b}^\dagger]=0$. Thus, the coefficients u,v have to satisfy the relationship

$$|u|^2 - |v|^2 = 1. \tag{3.23}$$

We choose the phase of the coefficients to be real and introduce the new parameter $\rho = v/u$ such that

$$\hat{b} = \frac{\hat{a} - \rho\hat{a}^\dagger}{\sqrt{1-\rho^2}} \;\Leftrightarrow\; \hat{a} = \frac{\hat{b} + \rho\hat{b}^\dagger}{\sqrt{1-\rho^2}}, \quad \rho \in [0,1[. \tag{3.24}$$

TABLE III. Energies $E_n^{(2)}$ of the ground state and excited states of the quartic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 100 basis functions and an accuracy of 30 decimal digits. The number of iterations varies between 25 and 250. The values marked by $)^+$ are the real parts of resulting complex numbers.

β	0.2	2.0	10.0	100.0	400.0	2000.0
E_0	1.118 292 654	1.607 541 302	2.449 174 072	4.999 417 545	7.861 862 678	13.388 441 701
E_1	3.539 005 288	5.475 784 536	8.599 003 455	17.830 192 716	28.118 453 544	47.944 412 113
E_2	6.277 248 617	10.358 583 375	16.635 921 492	34.873 984 262	55.102 869 334	94.034 677 465
E_3	9.257 765 618	15.884 807 969	25.806 276 215	54.385 291 572	86.010 541 609	146.838 227 689
E_4	12.440 601 800	21.927 166 188	35.885 171 222	75.877 004 029	120.067 986 129	205.032 314 268
E_5	15.799 534 456	28.406 278 209	46.729 080 901	99.032 837 315	156.771 246 445	267.753 782 438
E_6	19.315 679 984	35.268 098 232	58.241 298 740	123.640 697 627	195.782 663 025	334.424 516 387
E_7	22.974 631 159	42.472 870 974	70.351 051 939	149.545 657 443	236.855 659 414	404.622 399 351
E_8	26.764 949 615	49.989 872 819	83.003 867 038	176.628 655 958	279.800 791 267	478.023 155 101
E_9	30.677 284 079	57.794 502 238	96.156 262 981	204.794 774 513	324.467 058 269	554.368 335 158
E_{10}	34.703 815 271	65.866 526 080	109.772 570 864	233.966 225 876	370.730 733 552	633.446 186 453
E_{11}	38.837 886 729	74.188 952 302	123.822 898 910	264.077 875 649	418.488 229 608	715.079 433 896
E_{12}	43.073 748 536	82.747 268 756	138.281 763 471	295.074 233 703	467.651 306 959	799.117 075 807
E_{13}	47.406 373 217	91.528 908 647	153.127 130 748	326.907 350 786	518.143 725 014	885.428 649 405
E_{14}	51.831 319 630	100.522 862 999	168.339 723 962	359.535 299 359	569.898 823 586	973.900 090 109
E_{15}	56.344 629 992	109.719 392 149	183.902 508 794	392.921 046 372	622.857 728 632	1064.430 659 770
E_{16}	60.942 750 318	119.109 806 103	199.800 302 462	427.031 597 557	676.967 990 360	1156.930 615 236
E_{17}	65.622 467 906	128.686 294 076	216.019 470 890	461.837 335 032	732.182 529 124	1251.319 403 918
E_{18}	70.380 861 448	138.441 789 975	232.547 690 138	497.311 495 801	788.458 805 607	1347.524 243 372
E_{19}	75.215 260 686	148.369 864 702	249.373 755 670	533.429 755 055	845.758 157 846	1445.478 986 490
E_{20}	80.123 213 400	158.464 638 796	266.487 427 865	570.169 888 845	904.045 264 571	1545.123 202 954
E_{21}	85.102 458 099	168.720 710 776	283.879 305 433	607.511 497 810	963.287 705 721	1646.401 427 036
E_{22}	90.150 901 225	179.133 097 747	301.540 720 623	645.435 778 559	1023.455 598 782	1749.262 535 191
E_{23}	95.266 597 953	189.697 185 707	319.463 651 640	683.925 332 697	1084.521 295 032	1853.659 226 198
E_{24}	100.447 735 895	200.408 687 647	337.640 648 847	722.964 005 941	1146.459 123 665	1959.547 583 249
E_{25}	105.692 621 167	211.263 607 916	356.064 64)$^+$	762.52)$^+$	1209.23)$^+$	2066.86)$^+$

TABLE IV. Ground-state energies $E_0^{(3)}$ of the sextic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 200 basis functions and an accuracy of 50 decimal digits. The number k counts the iteration steps.

β	k	$E_0^{(3)}$
0.2	2998	1.173 889 345 125 433 152 981 773 27
	2999	1.173 889 345 125 433 152 981 773 61
	3000	1.173 889 345 125 433 152 981 773 95
0.6	2998	1.332 895 943 373 392 802 564 23
	2999	1.332 895 943 373 392 802 564 36
	3000	1.332 895 943 373 392 802 564 49
1.0	2998	1.435 624 619 003 392 315 564 4
	2999	1.435 624 619 003 392 315 565 2
	3000	1.435 624 619 003 392 315 565 9
2.0	2998	1.609 931 952 023 083 569 926
	2999	1.609 931 952 023 083 569 930
	3000	1.609 931 952 023 083 569 935
4.0	2998	1.830 437 343 750 106 212 601
	2999	1.830 437 343 750 106 212 616
	3000	1.830 437 343 750 106 212 631
100.0	2998	3.716 974 729 208 620 146 11
	2999	3.716 974 729 208 620 146 35
	3000	3.716 974 729 208 620 146 60
400.0	2998	5.188 358 854 438 675 605 01
	2999	5.188 358 854 438 675 605 46
	3000	5.188 358 854 438 675 605 90
2000.0	2998	7.701 738 364 609 832 717 2
	2999	7.701 738 364 609 832 718 0
	3000	7.701 738 364 609 832 718 7
16 000.0	2998	12.902 759 971 023 155 867 8
	2999	12.902 759 971 023 155 869 1
	3000	12.902 759 971 023 155 870 5
40 000.0	2998	16.211 718 264 749 243 084 9
	2999	16.211 718 264 749 243 086 6
	3000	16.211 718 264 749 243 088 4

This representation of the Bogoliubov transformation can be interpreted as a rotation (plus translation if $w \neq 0$) of the original Hilbert space yielding a new Hilbert space (see p. 2212 of Ref. [12]).

Expressing the Hamiltonian (3.20) in terms of the operators $\hat{b}, \hat{b}^\dagger$ yields

$$\hat{H}^{(m)}(\beta;\rho) = \frac{1+\rho^2}{1-\rho^2}(\hat{1} + 2\hat{b}^\dagger\hat{b}) + \frac{2\rho}{1-\rho^2}(\hat{b}^2 + \hat{b}^{\dagger 2}) + \frac{\beta}{2^m}\frac{(1+\rho)^{2m}}{(1-\rho^2)^m}(\hat{b}+\hat{b}^\dagger)^{2m}, \quad m = 2,3,4, \ldots . \tag{3.25}$$

In the quartic case the Hamiltonian (3.25) is often written in normal-ordered form [12,13,52].

Next, a parameter [see Eq. (2.13) of Ref. [12], or Eq. (60) of Ref. [52]]

$$\omega = \frac{1-\rho}{1+\rho}, \quad \omega \in]0,1] \tag{3.26}$$

is introduced. This parameter ω will be determined by the variation of $\langle \phi_n | \hat{H}^{(m)}(\beta;\omega) | \phi_n \rangle$ with respect to ω according to

$$\frac{d}{d\omega}\left\{ \frac{1+\omega^2}{2\omega} E_n^0 + \frac{\beta}{(2\omega)^m} D_m^n \right\} = 0. \tag{3.27}$$

This corresponds to Eq. (3.8) if ω is used instead of τ. Here,

$$E_n^0 = 1 + 2n, \quad D_m^n = \langle \phi_n | (\hat{b} + \hat{b}^\dagger)^{2m} | \phi_n \rangle. \tag{3.28}$$

This leads for arbitrary $m = 2,3,4, \ldots$ to a simple nonlinear algebraic expression between the coupling constant β and the variational parameter ω [Eq. (5.5-10) of Ref. [2]]

$$\omega^{m+1} - \omega^{m-1} - B_m^n \beta = 0, \quad B_m^n = \frac{m D_m^n}{2^{m-1} E_n^0}. \tag{3.29}$$

The constant B_m^n is identical with the one in Eq. (3.10) obtained by generalizing the renormalization scheme of Vinette and Čížek [17]. By comparing Eq. (3.9) for τ with Eq. (3.29) for ω, we see that Eq. (3.29) leads to Eq. (3.9) if we set $\omega = \tau^{-1}$.

Thus, both transformation schemes are equivalent. In other words, the Bogoliubov transformation (with $w = 0$) used in the second quantization is equivalent to Symanzik scaling if the parameters τ and ω are determined by Eq. (3.8) and Eq. (3.27), respectively. Hence, for our calculations we can use the renormalization technique which is based on the Symanzik scaling as well as the one which is based on the Bogoliubov transformation.

IV. ANHARMONIC OSCILLATORS

In this section we apply the WEC-iteration method, described in Sec. II, and the renormalization technique, described in Sec. III, to the anharmonic oscillators defined by Eq. (1.3).

For that purpose, we have to determine the matrix elements of the Hamiltonian (3.7),

$$\hat{H}^{(m)}(\beta;\tau) = \hat{H}^{(m)}(\beta(\kappa);(1-\kappa)^{1/2}) = (1-\kappa)^{-1/2}\hat{\mathcal{H}}^{(n,m)}(\kappa) = \hat{H}^{(n,m)}(\kappa), \tag{4.1}$$

with respect to the eigenfunctions of the Hamiltonian $\hat{\mathcal{H}}_0 = \hat{p}^2 + \hat{x}^2$. For a given $\beta \geqslant 0$ the renormalized coupling constant κ is determined according to Eq. (3.15).

In the following, we will consider the quartic, sextic, and octic anharmonic oscillator ($m = 2,3,4$) using only a one-dimensional reference space which contains the ground state $|\phi_0\rangle$ or an excited state $|\phi_n\rangle$, $n > 0$, of the harmonic oscillator.

TABLE V. Energies $E_n^{(3)}$ of the ground state and excited states of the sextic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 100 basis functions and an accuracy of 30 decimal digits. The number of iterations varies between 25 and 250. The values marked by $)^+$ are the real parts of resulting complex numbers.

β	0.2	2.0	10.0	100.0	400.0	2000.0
E_0	1.173 889 345	1.609 931 952	2.205 723 268	3.716 974 729	5.188 358 854	7.701 738 365
E_1	3.900 835 570	5.749 347 753	8.114 843 119	13.946 206 623	19.563 130 002	29.121 275 718
E_2	7.381 647 216	11.543 934 572	16.641 218 108	28.977 293 817	40.778 190 628	60.810 583 703
E_3	11.547 467 607	18.649 694 591	27.155 085 605	47.564 984 582	67.029 670 737	100.036 400 295
E_4	16.295 106 578	26.830 242 757	39.289 330 657	69.046 576 526	97.377 734 917	145.391 321 051
E_5	21.559 198 785	35.957 488 954	52.849 512 678	93.073 891 695	131.329 254 341	196.137 354 955
E_6	27.293 159 807	45.941 185 837	67.698 071 648	119.399 778 937	168.533 879 957	251.749 926 949
E_7	33.461 170 767	56.712 885 988	83.730 950 282	147.837 547 352	208.727 055 860	311.832 992 247
E_8	40.034 560 162	68.218 416 493	100.865 986 116	178.239 969 897	251.700 207 862	376.074 359 579
E_9	46.989 696 992	80.413 494 473	119.036 133 924	210.487 018 157	297.283 328 838	444.219 593 327
E_{10}	54.306 663 460	93.261 028 760	138.185 313 922	244.478 367 578	345.334 343 437	516.056 080 299
E_{11}	61.958 166 340	106.703 944 069	158.224 311 899	280.051 349 559	395.621 856 064	591.236 681 542
E_{12}	69.934 866 491	120.731 046 132	179.139 196 688	317.184 225 138	448.116 156 660	669.717 834 584
E_{13}	78.215 556 365	135.300 198 585	200.865 037 003	355.759 552 652	502.650 498 840	751.249 647 730
E_{14}	86.782 276 497	150.377 664 550	223.350 707 147	395.685 753 941	559.095 155 489	835.637 955 256
E_{15}	95.615 703 768	165.926 701 478	246.540 302 082	436.862 448 281	617.307 847 977	922.669 736 684
E_{16}	104.700 590 690	181.921 170 110	270.395 316 428	479.221 808 119	677.192 875 742	1012.202 072 551
E_{17}	114.018 320 473	198.326 502 826	294.863 466 008	522.670 259 145	738.617 706 750	1104.036 617 016
E_{18}	123.555 550 426	215.28)$^+$	320.35)$^+$	567.84)$^+$	803.41)$^+$	1200.96)$^+$
E_{19}	132.97)$^+$	232.48)$^+$	347.70)$^+$	615.90)$^+$	834.02)$^+$	1300.39)$^+$

The matrices of the Hamiltonian (4.1), with $m=2,3,4$, are sparse matrices. The matrix elements are explicitly shown in Sec. 5.5 of Ref. [2]. Therefore, the energy of the ground state $E_0^{(m)}$ or an excited state $E_n^{(m)}$ for $m=2,3,4$ can be written as

$$E_n^{(m)}=H_{n,n}^{(n,m)}+\sum_{\substack{i=-m\\ i\neq 0}}^{m} H_{n,n-2i}^{(n,m)} C_{n-2i}^n . \tag{4.2}$$

Here,

$$H_{\mu,\nu}^{(n,m)}=\langle \phi_\mu|\hat{H}^{(n,m)}(\kappa)|\phi_\nu\rangle \tag{4.3}$$

are the matrix elements of the renormalized Hamiltonian (4.1).

With the help of Eq. (2.21), using $\tilde{\sigma}$ instead of σ, we obtain the following WECs:

$$C_\mu^n=\frac{1}{2H_{n,\mu}}\{\Lambda_\mu^n-\tilde{\sigma}[\{\Lambda_\mu^n\}^2+4H_{n,\mu}(H_{\mu,n}+\Gamma_{\mu,n})]^{1/2}\}. \tag{4.4}$$

Here

$$\Lambda_\mu^n=\Delta E_{n,\mu}-\Delta_{n,\mu}, \tag{4.5}$$

$$\Delta E_{n,\mu}=H_{\mu,\mu}-H_{n,n}, \quad H_{\mu,\nu}=H_{\mu,\nu}^{(n,m)}, \tag{4.6}$$

$$\Delta_{n,\mu}=\sum_{\substack{i=-m\\ n-2i\neq n,\mu}}^{m} H_{n,n-2i}\, C_{n-2i}^n , \tag{4.7}$$

$$\Gamma_{\mu,n}=\sum_{\substack{i=-m\\ \mu-2i\neq n,\mu}}^{m} H_{\mu,\mu-2i}\, C_{\mu-2i}^n . \tag{4.8}$$

Moreover, we choose according to Eqs. (2.26) and (2.27),

$$\tilde{\sigma}=\mathrm{sgn}(D_\mu^n)=\mathrm{sgn}(\Delta E_{n,\mu}). \tag{4.9}$$

Here, $n\geqslant 0$ is the index of the reference state whose WEC satisfies $C_n^n=1$, and $\mu\neq n$ is the index of those basis functions whose matrix elements $H_{n,\mu}$ do not vanish.

If the matrix element $H_{n,\mu}$ vanishes we obtain for the WECs according to Eq. (2.22)

$$C_\mu^n=\frac{\Gamma_{\mu,n}}{\Delta-\Delta E_{n,\mu}}, \tag{4.10}$$

$$\Delta=\sum_{\substack{i=-m\\ i\neq 0}}^{m} H_{n,n-2i}\, C_{n-2i}^n . \tag{4.11}$$

For the calculation of the WECs and the energy, respectively, we used a one-step iteration scheme of the following type:

$$C_j^{(\kappa+1)}=f_j(C_1^{(\kappa+1)},\ldots,C_{j-1}^{(\kappa+1)},C_j^{(\kappa)},C_{j+1}^{(\kappa)},\ldots). \tag{4.12}$$

TABLE VI. Ground-state energies $E_0^{(4)}$ of the octic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 200 basis functions and an accuracy of 50 decimal digits. The number k counts the iteration steps.

β	k	$E_0^{(4)}$
0.2	3498	1.241 027 905 768 2
	3499	1.241 027 905 767 4
	3500	1.241 027 905 766 7
0.6	3498	1.397 708 765 129 9
	3499	1.397 708 765 126 6
	3500	1.397 708 765 123 3
1.0	3498	1.491 019 900 788
	3499	1.491 019 900 783
	3500	1.491 019 900 778
2.0	3498	1.641 370 366 053
	3499	1.641 370 366 044
	3500	1.641 370 366 035
4.0	3498	1.822 179 884 013
	3499	1.822 179 883 999
	3500	1.822 179 883 986
100.0	3498	3.188 654 398 359
	3499	3.188 654 398 311
	3500	3.188 654 398 263
400.0	3498	4.146 188 636 727
	3499	4.146 188 636 657
	3500	4.146 188 636 587
2000.0	3498	5.666 203 972 945
	3499	5.666 203 972 842
	3500	5.666 203 972 739
16 000.0	3498	8.536 651 143 218
	3499	8.536 651 143 056
	3500	8.536 651 142 893
40 000.0	3498	10.238 868 450 82
	3499	10.238 868 450 62
	3500	10.238 868 450 42

The numerical calculations were performed with the help of the symbolic computation language MAPLE [20–22].

The iteration starts by setting $C_n^n=1$ for the reference state with index n. All residual WECs are equal to zero. Then, we calculate the WECs which occur in the expression of the energy (4.2) in the sequence C_{n-2}^n, $C_{n+2}^n,\ldots,C_{n-2m}^n,C_{n+2m}^n$. Next, the residual WECs will be calculated. This will be done by the following one-step iteration scheme:

$$C_\mu^{(\kappa+1)}=f_\mu(C_i^{(\kappa)},\ldots,C_\mu^{(\kappa)},C_{\mu+2}^{(\kappa+1)},\ldots,C_{n-4}^{(\kappa+1)},C_{n-2}^{(\kappa+1)}),\quad n-2m>\mu\geqslant i, \tag{4.13}$$

$$C_\mu^{(\kappa+1)}=f_\mu(C_{n+2}^{(\kappa+1)},C_{n+4}^{(\kappa+1)},\ldots,C_{\mu-2}^{(\kappa+1)},C_\mu^{(\kappa)},\ldots,C_N^{(\kappa)}),\quad n+2m<\mu\leqslant N. \tag{4.14}$$

We have $i=0$ if the reference state $|\phi_n\rangle$ has an even index, and $i=1$ if the reference state $|\phi_n\rangle$ has an odd index. Within the set of all indices μ specifying the basis functions $|\phi_\mu\rangle$, which are used in the calculation, the index N stands for the maximal index. The quantity Δ in the iteration function f_μ according to Eq. (4.10) is fixed by the WECs in the expression of the energy Eq. (4.2).

With the help of Eq. (4.2), the ground-state energy of the quartic anharmonic oscillator can be written as follows:

$$E_0^{(2)}=H_{0,0}^{(0,2)}+H_{0,4}^{(0,2)}C_4^0, \tag{4.15}$$

where we use that

$$\langle\phi_0|\hat{H}^{(n,2)}(\kappa)|\phi_2\rangle=H_{0,2}^{(0,2)}=0. \tag{4.16}$$

Equation (4.16) is a result of the renormalization of the Hamiltonian. An analogous expression holds also for the energy of the first excited state:

$$\langle\phi_1|\hat{H}^{(n,2)}(\kappa)|\phi_3\rangle=H_{1,3}^{(n,2)}=0. \tag{4.17}$$

Since the matrix elements $H_{\mu,\nu}^{(n,2)}$ of the quartic anharmonic oscillator with functions of opposite parity vanish, the first excited state is the ''ground state'' for the basis functions with odd indices, like the ground state $|\phi_0\rangle$ for the basis functions with even indices. This is also true for the sextic and octic anharmonic oscillator.

Table I shows results of highly accurate calculations of the ground-state energy for the quartic anharmonic oscillator for different coupling constants. We used 200 basis functions and an accuracy of 70 decimal digits. If we compare these results with the upper and lower bounds obtained by Vinette and Čížek [17], the energies from Table I for $\beta=0.2$ through 100.0 lie between their upper and lower bounds. For $\beta=400.0$ through 40 000.0 the upper and lower bounds given by Vinette and Čížek are higher then the results of Table I. However, our results agree, for example for $\beta=40\,000.0$, with the 15 decimal digits of Banerjee's result [53] (see also [54]). The results in Table I given by Weniger [39] for the same coupling constants as used in Table I agree also with our results listed in Table I.

Table II shows results of the ground-state energy for different coupling constants β using an approximation for the C_4^0 coefficient in Eq. (4.15) deduced from Eq. (4.4):

TABLE VII. Energies $E_n^{(4)}$ of the ground state and excited states of the octic anharmonic oscillator for different coupling constants β using the WEC-iteration method. The calculations were performed in MAPLE, using 100 basis functions and an accuracy of 30 decimal digits. The number of iterations varies between 90 and 3000. The values marked by $)^+$ are the real parts of resulting complex numbers.

β	0.2	2.0	10.0	100.0	400.0
E_0	1.241 027 906	1.641 370 366	2.114 544 658	3.188 654 398	4.146 188 637
E_1	4.275 477 260	5.999 607 360	7.929 683 083	12.195 021 934	15.951 984 779
E_2	8.453 030 681	12.421 035 881	16.711 022 381	26.033 458 321	34.183 309 142
E_3	13.737 162 633	20.660 642 905	28.022 750 233	43.902 113 333	57.739 246 097
E_4	19.993 020 289	30.460 576 795	41.494 702 573	65.201 815 832	85.825 114 583
E_5	27.121 781 054	41.657 080 682	56.898 990 130	89.569 748 770	117.961 640 041
E_6	35.056 003 250	54.140 371 960	74.083 047 443	116.762 998 352	153.827 888 142
E_7	43.744 375 499	67.826 901 779	92.930 664 513	146.596 403 041	193.179 173 024
E_8	53.145 590 381	82.649 604 300	113.348 632 162	178.921 526 920	235.819 369 582
E_9	63.225 347 319	98.552 969 649	135.259 874 580	213.615 701 996	281.586 427 123
E_{10}	73.954 524 917	115.489 994 593	158.599 178 257	250.575 191 998	330.343 324 077
E_{11}	85.307 965 177	133.420 159 010	183.310 359 774	289.710 661 566	381.972 073 999
E_{12}	97.263 627 357	152.308 024 478	209.344 306 977	330.944 045 334	436.369 584 539
E_{13}	109.796 736 743	172.112 579 014	236.643 622 787	374.183 493 403	493.414 326 635
E_{14}	122.890 901 701	192.808 269 366	265.173 286 541	419.373 774 370	553.033 527 919
E_{15}	136.49)$^+$	214.66)$^+$	295.13)$^+$	466.93)$^+$	

$$E_0^{(2)}(app)=\frac{4-\kappa}{4\sqrt{1-\kappa}}+\frac{1}{2}[\Delta E_{4,0} - \{\Delta E_{4,0}^2+4(|H_{0,4}|^2+\widetilde{\Gamma}_{4,0})\}^{1/2}]. \quad (4.18)$$

Here,

$$\widetilde{\Gamma}_{4,0}=|H_{2,4}|^2\left(1-\frac{\Delta E_{2,0}}{D}\right)^{-1}+|H_{4,6}|^2\left(1-\frac{\Delta E_{6,0}}{D}\right)^{-1} + |H_{4,8}|^2\left(1-\frac{\Delta E_{8,0}}{D}\right)^{-1} \quad (4.19)$$

and

$$D=\tfrac{1}{2}[\Delta E_{4,0}-\{\Delta E_{4,0}^2+4|H_{0,4}|^2\}^{1/2}]. \quad (4.20)$$

If we compare these results with the energies in Table I, which were determined iteratively by the WEC-iteration method as described above, we see that this simple approximation (4.18) yields remarkably good results.

Table III shows highly accurate results for the energies of the first 26 states of the quartic anharmonic oscillator for different coupling constants. We used 100 basis functions and an accuracy of 30 decimal digits. Again, our results for E_0 through E_{10} for $\beta=10.0$ and 100.0 are in agreement with the energies given by Banerjee [53]. Furthermore, variational calculations by using the renormalized Hamiltonian Eq. (4.1) give the same energies as displayed in Table III. These variational calculations which utilized the procedure *Eigenvals* of MAPLE [20–22] were based on the same renormalized Hamiltonian which was used in the WEC calculations of E_{24} for even indices and in the WEC calculations of E_{23} for odd indices. For higher excited states the iteration of the WEC calculation apparently converges. However, it oscillates between a complex number and its complex conjugate. The values of Table III marked by $)^+$ are the real parts of the resulting complex numbers.

Table IV shows results of analogous WEC calculations for the ground-state energy of the sextic anharmonic oscillator. The same coupling constants as in the case of the quartic anharmonic oscillator were considered. These results were calculated by using 200 basis functions and an accuracy of 50 decimal digits. Here, the results lie between the upper-energy and lower-energy bounds of the ground-state of Vinette and Čížek [17], which are less accurate than in the quartic case. The results for the ground-state energy given by Banerjee [53] and by Weniger [39], which are of lower accuracy, are in agreement with the results of Table IV up to the relevant digits.

Energies of some excited states of the sextic anharmonic oscillator are listed in Table V. As in the quartic case the results for $\beta=10$ and $\beta=100$ for the first 11 states agree with the results given by Banerjee [53]. The values marked by $)^+$ are again the real parts of the resulting complex numbers as in the case of the x^4 anharmonic oscillator.

As in the quartic and sextic case, the results for the energies of the octic anharmonic oscillator are displayed in Table VI for the ground state, and in Table VII for the excited states. As before the values marked by $)^+$ are the real parts of the resulting complex numbers. Furthermore, as in the cases of the quartic and sextic anharmonic oscillators we reproduce up to the relevant digits the results of the calculations given by Banerjee [53] with coupling constants $\beta=10$ and $\beta=100$ for the first 11 states.

For the infinite coupling limit Eq. (3.19) of the ground state for the quartic, sextic, and octic anharmonic oscillator, we obtained with the help of the WEC-iteration method

$$k_2^0(3000) = 1.060\ 362\ 090\ 484\ 182\ 899\ 647\ 046\ 016\ 692\ 663\ 545\ 515\ 208\ 728\ 528$$
$$977\ 933\ 216\ 245\ 241\ 695\ 943\ 563\ 044\ 344\ 504\ 109\ 68, \quad (4.21)$$

$$k_3^0(3500) = 1.144\ 802\ 453\ 797\ 052\ 7, \quad (4.22)$$

$$k_4^0(4000) = 1.225\ 820\ 1. \quad (4.23)$$

The numbers in the parentheses are the numbers of iteration. These results agree with the results of Vinette and Čížek [17] up to all digits given by them. In the case of k_3 and k_4 the results of Vinette and Čížek are more accurate than our results.

Thus, the WEC-iteration method is a powerful tool which produces very accurate approximations to the energies of x^{2m}-anharmonic oscillators $(m=2,3,4)$, even if it is used with a one-dimensional reference space only.

V. SUMMARY

In this article, we applied the WEC-iteration method, which was introduced in [2,3], in combination with a one-dimensional reference space to the ground and excited states of the quartic, sextic, and octic anharmonic oscillator. Our approach yielded highly accurate results for the energies of the ground state and of some excited states for these anharmonic oscillators.

In our calculations we used a renormalization technique which was introduced by Vinette and Čížek[17], and generalized it to excited states. Furthermore, we showed that this renormalization scheme, which is based on Symanzik scaling [18], is identical with a renormalization based on the Bugoliubov transformation [12].

On the basis of the results presented in this article and elsewhere [2,3], one can expect that the WEC-iteration method should also give good results in the case of other quantum-mechanical problems.

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