# Functional representations in non-Fourier basis with applications

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Orthogonal trigonometric basis functions in $(-\pi,\pi)$ are considered and the suitability of Fourier-like expansions involving odd harmonics of the semifundamental frequency is noted. Comparison with the conventional representation is made, pointing out the advantages of employing non-Fourier bases. As a practical application, near-exact results of variational calculations for the ground state of the quartic-anharmonic-oscillator problem are presented both for small and large coupling strengths.

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## I. INTRODUCTION

Functional representation in terms of an orthogonal basis is often preferred over a straightforward power-series development for various reasons [1] and, in this context, *trigonometric* basis functions have become quite popular both in functional [2] and numerical [3] analyses. Here the basic strategy is to expand a function $F(x)$, satisfying $F(\pi)=F(-\pi)$, in the following way:

$$F(x)=a_0+\sum_{m=1,2,\ldots} a_m \cos mx+\sum_{n=1,2,\ldots} b_n \sin nx\ , \qquad -\pi\le x\le\pi\ . \tag{1}$$

One ascribes a *fundamental* frequency (unity) to $F(x)$ and calls the development (1) a harmonic series, keeping aside the rather trivial constant term $a_0$. Conventionally, however, Eq. (1) is termed a Fourier series.

The purpose of the present paper is threefold: (i) to emphasize that $\{\cos mx\}$ and $\{\sin nx\}$ $(m,n: 1,2,\ldots)$ are *not* the *only* possible symmetry-adapted orthogonal sets in $(-\pi,\pi)$, (ii) to present a comparative survey of the efficiency of all possible orthogonal trigonometric bases in $(-\pi,\pi)$ in representing various functions, and (iii) to demonstrate how the alternative sets may be computationally more advantageous, particularly a judicious choice of a variational trial function could be made by virtue of (ii) for the quartic-anharmonic-oscillator problem, leading to very accurate estimates of the ground-state energy and other properties, and hence the wave function.

## II. BASIS SETS

In a symmetric interval such as $(-\pi,\pi)$, cosine and sine functions are always orthogonal. So, let us consider first the orthogonality of two cosine functions $\cos px$ and $\cos qx$. Thus we require

$$\int_{-\pi}^{\pi} \cos px\,\cos qx\,dx=0,\quad p\neq q \tag{2}$$

for discrete variables $p$ and $q$, not necessarily integers. From (2), one is led to the condition

$$p\sin p\pi\cos q\pi=q\sin q\pi\cos p\pi,\quad p\neq q\ . \tag{3}$$

Similarly, for sine functions, the orthogonality relation becomes equivalent to the condition

$$p\sin q\pi\cos p\pi=q\sin p\pi\cos q\pi,\quad p\neq q\ . \tag{4}$$

It is easy to see by inspection that (3) and (4) are satisfied *at least* under two different conditions: (i) $p$ and $q$ are integers and (ii) $p$ and $q$ are odd half-integers. In the former situation, one recovers the Fourier bases $\{\cos mx\}$ and $\{\sin nx\}$, while the latter refers to alternative basis functions $\{\cos m_1 x/2\}$ and $\{\sin n_1 x/2\}$ $(m_1,n_1: 1,3,\ldots)$. At this point, however, it is not quite apparent whether (3) and (4) would also be satisfied for other sets of values of $p$ and $q$ (but see below).

We may now assert that the following four orthogonal sets are certainly possible in $(-\pi,\pi)$ to represent an arbitrary function $F(x)$, given the proper boundary conditions:

$$\begin{aligned}&\text{set I: } \cos mx,\ \sin nx\ ,\\ &\text{set II: } \cos m_1 x/2,\ \sin nx\ ,\\ &\text{set III: } \cos m_1 x/2,\ \sin n_1 x/2\ ,\\ &\text{set IV: } \cos mx,\ \sin n_1 x/2\ .\end{aligned} \tag{5}$$

An alternative way to arrive at (5) is to consider the Sturm-Liouville problem [4]. In terms of the eigenvalue equation

$$Y''(x)+\lambda Y(x)=0\ , \tag{6}$$

the above sets follow as *quantized* solutions, respectively, with the boundary conditions (i) $Y(\pi)=Y(-\pi)$, $Y'(\pi)=Y'(-\pi)$; (ii) $Y(\pi)=Y(-\pi)=0$; (iii) $Y(\pi)=-Y(-\pi)$, $Y'(\pi)=-Y'(-\pi)$; (iv) $Y'(\pi)=Y'(-\pi)=0$. Thus two conditions are required in each case. Let us note here that set I corresponds to the Fourier series (1). Set II may be identified with the solutions for the particle-in-a-box problem of quantum mechanics [5]. Sets III and IV, however, to the best of our knowledge, have found little practical use so far, and they do not appear in the course of discussions on trigonometric series [2,3]. One further point is that the way (6) has led us to the sets in (5) shows clearly that no other orthogonal set is possible. The reason is obvious. Imposing conditions

 

on higher derivatives of $F(x)$ at the boundaries would not alter the nature of restrictions on the arguments of sines and cosines from those already mentioned.

## III. DISCUSSION

Evidently, for each of the sets in (5), there will be a corresponding series representation, in very much the same way as the Fourier series (1) refers to set I. In this respect, we first observe that all the sets, except set I, involve *odd* harmonics of the *semifundamental* frequency. Second, we remark that set II applies with equal facility to represent a function $F(x)$, obeying $F(\pi)=F(-\pi)$, in place of set I. One has to consider only a trivially modified form of the function, $\bar{F}(x)=F(x)-F(\pi)$, amounting to an overall constant shift. Finally, and most importantly, rates of convergence of the coefficients $C_r$ [$C$: $a$ or $b$, as in (1); $r$: $m$, $m_1/2$, $n$, or $n_1/2$] will crucially determine the adequacy of the expansions concerned and, in this respect too, the alternative basis functions $\{\cos m_1 x/2\}$ and $\{\sin n_1 x/2\}$ perform at times very desirably. If the coefficient $C_r$ decays as

$$C_r \sim r^{-\alpha}, \quad \alpha > 0 , \tag{7}$$

one would find that the value of $\alpha$ depends both on the nature of $F(x)$ *and* the basis. A larger $\alpha$ value naturally implies faster convergence. In a nutshell, Table I presents a comparative survey of the performance of various bases.

In order to appreciate the usefulness of Table I, and hence the adequacy of representations based on the odd harmonics of the semifundamental frequency, let us first consider the case of $\sin n_1 x/2$. Table I shows that, in this case, $\alpha \geq 2$ always. For $\sin nx$, on the other hand, we have $\alpha \geq 1$. Thus, as an *odd* function set, $\{\sin n_1 x/2\}$ is, in general, *superior*. One may also observe from the table that, if we expand $\sin nx$ in terms of $\{\sin n_1 x/2\}$, coefficients would decay as $n_1^{-2}$ (*vide* entry 1 or 3 ). On the contrary, for the converse expansion, it turns out that $\alpha=1$ (*vide* entry 2), providing an additional testimony of our above remark.

To cite a practical case, we choose the problem of *analysis* of a sawtooth signal [6], given by the function $F(x)=x$, $-\pi \leq x \leq \pi$. Conventionally, here the Fourier representation goes as

$$x = 2 \sum_{n=1,2,\ldots,} (-1)^{n+1}[(1/n)\sin nx] , \tag{8}$$

showing (i) $\alpha=1$, in accordance with entry 4 of Table I and (ii) since $F(\pi)\neq F(-\pi)$ here, the right-hand side of (8) behaves wildly *near* the boundaries, converging wrongly at $[F(\pi)+F(-\pi)]/2$ at $x=\pm\pi$. The situation with $\{\sin n_1 x/2\}$, however, is quite comfortable. One obtains

$$x = (8/\pi) \sum_{n_1=1,3,\ldots} (-1)^{(n_1-1)/2}[(1/n_1^2)\sin n_1 x/2] , \tag{9}$$

which is a far better representative both from the standpoint of convergence ($\alpha=2$) *and* the behavior near $x=\pm\pi$. Thus the set $\{\sin n_1 x/2\}$ may be quite important in areas such as signal processing [6,7].

While expansions in $\{\sin n_1 x/2\}$ are *generally* recommendable, the set $\{\cos m_1 x/2\}$ may be of importance in specific situations. In what follows, we shall demonstrate how such a basis set may be very conveniently employed in certain variational calculations for bound states.

## IV. VARIATIONAL CALCULATION

Let us choose the problem of finding the eigenvalue and eigenfunction for the ground state of the quartic anharmonic oscillator, defined by the Hamiltonian

$$H = -\nabla^2 + x^2 + \lambda x^4 . \tag{10}$$

This problem has been treated in various ways from time to time [8,9]. While Ref. [8] presents very accurate data by using a variational scheme with *scaled* basis functions, other approaches are also in vogue and a selected list of works may be found in Ref. [9], which, by no means, is exhaustive. Here we shall essentially employ the basis $\{\cos m_1 x/2\}$ in a linear variational framework. Changing the domain to $(-L,L)$, the basis set becomes $\{\cos m_1 \pi x/2L\}$ and we consider the trial function in the form

$$\tilde{\psi}(N_1,L,x) = \sum_{m_1=1,3,\ldots}^{N_1} a_{m_1} \cos m_1 \pi x/2L, \quad -L \leq x \leq L , \tag{11}$$

and zero otherwise. The choice (11) is quite reasonable and straightforward, since the exact density also should approach zero well beyond the classical turning point ($L_c$). The Fourier basis $\{\cos mx\}$ cannot be directly employed here because these functions do not vanish at the boundaries $\pm\pi$. Integrals involved in such calculations

TABLE I. Dependence of $\alpha$ [Eq. (7)] on the nature of $F(x)$ and the various trigonometric bases in $(-\pi,\pi)$.

| Serial number | Nature of $F(x)$ | $\alpha$ | | | |
|---|---|---|---|---|---|
| | | $\cos mx$ | $\sin nx$ | $\cos m_1 x/2$ | $\sin n_1 x/2$ |
| 1 | $F(\pi)=F(-\pi)$ | 2 | 3 | 1 | 2 |
| 2 | $F(\pi)=-F(-\pi)$ | 2 | 1 | 3 | 2 |
| 3 | $F(\pi)=F(-\pi)=0$ | 2 | 3 | 3 | 2 |
| 4 | $F'(\pi)=F'(-\pi)$ | 4 | 1 | 1 | 2 |
| 5 | $F'(\pi)=-F'(-\pi)$ | 2 | 1 | 1 | 4 |
| 6 | $F'(\pi)=F'(-\pi)=0$ | 4 | 1 | 1 | 4 |

TABLE II. Approximate ground-state energies for the Hamiltonian (10) at $\lambda=1$ and 40 000 as function of the number of basis ($N$) employed in (11). The bracketed data in the last row show exact values [8].

| Number of basis ($N$) | $\lambda=1$ | | $\lambda=40\,000$ | |
|---|---|---|---|---|
| | $L_{\text{opt}}/\pi$ | $\bar{E}_0$ | $L_{\text{opt}}/\pi$ | $\bar{E}_0$ |
| 2 | 0.705 | 1.393 | 0.134 | 36.3 |
| 4 | 0.814 | 1.392 37 | 0.146 | 36.274 8 |
| 6 | 0.916 | 1.392 351 8 | 0.161 | 36.274 46 |
| 8 | 1.115 | 1.392 351 641 9 | 0.175 | 36.274 458 2 |
| 10 | 1.140 | 1.392 351 641 531 | 0.187 | 36.274 458 134 |
| | | [1.392 351 641 530 2] | | [36.274 458 133 7] |

are also quite easy to evaluate in the chosen basis. For convenience, we list below the relevant matrix elements in normalized bases, viz. $(1/\sqrt{L})\cos m_i\pi x/2L$ and $(1/\sqrt{L})\cos m_j\pi x/2L$:

$$\langle -\nabla^2\rangle_{ii}=m_i^2\pi^2/4L^2,\quad \langle -\nabla^2\rangle_{ij}=0\ ;$$

$$\langle x^2\rangle_{ii}=L^2(\tfrac{1}{3}-2/m_i^2\pi^2)\ ,$$

$$\langle x^2\rangle_{ij}=(8L^2/\pi^2)[(m_i+m_j)^{-2}\cos(m_i+m_j)\pi/2 +(m_i-m_j)^{-2}\cos(m_i-m_j)\pi/2]\ ;$$

$$\langle x^4\rangle_{ii}=L^4(\tfrac{1}{5}-4/m_i^2\pi^2+24/m_i^4\pi^4)\ ,$$

$$\langle x^4\rangle_{ij}=(16L^4/\pi^2)[(m_i+m_j)^{-2}\{1-24/(m_i+m_j)^2\pi^2\}\times\cos(m_i+m_j)\pi/2 +(m_i-m_j)^{-2}\{1-24/(m_i-m_j)^2\pi^2\}\times\cos(m_i-m_j)\pi/2]\ .$$

We note in addition that $L$ cannot be too large or too small. This is because, the average kinetic energy increases without limit as $L\to 0$ while the average potential energy behaves in the same manner as $L\to\infty$. Thus $L$ in (11) indeed appears as a nonlinear variational parameter, to be optimized ($L_{\text{opt}}$) subsequently.

Table II shows the results of our calculations for approximate ground-state eigenvalue $\bar{E}_0$. We have chosen two widely separated values of $\lambda$ (viz. $\lambda=1$ and 40 000) in order to check any instability in the scheme. A rather small number of basis functions ($N$) have been employed in each case [$N=(N_1+1)/2$], but we note that convergence is quite fast. This is expected. From Table I, we may easily infer that the rate of convergence of the coefficients $a_{m_1}$ would follow the power law $a_{m_1}\sim m_1^{-3}$ at large $m_1$. Thus, as a trial function, (11) possesses very good computational convenience, justifying the worth of employing non-Fourier bases. The results we obtain are also impressive. With just ten basis functions, we note that the error is already approximately $10^{-11}\%$ at $\lambda=1$ and $10^{-9}\%$ at $\lambda=40\,000$. For further improvement, one needs only to increase the number of basis. Finally, to convince ourselves about the suitability of the choice (11), a comparison should be made between $L_{\text{opt}}$ and $L_c$, the classical turning point. One finds that $L_c/\pi=0.281$ at $\lambda=1$ and the value changes to $L_c/\pi=0.055$ at $\lambda=40\,000$. Thus the inequality $L_{\text{opt}}\gg L_c$ is also satisfied, as we presumed. Had we taken larger $N$, it is transparent from Table II that such an inequality would have been more dominant.

To assess the quality of the optimized wave function, we have also computed $\langle x^2\rangle$ and $\langle x^4\rangle$. Results are presented in Table III. Since in a linear variational context, the virial theorem [10] is not *generally* satisfied with approximate functions, we have attempted to verify the same. In view of the unavailability of near-exact results for the aforesaid moments, we believe that this verification should furnish a reliable testing ground. For the exact function, we should have, from (10),

$$\langle -\nabla^2\rangle=\langle x^2\rangle+2\lambda\langle x^4\rangle\ , \tag{12}$$

so that the average energy, which is also the eigenenergy, would become, by virtue of the virial theorem,

$$E_v=2\langle x^2\rangle+3\lambda\langle x^4\rangle\ . \tag{13}$$

For the exact function $\psi_0$, then we should have

TABLE III. Expectation values $\langle x^2\rangle$ and $\langle x^4\rangle$ for the ground state of the oscillator (10) and verification of Eq. (14) for approximate estimates obtained from our calculations.

| $N$ | $\lambda=1$ | | | $\lambda=40\,000$ | | |
|---|---|---|---|---|---|---|
| | $\langle x^2\rangle$ | $\langle x^4\rangle$ | $\bar{E}_v/\bar{E}_0$ | $\langle x^2\rangle$ | $\langle x^4\rangle$ | $\bar{E}_v/\bar{E}_0$ |
| 2 | 0.307 | 0.260 1 | 0.999 7 | 0.010 51 | 0.000 302 7 | 0.999 4 |
| 4 | 0.305 82 | 0.260 245 | 0.999 996 | 0.010 584 | 0.000 302 11 | 1.000 02 |
| 6 | 0.305 813 61 | 0.260 241 5 | 0.999 999 998 | 0.010 583 883 | 0.000 302 110 9 | 0.999 999 8 |
| 8 | 0.305 813 650 | 0.260 241 448 | 1.000 000 000 21 | 0.010 583 881 27 | 0.000 302 110 76 | 0.999 999 993 |
| 10 | 0.305 813 650 72 | 0.260 241 446 70 | 1.000 000 000 01 | 0.010 583 881 29 | 0.000 302 110 75 | 1.000 000 000 03 |

TABLE IV. Demonstrative 4-basis ($N=4$) calculations of $\langle x^4 \rangle$ for the ground state via the Hellman-Feynman route, i.e., the derivative method given by Eq. (15). More accurate estimates are presented in Table III, with which these agree.

| | $\Delta E/\Delta\lambda$ | |
|---|---|---|
| $h/\lambda$ | $\lambda=1$ | $\lambda=40\,000$ |
| 0.1 | 0.260 5 | 0.000 302 7 |
| 0.01 | 0.260 25 | 0.000 302 12 |
| 0.001 | 0.260 243 | 0.000 302 111 |
| 0.0001 | 0.260 243 | 0.000 302 111 |

TABLE V. Verification of Symanzik scaling relation by the approach of $E_0/\lambda^{1/3}$ towards a constant value ($=1.06036$) in the present study.

| | $\bar{E}_0/\lambda^{1/3}$ | |
|---|---|---|
| $\lambda$ | $N=2$ | $N=4$ |
| 10 000 | 1.062 7 | 0.061 2 |
| 15 000 | 1.062 5 | 1.061 0 |
| 20 000 | 1.062 4 | 1.060 9 |
| 30 000 | 1.062 3 | 1.060 75 |
| 40 000 | 1.062 2 | 1.060 68 |

$$E_v/E_0=1\ , \tag{14}$$

where $E_0$ satisfies $H\psi_0=E_0\psi_0$. Thus a pertinent *goodness test* for an approximate wave function $\bar{\psi}_0$ would be to check how far (14) is satisfied with $\bar{E}_v$ and $\bar{E}_0$ replacing $E_v$ and $E_0$, respectively, where $\bar{E}_v=2\langle x^2\rangle+3\lambda\langle x^4\rangle$. Table III also shows the relevant data. It is now probably transparent that the present scheme furnishes sufficiently good-quality wave functions as well with little effort.

It may, however, be inferred from the form (11) for $\bar{\psi}_0$ that $1/L$ would act as a scale parameter to satisfy the virial theorem in an obvious way [10] at its *optimal* value. However, such an assertion is strictly valid only if the optimization is performed *analytically*. In a numerical scheme such as the present one, a sensitive dependence of $\bar{E}_v/\bar{E}_0$ on the level of accuracy to which $L_{\text{opt}}$ is determined is, in general, quite likely, especially when $\bar{\psi}_0$ is not a reasonably good approximation to $\psi_0$. This is why we have incorporated this aspect in Table III. What we observe in this respect here is again very desirable. The said dependence is noticeably weak in our scheme. Indeed, $L_{\text{opt}}$ is accurately estimated only up to the *third* decimal place (see, e.g., Table II). But we note that Table III respects the number of basis ($N$) much more than the accuracy level of $L_{\text{opt}}$ in the context of validity of the virial theorem. This is precisely why our results finally agree to *ten* decimal places. So, we may now conclude that $\bar{\psi}_0$ obeys $\bar{E}_v/\bar{E}_0\approx 1$ more because the individual average properties are accurately obtained; that it involves an optimally scaled coordinate has little decisive value here.

In order to examine the quality of $\bar{\psi}_0$ unambiguously, two more goodness tests are finally in order. One of these is concerned with satisfaction of the Hellmann-Feynman theorem. For $H$ in (10), it states that, at a given value of $\lambda$,

$$\langle x^4\rangle = dE/d\lambda \approx \Delta E/\Delta\lambda = [E(\lambda+h)-E(\lambda-h)]/2h\ , \quad h \ll \lambda\ . \tag{15}$$

Table IV shows how well (15) is satisfied for approximate estimates at various values of $h/\lambda$. Here we report merely 4-basis calculations, but note that the estimates obtained by employing the right-hand side of (15) agree very satisfactorily with the results of $\langle x^4\rangle$ presented in Table III, even for moderately high $h/\lambda$. The Symanzik scaling relation, pointed out by Simon [9], is another requirement to be checked. At large $\lambda$, for this oscillator problem, the eigenenergy $E(\lambda)$ should increase as $\lambda^{1/3}$, so that $E_0/\lambda^{1/3}$ approaches a constant value of 1.060 36. In Table V, we display how satisfactorily this asymptotic behavior is obeyed. Here too, we report small-basis calculations only in order to emphasize the remarkable performance of the present scheme. As $\bar{E}_0$ values themselves are quite accurately obtained in larger basis sets, it is quite natural that the required behavior would be followed much more closely in such situations.

The importance of form (11) in a variational context may now be appreciated. It is capable of furnishing very good-quality wave function and hence the average properties. We further observe that integral evaluations in and implementation of the present scheme are also recommendably easy in comparison with the prevalent methods [8,9] of approaching the problem in hand.

## V. CONCLUDING REMARKS

Non-Fourier basis functions have not so far found wide applicability. The present endeavor is a preliminary step towards this goal. We have demonstrated that, at times, such bases are computationally very convenient. Table I may be a helpful guide in this regard. Further work along this line is in progress.

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