

# Anharmonic oscillator and the optimized basis expansion

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## Abstract

We introduce various optimization schemes for highly accurate calculation of the eigenvalues and the eigenfunctions of the one-dimensional anharmonic oscillators. We present several methods of analytically fixing the nonlinear variational parameter specified by the domain of the trigonometric basis functions. We show that the optimized parameter enables us to determine the energy spectrum to an arbitrary accuracy. Also, using the harmonic oscillator basis functions, we indicate that the resulting optimal frequency agrees with the one obtained by the principle of the minimal sensitivity.

*Keywords:* anharmonic oscillator, basis expansion, Rayleigh-Ritz variational principle

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## 1. Introduction

Eight decades after the discovery of quantum mechanics, the Schrödinger's famous equation still remains an interesting subject for various investigations, aiming at extending its applications and at developing more efficient analytic and numerical methods for obtaining its energy eigenvalues and stationary states. The interest in this subject ranges from various branches of mathematics, physics, and chemistry. This has been the driving force behind the development of perturbative and nonperturbative methods for this kind of problems. Among them are the factorization method [1, 2], semiclassical approximation [3], finite-difference technique [4], optimized Rayleigh-Ritz variational scheme [5, 6], variational matrix solution [7], instanton method [8], transfer matrix method [9] and many other specific methods.

One general approach to construct a continuous wave function  $\psi(x)$  is to represent its values on a set of mesh (lattice) points  $x_n$  which is the starting point of the various mesh methods. Although this approach is simple, it is usually very inaccurate which is due to the fact that it only contains the local information of the wave function. To overcome this problem, Schwartz proposed a method based on a global construction of an approximate wave function which involves only the values  $\psi_n$  at the selected mesh points [10]. He showed that using an optimized mesh spacing the obtained errors are as small as  $A^{-N}$  or even  $1/N!$  where  $N$  is the number of the mesh points. This shows the priority of this method over the usual numerical methods that yield errors as small as  $1/N$ ,  $1/N^2$ , etc. The application of a set of orthogonal functions on a finite domain for solving a wide class of problems such as function interpolation and the numerical solution of the Schrödinger equation has attracted much attention in recent years (see Ref. [11] and references therein). For instance, the variational sinc collocation based on the principle of minimal sensitivity (PMS) method can be effectively used to obtain the highest precision with a given number of mesh points [12].

The second popular scheme is to expand the wave function in terms of an orthonormal set of the eigenfunctions of a Hermitian operator, i.e., the basis-set expansion method. For instance, the trigonometric basis functions obeying Dirichlet boundary condition (particle in a box basis) can be effectively used to find the spectrum of an unbounded problem. The low lying energy levels are approximately equal to the exact ones with high accuracy, if the boundedness parameter is in near vicinity of an optimal value upon implementing the Rayleigh-Ritz variational method [13, 14]. The extension of this method for the periodic

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boundary condition is also discussed in Ref. [15]. For these cases, the variational parameter is the width of the finite interval (the size of the box). On the other hand, if we expand the wave function in terms of the harmonic oscillator eigenfunctions, the frequency of the oscillator would be the variational parameter.

In this paper, first we briefly outline the Schwartz's method and its error analysis which is based on the large distance behavior of the wave function. Then by defining the Schwartz's length, which as we shall show has a useful application in diagonalization of the Hamiltonian with the particle in a box basis set, the nearly accurate results can be obtained if we use this length as the optimal width of the finite domain. By imposing a physically acceptable relation between the potential energy at the optimal length and the maximum available basis eigenenergy, we explain the physics behind the Schwartz's length and obtain the optimal length without need to the error analysis which is done in the Schwartz's original paper. As it is emphasized in Ref. [10], there is a close connection between the Schwartz's scheme and the Fourier expansion where we shall elaborate it in the next section. In this view, we improve our estimation and introduce some alternative and more accurate optimal lengths for the particle in a box basis functions. Also we present the optimal frequency for the expansion of the wave function in terms of the harmonic oscillator basis functions.

Another way for finding the optimal length is using the stationarity of the trace of the Hamiltonian [5, 6]. This method is based on the principle of minimal sensitivity but demands on fixing the values of nonlinear parameters before diagonalization of the truncated matrix. In fact, this optimal value extremizes the trace and results in highly accurate results. Here we apply this formalism for the trigonometric basis functions and find the related optimal length for the anharmonic oscillators.

## 2. The Schwartz's method

Let us consider an analytic reference function  $u(x)$  which has simple zeros at the real points  $x = x_n$  to approximate the wave function  $\psi(x)$ . We can define an interpolating wave function  $\bar{\psi}(x)$  to approximate  $\psi(x)$  as

$$\bar{\psi}(x) = \sum_m \psi_m \frac{u(x)}{x - x_m} \frac{1}{u'(x_m)}, \quad (1)$$

where  $\psi_m = \psi(x_m)$ . So at the mesh points  $x = x_n$ , the interpolating wave function takes the same values as  $\psi(x)$  there. With this definition, the derivatives of  $\bar{\psi}$  at the mesh points  $\left. \frac{d\bar{\psi}}{dx} \right|_{x_n}$  or its integrals  $\int_{x_0}^{x_n} \bar{\psi}(x) dx$  only depend on  $\psi_m$  not the derivatives or integrals (see Ref. [10] for details). However, all  $\psi_m$  would contribute to construct the corresponding values of  $\bar{\psi}$  which means that the global information about the wave function  $\psi$  is used to find the approximation.

We can write the above equation as an exact relation by introducing the error term  $\epsilon$  as

$$\psi(x) = \sum_m \psi(x_m) \frac{u(x)}{x - x_m} \frac{1}{u'(x_m)} + \epsilon. \quad (2)$$

Note that, we are usually interested for the cases where the wave functions decreases rapidly for large  $x$  (bound state solutions), so effectively the infinite sum over the mesh points can be truncated to a finite sum. In fact, there are two sources of error in our analysis. First one  $\epsilon_A$  due to the analytical approximation and the second  $\epsilon_T$  due to the truncation. If we make  $\epsilon_A$  approximately equal to  $\epsilon_T$  by choosing a relation between the mesh spacing  $h$  and the truncation at  $n < N$ , the total error will be reduces considerably. This will prevent us from using a too small  $h$  when the truncation error dominates or using a too large cutoff when the mesh error has the dominant role.

To compute the errors, consider a bound state wave function which has the following behavior at large distances

$$\psi(x) \sim e^{-ax^p}, \quad \text{for large } x, \quad (3)$$

so the truncation error reads

$$\epsilon_T \approx e^{-a(Nh)^p}. \quad (4)$$

For the mesh size error, we need to perform a contour integral in the complex plane. By taking the reference function as  $u(x) = \sin(\pi z/h)$ , the integral can be estimated by the stationary phase method and we obtain [10]

$$\epsilon_A \approx e^{-bh^{-q}}, \quad (5)$$

where  $q = p/(p-1)$  and

$$b = \left(\frac{\pi^p}{ap}\right)^{1/(p-1)} \left(\frac{p-1}{p}\right) \sin\left[\frac{\pi}{2(p-1)}\right]. \quad (6)$$

Now the optimal value of  $h$  for each  $N$  can be obtained by equating Eqs. (4) and (5)

$$h_S = \left(\frac{b}{aN^p}\right)^{\frac{p-1}{p^2}}, \quad (7)$$

which results in the exponential decrease of the error by increasing the number of the mesh points

$$\epsilon \approx e^{-CN}, \quad (8)$$

where  $C = b(a/b)^{1/p}$ . To apply the method, let us consider the following dimensionless time-independent one-dimensional Schrödinger equation<sup>1</sup>

$$\left(-\frac{d^2}{dx^2} + x^k\right) \psi(x) = E \psi(x), \quad k = 2, 4, 6, \dots \quad (9)$$

For this case, the wave function has the asymptotic behavior for large  $x$  given by (3) with

$$p = \frac{k+2}{2}, \quad a = \frac{2}{k+2}, \quad (10)$$

which results in

$$b = \pi^{\frac{k+2}{k}} \left(\frac{k}{k+2}\right) \sin\left(\frac{\pi}{k}\right), \quad \text{and} \quad h_S = \left[\frac{1}{2}k \pi^{\frac{k+2}{k}} \sin\left(\frac{\pi}{k}\right)\right]^{\frac{2k}{(k+2)^2}} N^{-\frac{k}{k+2}}. \quad (11)$$

Now if we define the Schwartz's length  $L_S \equiv Nh_S$ , we have

$$L_S(N) = \left[\frac{1}{2}k \pi^{\frac{k+2}{k}} \sin\left(\frac{\pi}{k}\right)\right]^{\frac{2k}{(k+2)^2}} N^{\frac{2}{k+2}}, \quad (12)$$

where, as we shall show in the next section, it can be used as an accurate candidate for the optimal length in the context of the Fourier expansion of the wave function.

At this point, it is worth to mention the connection between the above collocation method and the Fourier expansion scheme. So let us define the generalized sinc functions as

$$S_m(h, x) \equiv \frac{\sin[\pi(x-mh)/h]}{\pi(x-mh)/h}, \quad (13)$$

where  $m \in \mathbb{Z}$ , uniform grid spacing  $h$  and  $x \in \mathbb{R}$ . Now using Eq. (1) and  $u(x) = \sin(\pi x/h)$  we obtain

$$\bar{\psi}(x) = \sum_m \psi_m S_m(h, x), \quad (14)$$

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<sup>1</sup>Note that for  $V(x) = \beta x^k$  we have  $E \rightarrow \beta^{\frac{2}{k+2}} E$ .

which defines the sinc collocation method. It is also possible to write a similar equation in terms of the little sinc functions [11]. Consider an orthonormal set of particle in a box basis functions vanishing at  $x = \pm L$

$$\varphi_n(x) = \frac{1}{\sqrt{L}} \sin \left[ \frac{n\pi}{2L}(x + L) \right], \quad n = 1, 2, \dots, \quad (15)$$

and define

$$\begin{aligned} \bar{\delta}_N(x, y) &= \frac{2L}{N} \sum_{n=1}^N \varphi_n(x)\varphi_n(y), \\ &= \frac{1}{2N} \left\{ \frac{\sin \left[ \frac{(2N+1)\pi(x-y)}{4L} \right]}{\sin \left[ \frac{\pi(x-y)}{4L} \right]} - (-1)^N \frac{\cos \left[ \frac{(2N+1)\pi(x+y)}{4L} \right]}{\cos \left[ \frac{\pi(x+y)}{4L} \right]} \right\}, \end{aligned} \quad (16)$$

where  $N$  takes even values. Because of the completeness of the basis functions we have

$$\lim_{N \rightarrow \infty} \frac{N}{2L} \bar{\delta}_N(x, y) = \delta(x - y). \quad (17)$$

By setting  $h = 2L/N$ ,  $y_k = kh$  and selecting even values of  $N$ , we define the set of  $(N - 1)$  little sinc functions (LSF) as

$$s_k(h, N, x) \equiv \frac{1}{2N} \left\{ \frac{\sin \left[ \left(1 + \frac{1}{2N}\right) \frac{\pi}{h}(x - kh) \right]}{\sin \left[ \frac{\pi}{2Nh}(x - kh) \right]} - \frac{\cos \left[ \left(1 + \frac{1}{2N}\right) \frac{\pi}{h}(x + kh) \right]}{\cos \left[ \frac{\pi}{2Nh}(x + kh) \right]} \right\}. \quad (18)$$

Therefore, LSF become the standard sinc functions when  $N$  goes to infinity, i.e.,

$$\lim_{N \rightarrow \infty} s_k(h, N, x) = \frac{\sin[\pi(x - kh)/h]}{\pi(x - kh)/h} = S_k(h, x). \quad (19)$$

The LSF have some common properties with the sinc functions, for instance, we can approximate the wave function on the interval  $(-L, L)$  as

$$\bar{\psi}(x) = \sum_m \psi_m s_m(h, N, x), \quad (20)$$

where can be understood using the definition of  $s_k(h, N, x)$  in terms of the completeness relation. Therefore, we can rewrite Eq. (20) as

$$\bar{\psi}(x) = \sum_m \left[ h \sum_k \psi_k \varphi_m(x_k) \right] \varphi_m(x). \quad (21)$$

In the limit  $N \rightarrow \infty$  this relation becomes

$$\psi(x) = \sum_m \left[ \int_{-L}^L \psi(x) \varphi_m(x) dx \right] \varphi_m(x) = \sum_m a_m \varphi_m(x), \quad (22)$$

which is the well-known Fourier expansion. So there is a close relation between the sinc collocation method and the trigonometric basis expansion.

### 3. The trigonometric basis expansion

In this section we study the diagonalization of the Hamiltonian in terms of the particle in a box eigenfunctions that is basically different from the Schwartz's method. Then by imposing a constraint on the potential energy at the optimal length and the maximum available basis eigenenergy, we analytically fix the variational parameter. Before going further note that in the Schwartz's scheme  $N$  is the number of mesh

points whereas in this section  $N$  is the number of basis functions. However, in the Schwartz's method the reference function vanishes at the  $N$  mesh points and the  $N$  trigonometric basis functions have at most  $N$  nodes. Also we have  $Nh = L$ . So we expect that there would be a close connection between the Schwartz's method and the trigonometric basis expansion which is also explicitly elaborated in the previous section.

For the potentials which are even functions of  $x$ , to avoid large matrices, we can use

$$\phi_m(x) = \sqrt{\frac{1}{L}} \cos \left[ \left( m - \frac{1}{2} \right) \frac{\pi x}{L} \right], \quad \text{and} \quad \phi_m(x) = \sqrt{\frac{1}{L}} \sin \left( \frac{m\pi x}{L} \right), \quad (23)$$

basis functions ( $m = 1, 2, \dots, N$ ) for even and odd parity solutions, respectively, and write the wave function as  $\psi(x) = \sum_{m=1}^N A_m \phi_m(x)$  which vanishes at  $\pm L$ . Now the approximate solutions are the eigenvalues and the eigenfunctions of the  $(N \times N)$  Hamiltonian matrix  $\mathbf{H}_N$  where can be written as

$$H_{mn} = \left( m - \frac{1}{2} \right)^2 \frac{\pi^2}{L^2} \delta_{mn} + \left( \frac{L}{\pi} \right)^k \left( D_{m+n-1} + D_{m-n} \right), \quad (24)$$

and

$$H_{mn} = \frac{m^2 \pi^2}{L^2} \delta_{mn} + \left( \frac{L}{\pi} \right)^k \left( D_{m-n} - D_{m+n} \right), \quad (25)$$

for even and odd states, respectively. Here,  $\delta_{mn}$  is the kronecker's delta and  $D_s$  is defined as

$$D_s = \frac{1}{\pi} \int_0^\pi dx x^k \cos(sx) = \begin{cases} \sum_{i=0}^{\frac{k}{2}-1} \frac{(-1)^{i+s}}{s^{2(i+1)}} \frac{k!}{(k-2i-1)!} \pi^{k-2i-2}, & s > 0, \\ \frac{\pi^k}{k+1}, & s = 0. \end{cases} \quad (26)$$

Now the good strategy is to choose a relation between the basis domain  $L$  and the truncation at  $n < N$  so that the errors due to the basis domain and the truncation approximately suppress each other. This will prevent us from choosing a too large domain for small  $N$  or a too large cutoff for small  $L$ .

Note that, the expansion the solutions in terms of particle in a box basis functions approximately corresponds to confining the potential in an infinite potential well,<sup>2</sup> i.e.,  $V(x) = x^k$  for  $|x| < L$  and  $V(x) = \infty$  elsewhere. Moreover, each energy eigenvalue is a superposition in the form  $E_n = \sum_{m=1}^N P_{nm} \varepsilon_m$  where  $\sum_{m=1}^N P_{nm} = 1$ ,  $P_{nm} \geq 0$ , and  $\varepsilon_n = n^2 \pi^2 / L^2$ . Since for  $|x| \geq L$  this model is not identical with the original potential, the basis functions with energies larger than  $V(L)$  would not have a useful contribution to the sought-after solutions. In this case, we lose accuracy which is due to the small well's width. Also, when  $V(L) \gg \varepsilon_N$  the solutions would be inaccurate which means that  $L$  is too large. Keeping these two points in mind, we conclude that the value of the potential at  $L_{\text{op}}$  should be proportional to the maximum energy of the basis functions  $\varepsilon_N$ , namely

$$L_{\text{op}}^k = \alpha(k) \frac{N^2 \pi^2}{L_{\text{op}}^2}, \quad (27)$$

where  $\alpha(k) \geq 1$  and it is of order of one. From this equation we can find the optimal value of  $L$  as

$$L_{\text{op}}(N) = \left( \pi^2 \alpha(k) \right)^{\frac{1}{k+2}} N^{\frac{2}{k+2}}, \quad (28)$$

which has the same functional form as  $L_S(N)$  (12). This similarity is due to the relation  $L = Nh$  and the fact that the maximum number of nodes in this method agrees with the number of mesh points in the

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<sup>2</sup>This correspondence is exact as  $N$  goes to infinity.

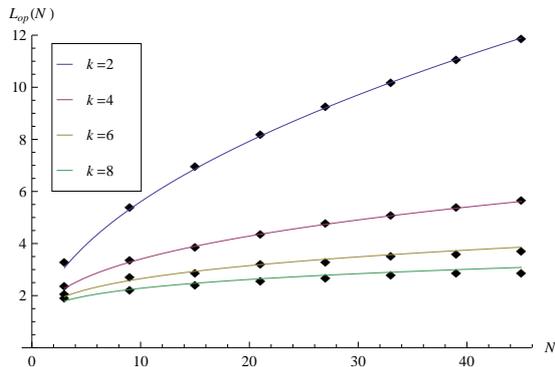


Figure 1: The variationally obtained optimal lengths (black diamonds) versus  $N$  for  $V(x) = x^k$  and the predicted optimal length curves (29).

Schwartz's method which both are represented by  $N$ . Now, it is only remained to determine  $\alpha(k)$  which can be found by choosing an acceptable ansatz and comparing with the variationally obtained results (Fig. 1).<sup>3</sup> It is straightforward to check that for the simple harmonic oscillator ( $k = 2$ ), the most accurate solutions can be obtained when the value of the potential at  $L_{\text{op}}$  is equal to the maximum energy of the basis functions  $\varepsilon_N$ , i.e.,  $\alpha(2) = 1$ . For this case using (28) we have  $L_{\text{op}} = \sqrt{\pi N} = L_S$ . For other values of  $k$ , the simplest choice is looking for a relation in the form  $\alpha(k) = \eta^{\frac{k-2}{2}}$  with constant  $\eta$  to ensure  $\alpha(2) = 1$ . As Fig. 1 shows, we can properly fit Eq. (28) to the variational values upon choosing  $\eta = \pi/2$  which results in

$$\alpha_{\text{op}}(k) = \left(\frac{\pi}{2}\right)^{\frac{k-2}{2}}, \quad \text{and} \quad L_{\text{op}}(N) = \sqrt{\frac{\pi}{2^{\frac{k-2}{k+2}}}} N^{\frac{2}{k+2}}, \quad (29)$$

Note that, although the coefficients of  $N^{\frac{2}{k+2}}$  in  $L_S$  (12) and  $L_{\text{op}}$  (29) seems to be very different, they are approximately equal especially for  $k < 10$ . For instance, for  $k = 4$  we have  $L_{\text{op}} = \sqrt{\pi/2^{1/3}} N^{1/3} \simeq 1.579 N^{1/3}$  which is nearly equal to  $L_S = 2^{1/9} \pi^{1/3} N^{1/3} \simeq 1.582 N^{1/3}$ . In Table 1, we have reported the accuracy of the energy eigenvalues for  $k = \{2, 4, 6, 8\}$  which are in complete agreement with the variationally obtained solutions [13].

Since  $\alpha(k)$  for  $k \gg 1$  will not be of  $\mathcal{O}(1)$ , we expect that the validity of Eq. (29) breaks down for large  $k$ . At this limit we have  $V(L_{\text{op}}) \gg \varepsilon_N$  which would result in inaccurate solutions as a consequence of too large  $L_{\text{op}}$ . To check this point, we consider the problem of  $V(x) = x^k$  where  $k \rightarrow \infty$ . For this case, the predicted optimal length is  $\lim_{k \rightarrow \infty} L_{\text{op}}(N) \simeq \sqrt{\pi/2} \simeq 1.253$ . However, the optimal length predicted by the Schwartz's formula has the correct limiting value, i.e.,  $\lim_{k \rightarrow \infty} L_S(N) = 1$  and gives the following proportionality coefficient:

$$\alpha_S(k) = \left[ \frac{k}{2} \sin\left(\frac{\pi}{k}\right) \right]^{\frac{2k}{k+2}}, \quad (30)$$

where  $\alpha_S(2) = 1$  and as we have desired, it is of the order of unity for all  $k$ , i.e.,  $1 \leq \alpha_S \leq \pi^2/4$ . Also, Fig. 2 shows that the error exponentially decreases with respect to the number of the basis functions. In comparison, the calculations show that the usage of  $L_S$  results in more accurate energy spectrum than those obtained by  $L_{\text{op}}$ .

<sup>3</sup>From now on we show the relative error of the energy spectrum by  $\epsilon_n \equiv \left| \frac{E_n - E_n^{\text{exact}}}{E_n^{\text{exact}}} \right|$ .

$k$	$L_{\text{op}}$	$N$	$n$	$\epsilon_n$
2	$\sqrt{30\pi}$	30	0	$2.77 \times 10^{-40}$
			2	$9.57 \times 10^{-37}$
			4	$1.47 \times 10^{-33}$
4	$\frac{\sqrt{\pi} 35^{1/3}}{2^{1/6}}$	35	0	$4.95 \times 10^{-40}$
			2	$1.72 \times 10^{-38}$
			4	$1.04 \times 10^{-36}$
6	$\sqrt{2\pi} 5^{1/4}$	40	0	$3.31 \times 10^{-36}$
			2	$1.57 \times 10^{-35}$
			4	$8.22 \times 10^{-35}$
8	$\frac{\sqrt{\pi} 45^{1/5}}{2^{3/10}}$	45	0	$2.03 \times 10^{-32}$
			2	$7.19 \times 10^{-32}$
			4	$4.57 \times 10^{-31}$

Table 1: The relative errors of the energy spectrum of the anharmonic oscillator  $V(x) = x^k$ .

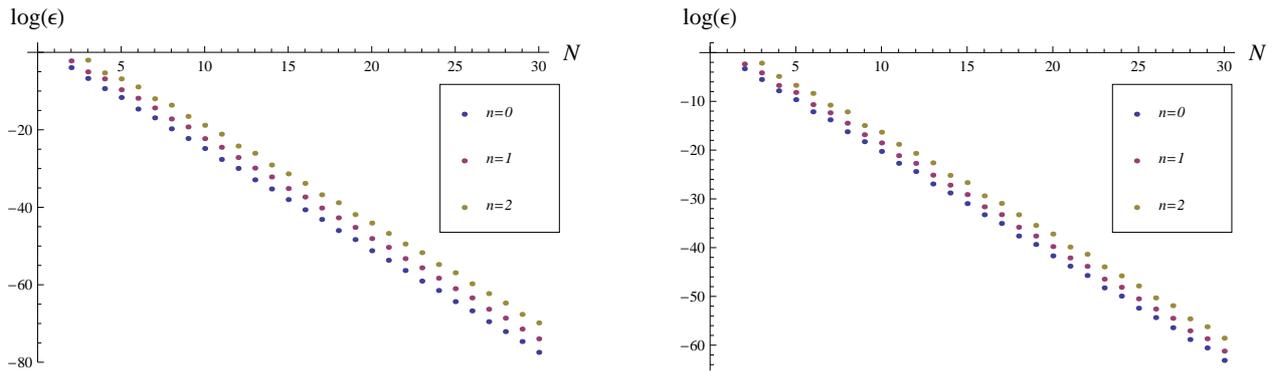


Figure 2: The error versus  $N$  for  $k = 4$  and  $L_{\text{op}}$  (left), and for  $k = 6$  and  $L_S$  (right).

#### 4. Other applications

The applicability of the introduced optimal lengths is not restricted to the particular form of the potentials, boundary conditions, or differential equations. Indeed, the optimal length can be effectively used for the following issues:

##### 4.1. Polynomial potentials

Let us consider a symmetric polynomial potential  $V(x) = \sum_{i=2}^k a_i x^i$  where  $a_k > 0$  and  $i = 2, 4, \dots$ . Since the optimal length related to each term behaves in a separate manner, we cannot simply use Eq. (29) for this polynomial potential. However, for the large values of  $L_{\text{op}}$ , the dominant term near the boundaries is  $x^k$ . In other words, we can also use this equation for the polynomial potentials when we work with a large set of the basis functions. To elaborate this fact, let us study the doubly anharmonic oscillator  $V(x) = a_2 x^2 + a_4 x^4 + a_6 x^6$ . The ground state wave function of this potential should not have nodes and it should vanish as  $x \rightarrow \pm\infty$ . Thus, we can examine the following solution

$$\Psi_0(x) = \exp\left(-\frac{1}{4}b_4 x^4 + \frac{1}{2}b_2 x^2\right), \quad b_4 > 0. \quad (31)$$

It is easy to check that this trial wave function satisfies the corresponding Schrödinger with the eigenvalue  $E_0 = -b_2$ ,  $b_2 = -\frac{1}{2}a_4 a_6^{-1/2}$ ,  $b_4 = a_6^{1/2}$  and a constraint on the potential [13]

$$a_2 = b_2^2 - 3b_4. \quad (32)$$

For instance, the potential  $V(x) = -2x^2 + 2x^4 + x^6$  obeys this constraint and has the following ground state eigenvalue and eigenfunction

$$\Psi_0(x) = \exp\left(-\frac{1}{4}x^4 - \frac{1}{2}x^2\right), \quad E_0 = 1. \quad (33)$$

For this case, using the optimal length related to  $k = 6$ , i.e.,  $L_{\text{op}} = (\pi^2 N/2)^{1/4}$ , one can easily obtain the ground state energy  $E_0$  with 28 and 36 significant digits accuracy for  $N = 30$  and  $N = 40$  basis functions, respectively.

##### 4.2. Periodic boundary condition

We have deduced Eq. (29) from diagonalization scheme for the Hamiltonian with the basis functions which are vanishing at the boundaries, but we can also use it for the case of the periodic boundary condition under some circumstances. Note that, for this case, we observe an inflection point instead of a minimum value in the graph of the energy versus the domain of basis functions [15]. However, since for the large optimal lengths the low-lying wave functions are almost zero at the boundaries, Eq. (29) is still valid for case of the periodic boundary condition when  $L_{\text{op}}$  is large enough.

##### 4.3. Multidimensional problems

In a  $d$ -dimensional space which the Hamiltonian is invariant under parity transformation, the basis functions are in the form

$$\phi_{m_1 m_2 \dots m_d}^{\text{even}}(\vec{x}) = \prod_{i=1}^d \sqrt{\frac{1}{L_i}} \cos\left[\left(m_i - \frac{1}{2}\right) \frac{\pi x_i}{L_i}\right], \quad (34)$$

$$\phi_{m_1 m_2 \dots m_d}^{\text{odd}}(\vec{x}) = \prod_{i=1}^d \sqrt{\frac{1}{L_i}} \sin\left(\frac{m_i \pi x_i}{L_i}\right), \quad (35)$$

where  $m_i = 1, 2, \dots, N$ . Now the Hamiltonian is expressed as a  $N^d \times N^d$  matrix. Therefore, even for the small values of  $N$ , the resulting matrix is too large and the ordinary variational scheme cannot be applied

efficiently. In general, we need to find  $d$  optimal lengths for the accurate calculation of the eigenvalues and the eigenfunctions. For instance, for the separable potential  $V(\vec{x}) = \sum_{i=1}^d V(x_i)$ , we can use the introduced optimal length (29) which needs to be properly chosen for each direction to get the desired accuracy. Moreover, if the Hamiltonian has the rotational symmetry, i.e.,  $V(\vec{x}) = V(|\vec{x}|)$ , we only need one optimal length to diagonalize the  $N \times N$  Hamiltonian.

#### 4.4. Wheeler-DeWitt equation

One approach to quantize gravity is based on the well-known Wheeler-DeWitt equation (WDW), i.e.,  $\mathcal{H}\Psi = 0$  where  $\Psi$  is the wave function of the universe [16]. After freezing out many degrees of freedom, WDW equation is expressed in the minisuperspace and  $\Psi$  is a function of just a few variables such as the scale factor, the scalar field, etc. This equation is a hyperbolic partial differential equation and can be cast in the form of the Schrödinger-like equation in the vicinity of the boundaries. To solve the WDW equation, the proper adjusting the width of the domain of the basis functions with the number of the basis functions is also an important issue which results in accurate solutions [17–19].

### 5. Alternative proposals

To improve the estimation for the optimal length, we need to modify Eq. (29) in such a way that it takes a finite value as  $k$  goes to infinity. For instance, consider the following proposal

$$\alpha_{\text{op}}^{(1)}(k) = \left(\frac{\pi}{2}\right)^{\frac{k-2}{k/2}}, \quad \text{and} \quad L_{\text{op}}^{(1)}(N) = \left(\frac{\pi^{4(k-1)}}{4^{k-2}}\right)^{\frac{1}{k(k+2)}} N^{\frac{2}{k+2}}. \quad (36)$$

For  $k = 2$  and  $k = 4$  this proposal coincides with Eq. (29) and for large  $k$  it agrees with Eq. (30), i.e.,

$$\lim_{k \rightarrow \infty} \alpha_{\text{op}}^{(1)}(k) = \lim_{k \rightarrow \infty} \alpha_S(k) = \frac{\pi^2}{4}. \quad (37)$$

Since  $\alpha_{\text{op}}^{(1)}$  is nearly equal to  $\alpha_S$  for all  $k$  (see Fig. 3), the accuracy of this proposal is of the order of  $\alpha_S$ .

Up to now, the most accurate proposal for the optimal length is  $L_S$ . However, the calculations show that to find more accurate results, we need to slightly increase  $L_S$  for all  $k$  and  $N$ . Therefore, since we always have  $L_{\text{op}}^{(1)} < L_S$ , the accuracy of Eq. (36) is slightly lesser than Eq. (29) which can be also confirmed by explicit calculations. To find an optimal length that is more accurate than  $L_S$ , note that the factor  $\pi/2$  in Eq. (36) is the first term in the asymptotic expansion of the term  $\frac{k}{2} \sin\left(\frac{\pi}{k}\right)$  in Eq. (30), i.e.,

$$\frac{k}{2} \sin\left(\frac{\pi}{k}\right) = \frac{\pi}{2} - \frac{\pi^3}{12k^2} + \mathcal{O}(k^{-4}). \quad (38)$$

So a good idea is to add the second factor  $\frac{\pi^3}{12k^2}$  to  $\pi/2$  in Eq. (36) and write the optimal length as

$$\alpha_{\text{op}}^{(2)}(k) = \left(\frac{\pi}{2} + \frac{\pi^3}{12k^2}\right)^{\frac{k-2}{k/2}} = \left(1 + \frac{\pi^2}{6k^2}\right)^{\frac{k-2}{k/2}} \alpha_{\text{op}}^{(1)}(k), \quad (39)$$

and

$$L_{\text{op}}^{(2)}(N) = \left(\frac{\pi^{4(k-1)}}{4^{k-2}}\right)^{\frac{1}{k(k+2)}} \left(1 + \frac{\pi^2}{6k^2}\right)^{\frac{2(k-2)}{k(k+2)}} N^{\frac{2}{k+2}} = \left(1 + \frac{\pi^2}{6k^2}\right)^{\frac{2(k-2)}{k(k+2)}} L_{\text{op}}^{(1)}(N), \quad (40)$$

which satisfies  $\alpha_{\text{op}}^{(2)}(2) = 1$  and  $\lim_{k \rightarrow \infty} \alpha_{\text{op}}^{(2)}(k) = \pi^2/4$ . It is straightforward to check that  $L_{\text{op}}^{(2)}$  ( $\alpha_{\text{op}}^{(2)}$ ) is always slightly greater than  $L_S$  ( $\alpha_S$ ) (see Fig. 3). Indeed, calculations show that between the several mentioned candidates for the optimal length,  $L_{\text{op}}^{(2)}$  gives the most accurate energy spectrum. As a simple application, in Table 2, we have reported the ground state energy of the anharmonic oscillators using only one basis function ( $N = 1$ ) and the optimal length  $L_{\text{op}}^{(2)}$ . For these cases, the matrix of the Hamiltonian has only one element and the relative error is less than 20%.

$k$	$E_0$	$E_0^{\text{exact}}$	$\epsilon_0$
2	1.19	1.00	$1.9 \times 10^{-1}$
4	1.23	1.06	$1.6 \times 10^{-1}$
6	1.34	1.14	$1.7 \times 10^{-1}$
8	1.45	1.23	$1.8 \times 10^{-1}$

Table 2: The ground state energies and their relative errors using one basis function ( $N = 1$ ) and  $L_{\text{op}}^{(2)}$ .

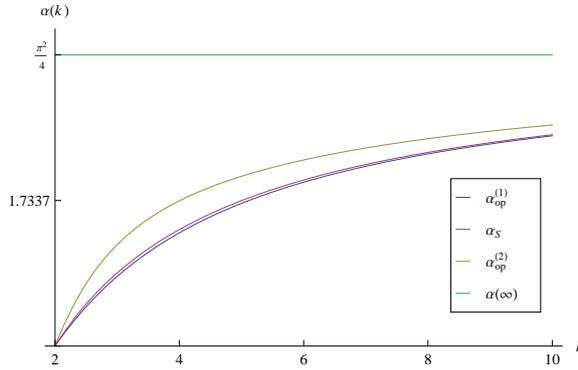


Figure 3: The proportionality coefficient  $\alpha(k)$ .

## 6. Stationarity of the trace of the Hamiltonian

In this section we apply the optimized Rayleigh-Ritz method proposed by Okopinska [5, 6] for the trigonometric basis functions. This method is originally used for the harmonic oscillator eigenfunctions and it is based on fixing the values of nonlinear parameters before diagonalization of the truncated matrix. Before diagonalization, the only physical quantity that can be determined is the trace of the Hamiltonian

$$\text{Tr}_N H = \sum_{n=1}^N \langle n | \hat{H} | n \rangle, \quad (41)$$

which represents the  $N$ th-order approximation to the sum of energies of the  $N$  lowest bound states. Now the strategy is to choose the values of nonlinear parameters so as to make  $\text{Tr}_N H$  stationary. Since the only nonlinear parameter for the trigonometric basis functions is  $L$  we have

$$\frac{d}{dL} \text{Tr}_N H = 0. \quad (42)$$

Using Eq. (24) we can find  $\text{Tr}_N H$  as

$$\text{Tr}_N H = \frac{\pi^2}{12L^2} (4N^2 - 1)N + \left(\frac{L}{\pi}\right)^k \left[ \sum_{n=1}^N D_{2n-1} + ND_0 \right], \quad (43)$$

where  $D_0 = \pi^k / (k+1)$  and

$$\sum_{n=1}^N D_{2n-1} = \sum_{i=0}^{\frac{k}{2}-1} \frac{\pi^{k-2i-2} k!}{(-4)^{i+1} (k-2i-1)!} \left[ (4^{i+1} - 1) \zeta(2i+2) - \zeta(2i+2, N+1/2) \right], \quad (44)$$

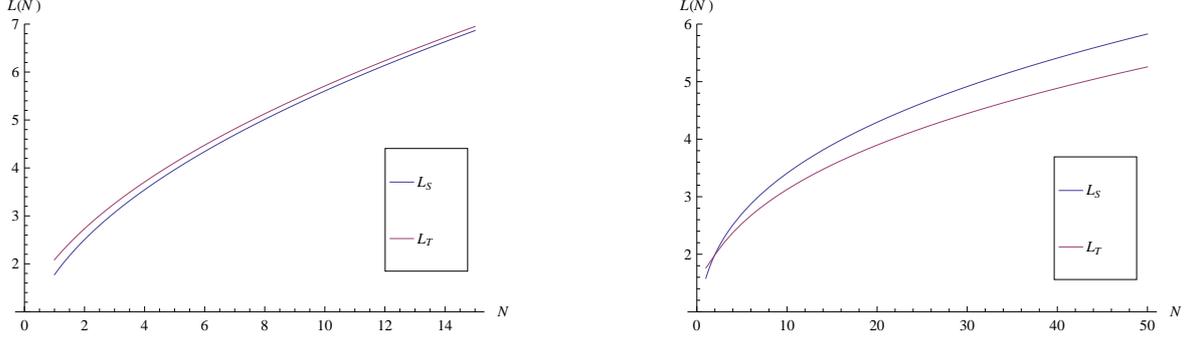


Figure 4: The optimal lengths versus  $N$  for  $k = 2$  (left) and  $k = 4$  (right).

where  $\zeta(s)$  and  $\zeta(s, a)$  are the Riemann zeta function and the generalized Riemann zeta function, respectively. After some algebra, Eq. (42) results in the following optimal length and  $\alpha_T$

$$L_T(N) = \pi \left( \frac{(4N^2 - 1)N/(6k)}{\frac{N\pi^k}{k+1} + \sum_{i=0}^{\frac{k}{2}-1} \frac{\pi^{k-2i-2}k!}{(-4)^{i+1}(k-2i-1)!} \left[ (4^{i+1} - 1) \zeta(2i+2) - \zeta(2i+2, N+1/2) \right]} \right)^{\frac{1}{k+2}},$$

$$\simeq \left( \frac{2(k+1)\pi^2}{3k} \right)^{\frac{1}{k+2}} N^{\frac{2}{k+2}}, \quad (45)$$

$$\alpha_T(k) \simeq \frac{2(k+1)}{3k}. \quad (46)$$

For  $k = 2$  we have  $L_T(N) \simeq \sqrt{\pi N}$  which agrees well with  $L_S$  and  $L_{op}$ . However, the accuracy of this method reduces for  $k > 2$ . In comparison with  $L_{op}$ , we should mention that for  $k < 10$ ,  $L_{op}$  is more accurate as it is apparent from Fig. 4 and l.h.s of Fig. 5.<sup>4</sup> But for  $k > 10$ ,  $L_T$  is more closer to  $L_S$  (r.h.s of Fig. 5) and similar to  $L_S$  tends to one as  $k$  goes to infinity. The accuracy of the energy spectrum of the anharmonic oscillators for  $k = \{2, 4, 6, 8\}$  and  $N = 10$  is reported in Table 3. As the table shows, the optimal length obtained using  $L_S$  or  $L_{op}$  formulas gives more accurate results in comparison with  $L_T$  formula for a given  $N$ . In Fig. 6, we depicted the coefficient of proportionality  $\alpha(k)$  for the proposed schemes. Since  $\alpha_{op}$  grows exponentially, it cannot be used efficiently for large  $k$ . On the other hand,  $\alpha_S$ ,  $\alpha_{op}^{(1)}$ , and  $\alpha_{op}^{(2)}$  go to  $\pi^2/4$  and  $\alpha_T$  goes to  $2/3$  at this limit.

## 7. The harmonic oscillator basis expansion

We can also find the energy spectrum of the anharmonic oscillators using the basis of the harmonic oscillator eigenfunctions

$$\phi_n(x) = \left[ \frac{\Omega}{\sqrt{\pi} 2^n n!} \right]^{1/2} H_n(\Omega x) e^{-\Omega^2 x^2/2}, \quad (47)$$

<sup>4</sup>Note that for  $k = 2$ , we have  $L_{op} = L_S$ , and for  $k = 4$ ,  $L_{op}$  nearly coincides with  $L_S$ .

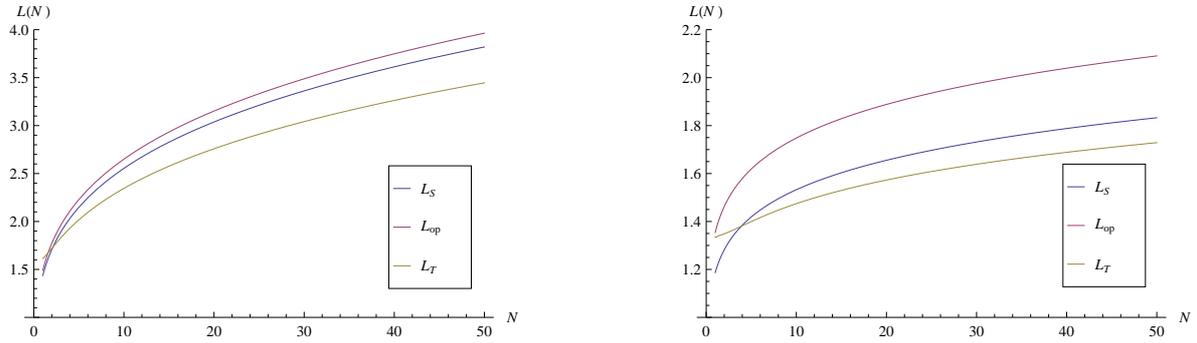


Figure 5: The optimal lengths versus  $N$  for  $k = 6$  (left) and  $k = 16$  (right).

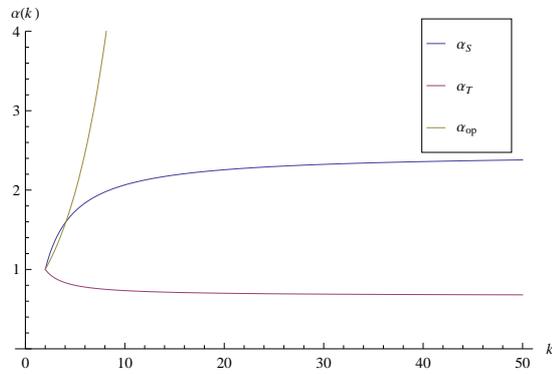


Figure 6: The proportionality coefficient versus  $k$ .

$k = 4$			$k = 6$			$k = 8$		
$n$	$L$	$\epsilon_n$	$n$	$L$	$\epsilon_n$	$n$	$L$	$\epsilon_n$
0	$L_S$	$1.53 \times 10^{-11}$	0	$L_S$	$1.57 \times 10^{-9}$	0	$L_S$	$4.10 \times 10^{-8}$
	$L_{op}$	$1.65 \times 10^{-11}$		$L_{op}$	$1.14 \times 10^{-10}$		$L_{op}$	$7.36 \times 10^{-8}$
	$L_T$	$4.51 \times 10^{-9}$		$L_T$	$5.00 \times 10^{-7}$		$L_T$	$6.85 \times 10^{-6}$
2	$L_S$	$1.88 \times 10^{-10}$	2	$L_S$	$9.03 \times 10^{-9}$	2	$L_S$	$1.30 \times 10^{-7}$
	$L_{op}$	$2.10 \times 10^{-10}$		$L_{op}$	$2.48 \times 10^{-9}$		$L_{op}$	$1.91 \times 10^{-7}$
	$L_T$	$5.96 \times 10^{-8}$		$L_T$	$2.15 \times 10^{-6}$		$L_T$	$1.75 \times 10^{-5}$
4	$L_S$	$6.05 \times 10^{-9}$	4	$L_S$	$8.07 \times 10^{-8}$	4	$L_S$	$7.04 \times 10^{-7}$
	$L_{op}$	$6.59 \times 10^{-9}$		$L_{op}$	$8.93 \times 10^{-8}$		$L_{op}$	$5.70 \times 10^{-7}$
	$L_T$	$9.92 \times 10^{-7}$		$L_T$	$1.36 \times 10^{-5}$		$L_T$	$6.46 \times 10^{-5}$
6	$L_S$	$2.12 \times 10^{-7}$	6	$L_S$	$4.88 \times 10^{-7}$	6	$L_S$	$4.03 \times 10^{-6}$
	$L_{op}$	$2.08 \times 10^{-7}$		$L_{op}$	$1.58 \times 10^{-6}$		$L_{op}$	$8.73 \times 10^{-7}$
	$L_T$	$1.25 \times 10^{-5}$		$L_T$	$7.91 \times 10^{-5}$		$L_T$	$2.40 \times 10^{-4}$

Table 3: The relative errors of various optimized schemes for  $N = 10$  basis functions.

where  $H_n(\Omega x)$  are Hermite polynomials and the frequency  $\Omega$  is the variational parameter. This frequency can be fixed by the principle of minimal sensitivity, requiring the dependence on the variational parameter be as weak as possible [20]. For the Hamiltonian

$$H = \frac{1}{2} \left[ -\frac{d^2}{dx^2} + \omega^2 x^2 \right] + \lambda x^4, \quad (48)$$

the application of the PMS to the sum of  $N$  even and  $N$  odd basis functions gives [5]

$$\Omega_{\text{PMS}}^3 - \omega^2 \Omega_{\text{PMS}} = 8\lambda \left( N + \frac{1}{8N} \right). \quad (49)$$

It is also possible to find a similar relation for the optimal frequency  $\Omega_{\text{op}}$  using the prescription presented in Sec. 3. Here we have two potentials: one physical  $\frac{1}{2}\omega^2 x^2 + \lambda x^4$  and one unphysical  $\frac{1}{2}\Omega^2 x^2$  which we use the eigenfunctions of the latter to approximate the solution of the former. The intersection points of these potentials are given by  $x_{\text{int}} = \pm \sqrt{\frac{\Omega^2 - \omega^2}{2\lambda}}$ . So the potentials take the following value at these points:

$$V(x_{\text{int}}) = \frac{\Omega^2}{4\lambda} (\Omega^2 - \omega^2). \quad (50)$$

On the other hand, for  $N$  even and  $N$  odd basis functions, the maximal quantum number is  $2N - 1$  and therefore the maximal energy reads

$$E_{\text{max}} = \Omega \left( 2N - \frac{1}{2} \right). \quad (51)$$

Now since the basis functions with the energy larger than  $V(x_{\text{int}})$  would have no useful contribution to the sought-after solutions, by equating Eq. (50) and Eq. (51) we obtain the relation for the optimal frequency as

$$\Omega_{\text{op}}^3 - \omega^2 \Omega_{\text{op}} = 8\lambda \left( N - \frac{1}{4} \right), \quad (52)$$

which agrees well with Eq. (49) especially for large  $N$ . At this limit, we have  $\Omega_{\text{op}} \approx \Omega_{\text{PMS}} \approx 2(\lambda N)^{1/3}$ . Also, the  $N$  dependence of the optimal frequency coincides with the  $N$  dependence of the optimal length in the trigonometric expansion for  $k = 4$ , i.e.,  $\Omega_{\text{op}} \sim N^{1/3} \sim L_{\text{op}}$ . Note that, the accuracy of  $\Omega_{\text{op}}$  is of the order of  $\Omega_{\text{PMS}}$  even for small  $N$ . In Fig. 7, we have depicted  $\frac{\Omega_{\text{PMS}}}{2\lambda^{1/3}}$  in terms of the total number of the basis functions  $2N$  for  $\omega^2 = \{0, 12\lambda^{2/3}, 20\lambda^{2/3}\}$ .

## 8. Conclusions

In this paper, we presented several optimal lengths for accurate calculation of the eigenvalues and eigenfunctions of the anharmonic oscillators using trigonometric basis functions obeying Dirichlet boundary condition and the harmonic oscillator eigenfunctions. We indicated that the value of the potential at the optimal length should be proportional to the maximum energy of the used basis functions. Since both  $V(L_{\text{op}}) \gg \varepsilon_N$  and  $V(L_{\text{op}}) \ll \varepsilon_N$  are two sources of error, we demanded that the proportionality coefficient  $\alpha(k)$  to be of the order of one. For the trigonometric basis set, we suggested some ansatz for  $\alpha(k)$  with the condition  $\alpha(2) = 1$  and found that  $L_{\text{op}}^{(2)}$  gives the most accurate results. By defining  $L_S$  we showed that it can be also used as an accurate optimal length. Indeed, it is shown that the optimal number of the mesh points (for fixed  $h$ ) in the Schwartz's scheme, where the reference function vanishes there nearly coincides with the optimal number of the basis functions (for fixed  $L$ ) which at most have the same number of nodes. Moreover,  $\alpha_S$  is of the order of unity for all  $k$ . An alternative proposal is using the trace of the Hamiltonian as an only physical quantity before diagonalization and to make it stationary at the optimal value  $L_T$ . We

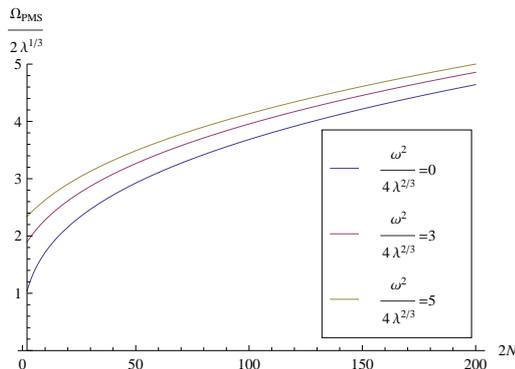


Figure 7: The optimal frequency parameter versus  $2N$  obtained via the principle of minimal sensitivity for  $\omega^2 = \{0, 12\lambda^{2/3}, 20\lambda^{2/3}\}$ .

showed that this optimal length has the correct asymptotic value for large  $k$  and can be used as a good approximation for  $k > 10$ . For all proposals except  $L_{\text{op}}$  the proportionality coefficient  $\alpha(k)$  remains of order of one for all  $k$  and they have the correct asymptotic value, i.e.,  $\lim_{k \rightarrow \infty} L(N) = 1$ . We indicated that these proposals can be also used for the multidimensional problems, and for large  $N$ , for the periodic boundary condition and the polynomial potentials. The following schematic diagram shows the relative efficiency of the proposed optimal lengths

$$\begin{array}{ccccccc}
 L_{\text{T}} & \xrightarrow{k < 10} & L_{\text{op}} & \longrightarrow & L_{\text{op}}^{(1)} & \longrightarrow & L_{\text{S}} & \longrightarrow & L_{\text{op}}^{(2)}, \\
 L_{\text{op}} & \xrightarrow{k > 10} & L_{\text{T}} & & & & & & 
 \end{array} \tag{53}$$

where the right arrow indicates the direction of the increasing of the accuracy. For the harmonic oscillator basis functions, we showed that the resulting optimal frequency agrees with the one obtained using the principle of the minimal sensitivity.

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