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## Self-rotating wave approximation via symmetric ordering of ladder operators

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We show how some Hamiltonians may be approximated using rotating wave approximation methods. In order to achieve this we use the algebra of boson ladder operators, and transformation formulas between normal and symmetric ordering of the operators. The method presented is studied in two special cases; the Morse and the Mathieu models. The connection with regular perturbation theory is given and the validity of the approximation is discussed.

### 1. Introduction

In this contribution we produce approximations for some Hamiltonians such as the ones related with the Morse potential and cosine potential (quantum rotor, or Mathieu differential equation). The approximation is based on the rotating wave approximation (RWA) [1, 2] and symmetric ordering of ladder operators [3]. The RWA is widely used in quantum optical systems and particularly in Jaynes–Cummings types of models [4, 5] and its extensions [6], for example in ion traps [7], cavity quantum electrodynamics [8] and population transfer in atoms and molecules [9]. Also the breakdown of the approximations in similar systems has been considered in several papers [10]. The RWA is usually used for two (or more) interacting subsystems, and in all the above examples, interaction between different subsystems are considered. When passing to the interaction picture with respect to the free Hamiltonian, one remains with a time-dependent Hamiltonian, which under certain conditions on the frequencies involved may take a simpler form by neglecting terms that oscillate rapidly [2, 4]. A phenomenological motivation for the approximation is that the neglected terms usually describe non-energy conserving processes, which in the Jaynes–Cummings model describe simultaneous excitation of

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the atom/ion and the quantized field. The neglected terms, usually very small within the experimental parameter regimes, give rise to the Bloch–Siegert shift of the energies [11]. In this paper we show that we can also apply a RWA in a single Hamiltonian system. Developing the potential in a Taylor series and grouping the quadratic term of the Hamiltonian with the kinetic energy to produce a harmonic oscillator term plus an infinite sum. The frequency of the *artificially* produced harmonic oscillator (HO) is then used as a reference to apply the RWA to the remaining sum. We call this HO a self-HO for the Hamiltonian studied. Using the underlying algebra of the oscillator ladder operators and the RWA, closed forms of the infinite sums are given in two special cases. Only Hamiltonian systems containing bound or quasi bound states may be approximated, and the validity depends on the relative ‘depth/width’ of the potential; the deeper and narrower potential the better the approximation. Thus, it is best suited for low excited bound states, which is verified by numerical simulations. It is also shown that the RWA gives the result of regular first-order perturbation theory of the self-HO, which again underlines the validity regimes of the approximation.

We proceed as follows, in the next section we introduce the self-HO and its Fock states of an arbitrary Hamiltonian and derive expressions for the diagonal elements of this Hamiltonian in the Fock basis. This is achieved using the properties of the ladder operators. In sections 3 and 4, the connection with the RWA is given and two specific models are considered; the Mathieu and Morse equations respectively. The validity of the approximation is investigated in section 5 for both studied cases. Section 6 is left for a summary, and Appendix A shows how the methods may be used in a more general way for calculating various sums.

## 2. Diagonal matrix elements in the Fock basis of an arbitrary Hamiltonian

Given an arbitrary Hamiltonian we expand the potential term in a Taylor series (in the following we consider for simplicity the case of unit mass and  $\hbar = 1$ )

$$H = \frac{\hat{p}^2}{2} + V(\hat{x}) = V^{(0)}(0) + V^{(1)}(0)\hat{x} + \frac{\hat{p}^2}{2} + \frac{\omega^2 \hat{x}^2}{2} + \sum_{k=3}^{\infty} \frac{V^{(k)}(0)}{k!} \hat{x}^k \quad (1)$$

with  $\omega^2 = V^{(2)}(0)$ . We let this frequency  $\omega$  define the ladder operators [12] for the Hamiltonian systems as

$$\hat{a} = \left(\frac{\omega}{2}\right)^{1/2} \hat{x} + i \frac{\hat{p}}{(2\omega)^{1/2}}, \quad \hat{a}^\dagger = \left(\frac{\omega}{2}\right)^{1/2} \hat{x} - i \frac{\hat{p}}{(2\omega)^{1/2}}. \quad (2)$$

The eigenstates of the number operator  $N = \hat{a}^\dagger \hat{a}$  are the Fock states, labelled  $|N\rangle$ . The ladder operators increase or decrease the quantum number  $N$  when acted on a Fock state;  $\hat{a}^\dagger |N\rangle = (N+1)^{1/2} |N+1\rangle$  and  $\hat{a} |N\rangle = N^{1/2} |N-1\rangle$ . Thus, only terms of the infinite sum

$$S = \sum_{k=3}^{\infty} \frac{V^{(k)}(0)}{2^{k/2} k!} (\hat{a}^\dagger + \hat{a})^k \quad (3)$$

of equation (1) that contain an equal number of  $\hat{a}^\dagger$ :s and  $\hat{a}$ :s will contribute to the diagonal matrix elements  $S_N = \langle N|S|N\rangle$ . When considering those elements we may therefore neglect all other terms of the sum. We have

$$(\hat{a}^\dagger + \hat{a})^k \Rightarrow \begin{cases} \binom{k}{k/2} :(\hat{a}^\dagger \hat{a})^{k/2}:_W, & k \text{ even,} \\ 0, & k \text{ odd,} \end{cases} \tag{4}$$

where  $:(\hat{a}^\dagger \hat{a})^k:_W$  denotes the Weyl (symmetric) ordering of the operator  $\hat{N}^k$ . It may be transformed into normal ordering using [13]

$$:(\hat{a}^\dagger \hat{a})^k:_W = \sum_{l=0}^k \frac{l!}{2^l} \binom{k}{l}^2 \hat{a}^{\dagger k-l} \hat{a}^{k-l}. \tag{5}$$

Thus, the new sum  $\tilde{S}(\hat{x}, \hat{p})$ , when the ‘off-diagonal’ terms have been neglected (this sum will now depend on the operator  $\hat{p}$ ), may be written as

$$\tilde{S} = \sum_{k=0}^{\infty} \sum_{l=0}^k \frac{V^{(2k)}(0)}{2^k (k!)^2} \frac{l!}{2^l} \binom{k}{l}^2 \hat{a}^{\dagger k-l} \hat{a}^{k-l}. \tag{6}$$

The second sum may be taken to infinity (as we may only add zeros)

$$\tilde{S} = \sum_{l=0}^{\infty} \sum_{k=0}^{\infty} \frac{V^{(2k)}(0)}{2^{k+l} (k-l)!^2 l!} \hat{a}^{\dagger k-l} \hat{a}^{k-l}. \tag{7}$$

For  $k < l$  the above expression is zero and thus we make the substitution  $j = k - l$  and get

$$\tilde{S} = \sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j (j!)^2} \hat{a}^{\dagger j} \hat{a}^j. \tag{8}$$

By using the identity

$$\hat{a}^{\dagger j} \hat{a}^j = \frac{\hat{N}!}{(\hat{N} - j)!}, \tag{9}$$

the sum is diagonalized in the number basis  $\{|N\rangle\}$  and we get the diagonal elements of (1)

$$\langle N|H|N\rangle = \omega \left( N + \frac{1}{2} \right) + \sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j (j!)^2} \frac{N!}{(N - j)!}, \tag{10}$$

where we have used that  $\langle N|\hat{p}^2/2|N\rangle = \langle N|\omega^2 \hat{x}^2/2|N\rangle = (\omega/2)(N + \frac{1}{2})$ . Note that the Fock basis used to calculate the diagonal elements of the Hamiltonian are obtained from the quadratic term of the Hamiltonian and we call them  $|N\rangle$  instead of the usual notation  $|n\rangle$ . In the following sections we apply the above to some specific examples.

### 3. Cosine potential

Using the fact that we can obtain closed forms for the diagonal elements of some of the potentials studied in section 2, and noting that the RWA is used to keep constant terms (terms that do not rotate), in this section we show that for some Hamiltonians we can produce approximations under certain circumstances, namely, when some parameters allow us to perform the RWA.

One very important equation for scientists is the Mathieu equation [14–16] which is identical to the Schrödinger equation with a sine or cosine potential, also known as the quantum rotor. During the last decade it has gained a new shove of attention due to the growing field of cold atoms in optical lattices [17]. Approximate results of the eigenfunctions and eigenvalues of the Mathieu equation have been studied earlier [18–20]. Known approximation methods from physics, such as the WKB and the Raman–Nath have been applied to the Mathieu equation [19]. Given the Hamiltonian (reminding that we set  $\hbar = 1$  and  $m = 1$ )

$$H = \frac{\hat{p}^2}{2} - g_0^2 \cos q\hat{x} \tag{11}$$

we can expand the cosine as (we neglect the constant term as it only displaces the energies)

$$H = \frac{\hat{p}^2}{2} + \frac{g_0^2 q^2}{2} \hat{x}^2 - g_0^2 \sum_{k=2}^{\infty} \frac{(q\hat{x})^{2k}}{(2k)!} (-1)^k. \tag{12}$$

With the above definition of the creation and annihilation operators (2), we get

$$\hat{a} = \left(\frac{g_0 q}{2}\right)^{1/2} \hat{x} + i \frac{\hat{p}}{(2g_0 q)^{1/2}}, \quad \hat{a}^\dagger = \left(\frac{g_0 q}{2}\right)^{1/2} \hat{x} - i \frac{\hat{p}}{(2g_0 q)^{1/2}}, \tag{13}$$

and rewrite the Hamiltonian as

$$H = g_0 q \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) - g_0^2 \sum_{k=2}^{\infty} \left( \frac{q}{2g_0} \right)^k \frac{(\hat{a}^\dagger + \hat{a})^{2k}}{(2k)!} (-1)^k. \tag{14}$$

In the case  $g_0 \gg q/4$  we can do RWA, and thus go to a rotating frame with respect to the free Hamiltonian,  $U(t) = \exp(-ig_0 q \hat{a}^\dagger \hat{a} t)$ . Using the relations

$$U^\dagger(t) \hat{a} U(t) = \hat{a} \exp(ig_0 q t), \quad U^\dagger(t) \hat{a}^\dagger U(t) = \hat{a}^\dagger \exp(-ig_0 q t), \tag{15}$$

and by only keeping non-rotating terms in the Hamiltonian we find

$$H = g_0 q \left( \hat{N} + \frac{1}{2} \right) - g_0^2 \sum_{k=2}^{\infty} \left( \frac{q}{2g_0} \right)^k \frac{(-1)^k}{(k!)^2} : (\hat{a}^\dagger \hat{a})^k :_W. \tag{16}$$

We now proceed as in section 2. Inserting (5) into (16) we have  $H = g_0 q (\hat{N} - 1/2) - g_0^2 S$  with

$$S \equiv \sum_{k=2}^{\infty} \sum_{l=0}^k \left( \frac{q}{2g_0} \right)^k \frac{(-1)^k}{(k!)^2} \frac{l!}{2^l} \binom{k}{m}^2 \hat{a}^{\dagger k-l} \hat{a}^{k-l}. \tag{17}$$

Rearranging terms and like in equation (7) we can sum  $l$  to infinity to get

$$S = \sum_{l=0}^{\infty} \frac{1}{2^l l!} \sum_{k=2}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-l} \hat{a}^{k-l}. \tag{18}$$

By expressing

$$\begin{aligned} \sum_{k=0}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-l} \hat{a}^{k-l} &= \sum_{k=2}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-l} \hat{a}^{k-l} \\ &+ 1 - \left(\frac{q}{2g_0}\right) \frac{1}{(1-l)!^2} \hat{a}^{\dagger 1-l} \hat{a}^{1-l}, \end{aligned} \tag{19}$$

we can write  $S = S_1 + S_2$  with

$$S_1 = \sum_{l=0}^{\infty} \frac{1}{2^l l!} \sum_{k=0}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-m} \hat{a}^{k-l} \tag{20}$$

and

$$S_2 = \left(\frac{q}{2g_0}\right) \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2}\right) - 1. \tag{21}$$

Note that, like previously in section 2, the second sum in equation (20) may be started at  $k=l$ , i.e.

$$\begin{aligned} S_1 &= \sum_{l=0}^{\infty} \frac{1}{2^l l!} \sum_{k=l}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-l} \hat{a}^{k-l} \\ &= \sum_{l=0}^{\infty} \frac{(-1)^l}{2^l l!} \left(\frac{q}{2g_0}\right)^l \sum_{n=0}^{\infty} \left(\frac{q}{2g_0}\right)^n \frac{(-1)^n}{n!^2} \hat{a}^{\dagger n} \hat{a}^n \end{aligned} \tag{22}$$

or

$$S_1 \exp\left(-\frac{\beta}{4g_0}\right) : J_0\left(\frac{q}{2g_0} \hat{a}^{\dagger} \hat{a}\right) : \tag{23}$$

or using that  $\hat{a}^{\dagger j} \hat{a}^j = \hat{N}! / (\hat{N} - j)!$

$$S_1 = \exp\left(-\frac{q}{4g_0}\right) L_{\hat{N}}\left(\frac{q}{2g_0}\right). \tag{24}$$

The result obtained here agree with previous results were approximations to the Mathieu equation are obtained [18]. The result also gives an interesting relation between the zeroth Bessel function and Laguerre polynomials.

Combining the results we find the diagonalized RWA Hamiltonian

$$H = \frac{g_0 q}{2} \left(\hat{N} + \frac{1}{2}\right) - g_0^2 \exp\left(-\frac{q}{4g_0}\right) L_{\hat{N}}\left(\frac{q}{2g_0}\right). \tag{25}$$

If we develop the Laguerre polynomials in powers of  $q/g_0$ , which should be valid within the regimes of the RWA and remain to second order, we obtain

$$H \approx g_0 q \left( \hat{N} + \frac{1}{2} \right) - \frac{q^2}{16} \left( \hat{N}^2 + \hat{N} + \frac{1}{2} \right) - g_0^2. \quad (26)$$

It should also be pointed out that the method also works for superimposed cosine potentials;  $\sum_k g_k^2 \cos(q_k x)$ . This has interesting applications in for example solid state physics [21] and cold atoms in optical superlattices [22].

We conclude this section by making an analogy between the RWA and first-order perturbation theory. Given the Hamiltonian

$$H = g_0 q \left( \hat{N} + \frac{1}{2} \right) \quad (27)$$

with eigenstates  $|N\rangle$ , we perturb it with

$$V = -g_0^2 \cos(qx) - \frac{g_0^2 q^2}{2} x^2. \quad (28)$$

The first-order correction to the energy [23] becomes

$$\delta E = \langle \Psi_n | V | \Psi_n \rangle = -g_0^2 \exp\left(-\frac{q}{4g_0}\right) L_n\left(\frac{q}{2g_0}\right) - \frac{g_0 q}{2} \left(n + \frac{1}{2}\right), \quad (29)$$

which regains exactly the same result as the one obtained from the RWA method. This relation between first-order perturbation theory and the RWA method is easily shown, using equation (A4), to be valid in any general case.

#### 4. Morse potential

Now let us look at the Morse potential [24, 25], from which we get the Hamiltonian

$$H = \frac{\hat{p}^2}{2} + \lambda^2 (1 - \exp[-\alpha(\hat{x} - b)])^2. \quad (30)$$

This kind of Hamiltonian is commonly used to describe properties of diatomic molecules and other situations with anharmonicity [26]. The Morse Hamiltonian has turned out to have interesting properties in connection with the WKB approximation [27, 28] (the WKB quantization gives the exact spectrum), and with supersymmetric quantum mechanics [29].

One can transform the Hamiltonian by means of the displacement operator  $\exp(ib\hat{p})$  so that  $H_T = \exp(ib\hat{p})H \exp(-ib\hat{p}) = (\hat{p}^2/2) + \lambda^2(1 - \exp[-\alpha\hat{x}])^2$ . The transformed Hamiltonian is then written in the approximate form (we neglect odd powers because of RWA, i.e. we are in the regime  $\lambda \gg \alpha$ )

$$H = 2^{1/2} \lambda \alpha (\hat{N} + 1/2) + \lambda^2 (S_1 + S_2) \quad (31)$$

with

$$S_1 = \sum_{k=2} \frac{(2\alpha\hat{x})^{2k}}{(2k)!}, \quad S_2 = -2 \sum_{k=2} \frac{(\alpha\hat{x})^{2k}}{(2k)!}. \tag{32}$$

Following the procedure of the former section we may write

$$S_1 \exp\left(\frac{\alpha}{2^{1/2}\lambda}\right) L_{\hat{N}}\left(-\frac{2^{1/2}\alpha}{\lambda}\right) - \frac{2^{1/2}\alpha}{\lambda}(\hat{N} + 1/2) - 1 \tag{33}$$

and

$$S_2 = -2 \left( \exp\left(\frac{\alpha}{4(2^{1/2}\lambda)}\right) L_{\hat{N}}\left(-\frac{\alpha}{2(2^{1/2}\lambda)}\right) - \frac{\alpha}{2(2^{1/2}\lambda)}(\hat{N} + 1/2) - 1 \right) \tag{34}$$

giving the RWA Hamiltonian

$$H = \frac{2^{1/2}\lambda\alpha}{2} \left( \hat{N} + \frac{1}{2} \right) + \lambda^2 \exp\left(\frac{\alpha}{2^{1/2}\lambda}\right) L_{\hat{N}}\left(-\frac{2^{1/2}\alpha}{\lambda}\right) - 2\lambda^2 \exp\left(\frac{\alpha}{4(2^{1/2}\lambda)}\right) L_{\hat{N}}\left(-\frac{\alpha}{2(2^{1/2}\lambda)}\right) + \lambda^2. \tag{35}$$

Using the fact that  $\lambda \gg \alpha$  in the RWA validity regime, we expand the Hamiltonian to second order in  $\alpha/\lambda$

$$H \approx \frac{3}{4} 2^{1/2}\lambda\alpha \left( \hat{N} + \frac{1}{2} \right) + \frac{7\alpha^2}{16} \left( \hat{N}^2 + \hat{N} + \frac{1}{2} \right). \tag{36}$$

Note that if we write the (transformed) Morse Hamiltonian as

$$H = 2^{1/2}\lambda\alpha(\hat{N} + 1/2) + \lambda^2 \left( 1 - \exp\left[-\frac{\alpha(\hat{a} + \hat{a}^\dagger)}{(2^{1/2}\lambda\alpha)^{1/2}}\right] \right)^2 - \frac{2\lambda^2\alpha^2}{2} \frac{(\hat{a} + \hat{a}^\dagger)^2}{2(2^{1/2}\lambda)\alpha} \tag{37}$$

and express the exponentials in a factorized normal form

$$\exp[\alpha(\hat{a} + \hat{a}^\dagger)] = \exp(\alpha^2/2) \sum_{n=0} \sum_{k=0} \frac{\alpha^{n+k} \hat{a}^{\dagger n} \hat{a}^k}{n!k!}. \tag{38}$$

The RWA in the above expression keeps only terms  $n=k$ , i.e. the double sum becomes a single sum, leading to Laguerre polynomials of order (operator)  $N$ . In this form we can recover equation (31) via RWA and using equation (37).

### 5. Validity check of the approximation

In this section we numerically study the applicability of the above approximation as a function of the system parameters.

#### 5.1 Cosine potential

As pointed out, solutions of the Mathieu equation in closed analytical form do not exist. However, it is well known, from Floquet [30] and Bloch theory [31], that the



spectrum of a periodic operator in 1D is determined by a continuous quantum number  $k$  referred to as quasi momentum and a discrete number  $n$  called the band index. The spectrum is most often represented within the first Brillouin zone [31] as allowed energy bands separated by forbidden gaps. The characteristics of the spectrum are usually, in a phenomenological way, explained in two different ways; starting from a weak potential or a strong one. In the weak limit the particle is moving almost freely in a periodic background, which at the degenerate points split the degeneracy. In the opposite, strong potential limit, particles with energies smaller than the potential barriers will be quasi bound, and the tunnelling rate determines the width of the bound energies, band width. As soon as a particle has an energy exceeding the barriers, it will move almost freely. Thus, we expect that the  $k$ -dependence is weak only for the lowest quasi bound energy bands when the amplitude  $g_0$  of the cosine potential is large. This is confirmed in figure 1, which shows the lowest energy bands of the Mathieu equation for  $q=1$  and  $g_0^2 = 10$ .

The RWA is only supposed to work in the limit of  $g_0 \gg q$ , so it approximates only the lowest quasi bound energies. In figure 2 we present the results of numerical calculations of the error estimate  $\delta_E(n, g_0) = |E_n^{\text{RWA}} - E_n|$ , where  $E_n^{\text{RWA}}$  is the approximate result for the energy from equation (25),

$$E_n^{\text{RWA}} = g_0 q \left( n + \frac{1}{2} \right) - g_0^2 \left[ \exp \left( -\frac{q}{4g_0} \right) L_n \left( \frac{q}{2g_0} \right) + \frac{q}{2g_0} \left( n + \frac{1}{2} \right) - 1 \right] - g_0^2 \quad (39)$$

and  $E_n$  is the numerically calculated result of the energy by diagonalization of the truncated Hamiltonian. Here the size of the Hamiltonian is  $765 \times 765$  (well within the convergence limits for the eigenvalues). The reason why we show the absolute error, and not the relative one, is because for higher values of  $n$ , the energies become close to zero and the relative error fluctuates greatly in such cases. In the figure,

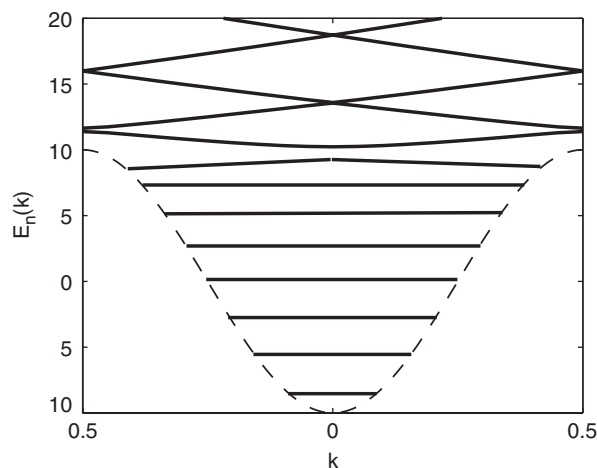


Figure 1. The spectrum  $E_n(k)$ , within the first Brillouin zone, of the Mathieu equation for a potential amplitude  $g_0^2 = 10$  and wave number  $q=1$ . The cosine function is plotted for clarity, showing that within the ‘wells’ the particle is quasi bound.

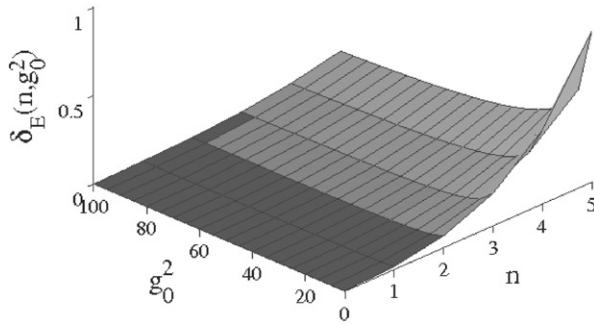


Figure 2. The absolute error  $\delta_E(n, g_0^2) = |E_n^{\text{RWA}} - E_n|$ , between the RWA result and the ‘exact’ numerical result, as a function of the band index  $n$  and the amplitude  $g_0^2$ . The approximation is most valid for low excited bands  $n$  and strong couplings  $g_0$ . Again the wave number  $q$  is set to unity.

the band index  $n$  runs between 0 and 5, hence showing the six lowest energies, and it is clear that the approximation breaks down for small couplings  $g_0$  and high excitations  $n$  as expected.

### 5.2 Morse potential

As the Morse potential is analytically solvable, no numerical diagonalization of the Hamiltonian is needed. The bound energies for the Morse potential are [24, 25]

$$E_n = 2^{1/2}\lambda\alpha\left(n + \frac{1}{2}\right) - \frac{\alpha^2}{2}\left(n + \frac{1}{2}\right)^2. \tag{40}$$

Clearly, since  $\lambda \gg \alpha$ , the second anharmonicity term becomes crucial only for larger excitations  $n$ . The anharmonicity term is purely negative resulting in that the highly excited bound states are more densely distributed. Interestingly, from the RWA result of equation (36) we note that the second term is positive causing the energies to be more sparse for high  $n$ 's. However, this is partly compensated for by the coefficient 3/4 in front of the first harmonic part. It should be emphasized that only the even terms in the sums (32) are included since within the RWA odd terms vanish. Thus, it is expected that the method may not be as efficient as for a situation with a purely even potential  $V(x)$ . It is more likely that the obtained eigenvalues approximate the ones for the Hamiltonian with a potential

$$\tilde{V}_{\text{eff}}(x) = \frac{V_{\text{eff}}(x)}{\lambda^2} = 1 + \sum_{k=0} \frac{(2\alpha x)^{2k}}{(2k)!} - 2 \sum_{k=0} \frac{(\alpha x)^{2k}}{(2k)!}. \tag{41}$$

Using that  $\exp(x^2) = \sum_k (x^{2k}/k!)$ , we expect that the potential (41) has some kind of ‘weak’ exponential behaviour. In figure 3 examples of the normalized effective potential  $\tilde{V}_{\text{eff}}(x)/V_{\text{eff}}(1)$  are given for  $\alpha = 0.1, 1$  and 10.

The relative error  $\Delta_E(n, \lambda) = |E_n^{\text{RWA}} - E_n|/E_n$  between the expanded RWA result  $E_n^{\text{RWA}}$  (36) and the exact result  $E_n$  (40) is shown in figure 4 for the first six eigenvalues

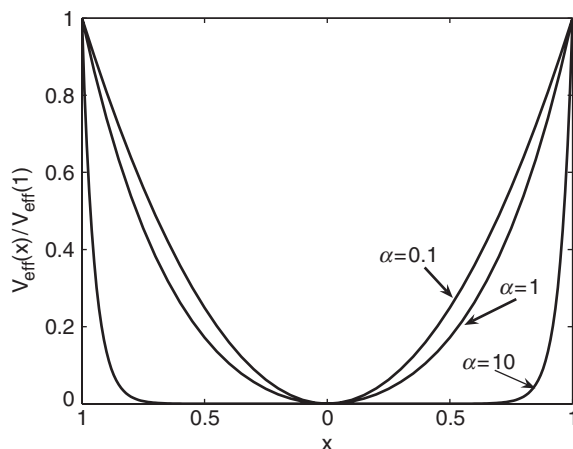


Figure 3. The normalized effective potential  $\tilde{V}_{\text{eff}}(x)/V_{\text{eff}}(1)$  defined in equation (41) for  $\alpha = 0.1, 1$  and  $10$ .

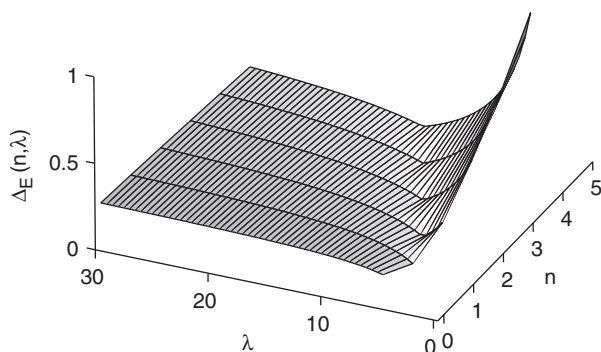


Figure 4. This plot displays the relative error  $\Delta_E(n, \lambda) = |E_n^{\text{RWA}} - E_n|/E_n$  for  $n = 0, 1, \dots, 5$  and as a function of  $\lambda$  and here  $\alpha = 1$ .

and as a function of  $\lambda$ . In the plot  $\alpha = 1$ , but similar results are obtained for other widths  $\alpha$ , however, with some increase of  $\Delta_E$  for larger  $\alpha$ .

## 6. Conclusions

We have developed a method to approximate Hamiltonians using a kind of self-RWA. We have shown how some of the involved sums may be calculated using symmetrically ordered expressions for Fock-states expectation values of powers of the position operator. We have used these expressions to obtain approximations for Hamiltonians corresponding to the quantum rotor and the Morse potential. A discussion of the validity of the approximation was given and the relation with perturbation theory was explained. The direct link between first-order perturbation

theory and the RWA deepens the understanding of the two methods, and a consequent question would be if higher orders in the RWA scheme could regain higher order perturbation theory. This seems possible, but has turned out to be more subtle than expected, mostly because of the non-commutability of the ladder operators.

**Appendix A: calculating sums via symmetric order**

In this Appendix we use the results of the previous sections and show how one may use it to calculate various sums. Like in section 2, no RWA is used and the results are exact.

We start with some function  $f(x)$  which we can expand according to

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{2^{k/2} k!} (\hat{a}^\dagger + \hat{a})^k. \tag{A1}$$

Here we have introduced the ‘symmetric’ ladder operators  $\hat{a}$  and  $\hat{a}^\dagger$  obeying the regular boson commutator algebra  $[\hat{a}, \hat{a}^\dagger] = 1$  and which are related to  $\hat{x}$  and  $\hat{p} = -i(\partial/\partial x)$  as

$$\begin{aligned} \hat{x} &= \frac{1}{2^{1/2}} (\hat{a}^\dagger + \hat{a}), \\ \hat{p} &= \frac{i}{2^{1/2}} (\hat{a}^\dagger - \hat{a}). \end{aligned} \tag{A2}$$

Further we have the normalized eigenstates and eigenvalues of the number operator  $\hat{N} = \hat{a}^\dagger \hat{a}$ ;  $\hat{N}|n\rangle = n|n\rangle$ , where  $n = 0, 1, 2, \dots$ , and which in  $x$ -basis are

$$\Psi_n(x) = \langle x|n\rangle = \frac{\pi^{-1/4}}{(2^n n!)^{1/2}} \exp(-x^2/2) H_n(x). \tag{A3}$$

As argued in section 2, the diagonal elements, in the Fock basis, of the function  $f(x)$  is identical to the diagonal elements of the function  $\tilde{f}(\hat{x}, \hat{p})$  where only terms containing an equal number of creation and annihilation operators are included. We thus have

$$\langle n|\tilde{f}|n\rangle = \langle n|f|n\rangle. \tag{A4}$$

The left-hand side (LHS) can be written, using equation (10), as

$$\tilde{f} = \sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{f^{(2j+2l)}(0)}{2^j (2!)^2} \frac{N!}{(N-j)!} \tag{A5}$$

and if we express the right-hand side (RHS) in the  $x$ -basis we obtain

$$\sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j (j!)^2} \frac{n!}{(n-j)!} = \frac{1}{2^n n! \pi^{1/2}} \int_{-\infty}^{+\infty} V(x) \exp(-x^2) H_n^2(x) dx, \tag{A6}$$

Below we give some analytically solvable examples. Approximate results are in principle easily achievable, but are left out in this paper.

**A1. Cosine function**

For a cosine function  $V(x) = \cos(qx)$  we have  $V^{(2k)}(0) = (-1)^k q^{2k}$  and we find [32] in (A6)

$$\begin{aligned} \text{LHS} &= \sum_{l=0}^{\infty} \frac{(-1)^l q^{2l}}{4^l l!} \sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!} = \exp\left(-\frac{q^2}{4}\right) \sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!}, \\ \text{RHS} &= \frac{1}{2^n n! \pi^{1/2}} \int_{-\infty}^{+\infty} \cos(qx) \exp(-x^2) H_n^2(x) dx = \exp\left(-\frac{q^2}{4}\right) L_n(q^2/2). \end{aligned} \tag{A7}$$

So that

$$\sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!} = L_n(q^2/2). \tag{A8}$$

Note that closed forms of  $V(x) = \exp(\pm iqx)$ ,  $V(x) = \cosh(qx)$ ,  $V(x) = \cosh^m(qx)$  or  $V(x) = \cos^m(qx)$ ,  $m = 0, 1, 2, \dots$  can also be obtained.

**A2. Gaussian function**

In the case of  $V(x) = \exp(-\alpha^2 x^2)$ ,  $\alpha^2 > 0$ , the integral in the RHS of equation (A6) is analytically solvable [32]

$$\begin{aligned} &\frac{1}{2^n n! \pi^{1/2}} \int_{-\infty}^{+\infty} \exp(-\alpha^2 x^2) \exp(-x^2) H_n^2(x) dx \\ &= 2^{n+1} \left(\frac{2\alpha^2}{\alpha^2 + 2}\right)^{n+1/2} \frac{\alpha^{-1}}{n} F\left(-n, n; -\frac{2n-1}{2}; \frac{\alpha^2 + 2}{2\alpha^2}\right), \end{aligned} \tag{A9}$$

where  $F(\dots, \dots; \dots; \dots)$  is the Gauss hypergeometric function. The derivatives are simply  $V^{(2k)}(0) = (-1)^k \alpha^{2k} [k!/(2k)!]$  resulting in the LHS

$$\text{LHS} = \sum_{l=0}^{\infty} \frac{(-1)^l \alpha^{2l}}{4^l l!} \sum_{j=0}^{\infty} \frac{(j+l)!}{(2j+2l)!} \frac{(-1)^j \alpha^{2j}}{2^j (j)!^2} \frac{n!}{(n-j)!}. \tag{A10}$$

The above holds also for exponential functions such that  $0 > \alpha^2 > -1$ , which, when applied to Hamiltonian systems, is of interest as they possess an infinite set of bound states.

**A3. Hermite polynomials**

When  $V_m(x) = H_{2m}(x)$ , where  $m = 0, 1, 2, \dots$  we find [32]

$$\text{RHS} = \frac{1}{2^n n! \pi^{1/2}} \int_{-\infty}^{+\infty} H_{2m}(x) \exp(-x^2) H_n^2(x) dx = \frac{2^{m/2} m! n!}{\left(\frac{m}{2}!\right)^2 \left(n - \frac{m}{2}!\right)}, \tag{A11}$$

while its derivatives are  $V_m^{(2k)}(0) = [2^{2k} (2m)! / (2k)!] H_{2m-2k}(0)$ .

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