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Confined One Dimensional Harmonic Oscillator as a Two-Mode System

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The one-dimensional harmonic oscillator in a box problem is possibly the simplest example of a two-mode system. This system has two exactly solvable limits, the harmonic oscillator and a particle in a (one-dimensional) box. Each of the two limits has a characteristic spectral structure describing the two different excitation modes of the system. Near each of these limits, one can use perturbation theory to achieve an accurate description of the eigenstates. Away from the exact limits, however, one has to carry out a matrix diagonalization because the basis-state mixing that occurs is typically too large to be reproduced in any other way. An alternative to casting the problem in terms of one or the other basis set consists of using an “oblique” basis that uses both sets. Through a study of this alternative in this one-dimensional problem, we are able to illustrate practical solutions and infer the applicability of the concept for more complex systems, such as in the study of complex nuclei where oblique-basis calculations have been successful.

Keywords: one-dimensional harmonic oscillator, particle in a box, exactly solvable models, two-mode system, oblique basis states, perturbation theory, coherent states, adiabatic mixing

PACS numbers: 03.65.-w, 02.70.-c, 02.60.-x, 03.65.Ge

I. INTRODUCTION

The understanding of a physical system is closely linked to how well one can determine its eigenstates. Typically a set of basis states that works well in one limit, fails in another. And more general methods, such as variational schemes, perturbation theory, or fixed-basis matrix diagonalizations typically begin with a reasonable Hamiltonian and some appropriate set of basis states that yield a good description of the system.

When applying perturbation theory, one is usually concerned with a small perturbation of an exactly solvable Hamiltonian system. However, there are many examples when the Hamiltonian has more than a single exactly solvable limit. This is a common situation when a dynamical symmetry group is used in the construction of the Hamiltonian. A simple example is the hydrogen atom in an external magnetic field: With increasing field strength, particularly for magnetic fields exceeding a so-called critical value of 2.35×10^5 T, the system changes from the spherical symmetry of the Coulomb problem to the cylindrical symmetry of the diamagnetic Hamiltonian.¹ Another example that occurs in a variety of condensed matter problems is a particle confined to two dimensions in an external magnetic field.² In nuclear physics, the Interacting Boson Model classifies many nuclei according to one of three dynamical symmetries.³ *But, what should be done if the system is nowhere near any of the exact limits?* In these situations, the problem may be approached better by using states associated with all the appropriate nearby limits. This set of

states will form an “oblique” (mixed-mode) basis for the calculation.^{4,5} In general, such a basis is non-orthogonal and may even be over complete. Nevertheless, as recent studies demonstrate, such oblique bases have merit. In this paper, we use a pedagogically simple problem to illustrate the oblique basis approach.

The one-dimensional harmonic oscillator in a one-dimensional box has been used to illustrate different aspects of mixing generated by two interactions. Barton, Bray, and Mackane used the model to study the effects of distant boundaries on the energy levels of a one-dimensional quantum system.⁶ Studies have also been done for the cylindrically symmetric system of a three-dimensional harmonic oscillator between two impenetrable walls.⁷ However, these studies did not discuss the bi-modal nature of the problem. Some authors have generalized the one-dimensional harmonic oscillator problem by introducing time-dependent parameters in the Hamiltonian⁸ to pass between the two limiting cases of a free particle and the harmonic oscillator solutions. The infinite square well and the harmonic oscillator have been considered as two limiting cases of a power-law potential within the context of wave packet collapses and revivals.^{9,10} Recent research in modified uncertainty relations has also shown related and interesting behavior.¹¹

In this paper, we demonstrate the concept of an oblique basis approach by considering the simple two-mode system of the one-dimensional harmonic oscillator in a box. First, in Sec. II, we discuss the concept as well as the exactly solvable limits of this toy model. A qualitative discussion of the expected spectrum of the one-dimensional harmonic oscillator in a box is given in Sec. III, along with an example spectrum and quantitative estimates. In Sec. IV some specific problems related to the structure of the Hilbert space are addressed. Sec. V contains specific toy model calculations and results as well as a

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discussion of a new interesting behavior, similar to that observed in nuclear structure studies.^{4,5} The discussion in Sec. V is focused on a quasi-perturbative behavior and a coherent structure within the “strong mixing” region¹² where the system is far from any exact limit. Our conclusions are given in Sec. VI and suggested student exercises in Sec. VII.

II. HARMONIC OSCILLATOR IN A ONE-DIMENSIONAL BOX

Let us start with an abstract two-mode system. For simplicity, we assume that the Hamiltonian of the system has two exactly solvable limits:

$$H = (1 - \lambda)H_0 + \lambda H_1. \quad (1)$$

Clearly this is set up so that $H \rightarrow H_0$ in the limit $\lambda \rightarrow 0$ and $H \rightarrow H_1$ when $\lambda \rightarrow 1$. In the vicinity of these two limits, one can use standard perturbation theory for one Hamiltonian perturbed by the other.¹³ Usually, somewhere in between these two limits there is a critical value of λ that is related to the strongly mixed regime of the system. This value of λ could be anywhere in the interval $(0, 1)$, a convenient choice being $\lambda \approx \frac{1}{2}$. Sometimes, a further symmetry breaking Hamiltonian H_2 can be explicitly introduced by adding $\lambda(1 - \lambda)H_2$ to H .

In Eq. (1), the variable λ has been introduced to simplify the discussion. In general, there will be more than just one such parameter in the Hamiltonian.¹⁴ Often the exactly solvable limits are described as hypersurfaces in the full parameter space. It could even be that there are three or more exactly solvable limits. For example, the Interacting Boson Model (IBM)³ for nuclear spectra has three exactly solvable limits.^{15,16} Another example with three exactly solvable limits is the commonly used schematic interaction with non-degenerate single-particle energies (ε_i), pairing (P^+P) two-body interactions,¹⁷ and quadrupole-quadrupole¹⁸ ($Q \cdot Q$) two-body interactions:

$$H = \varepsilon_i N_i - GP^+P - \chi Q \cdot Q.$$

Here, we consider what is perhaps the simplest two-mode system that shares the essential features of such problems while remaining pedagogically instructive. The Hamiltonian of a one-dimensional harmonic oscillator in a one-dimensional box¹⁹ of size $2L$ has the form:

$$H = \frac{1}{2m}p^2 + V_L(q) + \frac{m\omega^2}{2}q^2, \quad (2)$$

where $V_L(q)$ is the confining potential taking the value zero for $|q| < L$ and ∞ for $|q| \geq L$, and ω is the oscillator frequency. This system has two exactly solvable limits.

The first limit of the toy model in Eq. (2) is $\omega = 0$ when it reduces to a free particle in a one-dimensional box of size $2L$,

$$H_0 = \frac{1}{2m}p^2 + V_L(q). \quad (3)$$

The eigenvectors and energies are labeled by $n = 0, 1, \dots$ and given by

$$\Phi_n(q) = \begin{cases} \sqrt{\frac{1}{L}} \cos\left((n+1)\frac{\pi q}{2L}\right) & \text{if } n \text{ is even} \\ \sqrt{\frac{1}{L}} \sin\left((n+1)\frac{\pi q}{2L}\right) & \text{if } n \text{ is odd} \end{cases}, \quad (4)$$

$$E_n = \frac{1}{2m} \left((n+1)\frac{\pi}{2} \right)^2 \left(\frac{\hbar}{L} \right)^2.$$

This limit corresponds to extreme nuclear matter when the short range nuclear force can be described as an effective interaction represented by a square-well potential.²⁰ We can think of this limit as the one-dimensional equivalent of a three-dimensional model where nucleons are confined within a finite volume of space representing the nucleus. Recently such effective potentials for the Bohr Hamiltonian have been used to introduce symmetries in the critical point of quantum phase transitions.²¹

The other exactly solvable limit of the toy model in Eq. (2), when $L \rightarrow \infty$, is the harmonic oscillator in one dimension,

$$H_1 = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2. \quad (5)$$

In dimensionless coordinates,

$$q \rightarrow \tilde{q} \sqrt{\frac{\hbar}{m\omega}}, \quad p \rightarrow \tilde{p} \sqrt{m\hbar\omega},$$

we have

$$H_1 = \hbar\omega \frac{1}{2} (\tilde{p}^2 + \tilde{q}^2).$$

The eigenvectors and energies are labeled by $n = 0, 1, \dots$ and are given by

$$\Psi_n(q) = \sqrt{\frac{1}{b n! 2^n \sqrt{\pi}}} H_n\left(\frac{q}{b}\right) \exp\left(-\frac{1}{2} \frac{q^2}{b^2}\right), \quad (6)$$

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \quad b = \sqrt{\frac{\hbar}{m\omega}},$$

where H_n are the Hermite polynomials. This limit is essentially the harmonic oscillator model for nuclei.

In a one-dimensional toy model, the anharmonic oscillator with a quartic anharmonicity would be the appropriate counterpart of the $Sp(6, R)$ shell model²² since the quadrupole-quadrupole interaction $Q \cdot Q$ goes as $\sim r^4$ and Q connects harmonic oscillator shells with like parity. If we restrict the model space to only one harmonic oscillator shell, then we can use the algebraic quadrupole moment \tilde{Q} of Elliott²³ because within a single shell \tilde{Q} is the same as Q .¹⁵ Thus, for single shell studies, it is appropriate to consider the one-dimensional harmonic oscillator as representative of the $SU(3)$ shell model for nuclei.

III. SPECTRAL STRUCTURE AT DIFFERENT ENERGY SCALES

Often in physics the spectrum of a system has different characteristics over different energy regimes. This usually reflects the existence of different excitation modes of the system. For the toy model Hamiltonian in Eq. (2), we can define three spectral regions:

- Spectrum of a particle in a one-dimensional box as in Eq. (4) with quadratic dependence on n ($E_n \sim n^2$),
- Spectrum of the one-dimensional harmonic oscillator as in Eq. (6) with linear dependence on n ($E_n \sim n$),
- Intermediate spectrum that is neither of the above two types.

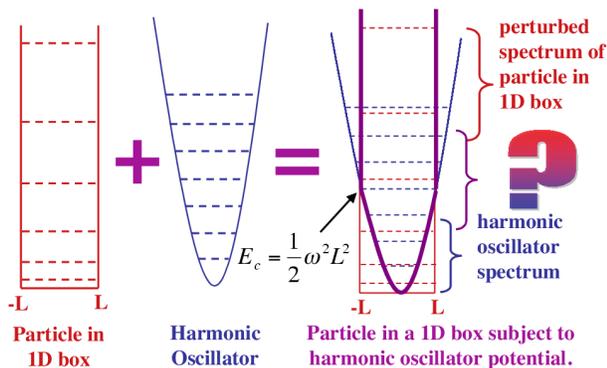


FIG. 1: Two-mode toy system consisting of a particle in a one-dimensional box subject to a central harmonic oscillator restoring force.

As shown in Fig. 1, one expects to see the particle in a box spectrum at high energies. These energies correspond to the box boundaries dominating over the harmonic oscillator potential. In this regime, one can use standard perturbation theory to calculate the energy for a particle in a box perturbed by a harmonic oscillator potential. It can be shown that perturbation theory gives better results for higher energy levels. For $n \rightarrow \infty$, the first correction (δE_n^1) approaches a constant value:

$$\delta E_n^1 = \frac{1}{6} m \omega^2 L^2 \left(1 - \frac{6}{(1+n)^2 \pi^2} \right) \rightarrow \frac{1}{6} m \omega^2 L^2.$$

Using $E_{n+1}^0 - E_n^0 \gg \langle n | V | n \rangle$, one estimates that perturbation calculations are valid when

$$n \gg \frac{2m^2 \omega^2 L^4}{3\hbar^2 \pi^2}. \quad (7)$$

This analysis is confirmed by the numerical calculations shown in Fig. 2 where the perturbed particle in a box spectrum provides a good description for $n > 6$ for the case of $m = \hbar = 2L/\pi = 1$ and $\omega = 4$. Actually, the agreement extends to lower n as is often the case, perturbation theory seemingly yielding valid results well past its expected region of validity. Note that the first order corrections are already close to the limiting constant value of $\frac{1}{6} m \omega^2 L^2$. On the other hand, first-order perturbation clearly fails for the ground state. Indeed, an earlier study¹⁹ of the inadequacy of fixed basis calculations showed that adequate convergence for the ground state when ω is large requires a large number of basis states of the one-dimensional box. This is related to the fact that for large values of ω , or equivalently large L values, a large number of particle-in-a-box wave functions (sin and cos) are needed to obtain the correct behavior (exponential fall off) of the low-energy harmonic oscillator wave functions in the classically forbidden zone.

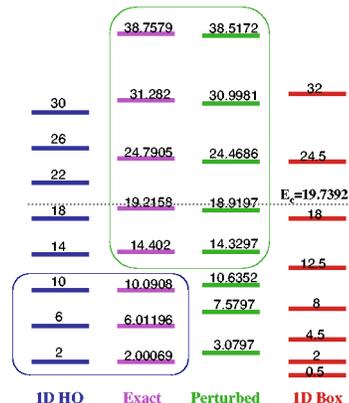


FIG. 2: Exact energies of a two-mode system with $m = \hbar = 2L/\pi = 1$ and $\omega = 4$ compared to the spectrum of the one-dimensional harmonic oscillator (left), spectrum of the free particle in a 1D box (right), and spectrum as calculated within a first order perturbation theory of a free particle in a 1D box perturbed by a 1D HO potential. The lowest three eigenenergies of the two-mode system nearly coincide with the 1D HO eigenenergies, while higher energy states are better described as perturbations of the other limit of a free particle in a 1D box.

The intermediate spectrum should be observed when the harmonic oscillator turning points coincide with the walls of the box. Therefore, the critical energy that separates the two extreme spectral structures is given by

$$E_c = \frac{m\omega^2}{2} L^2. \quad (8)$$

Notice that the constant energy shift $m\omega^2 L^2/6$ in the energy of the high energy levels $\delta E_{n \gg 1}^1$ is one-third of the critical energy ($E_c/3$).

At low energies, where the classical turning points of the oscillator lie far from the boundaries, we expect the spectrum to coincide essentially with that of the oscillator as shown in Fig. 2. The number of such nearly harmonic oscillator states is easily estimated using

$$E_c > E_n^{HO} \Rightarrow n_{\max}^{HO} = \frac{1}{2} \frac{m\omega L^2}{\hbar} - \frac{1}{2}. \quad (9)$$

There is also a compatible number of levels, usually larger than n_{\max}^{HO} , below the E_c corresponding to a free particle in a box,

$$E_c > E_n^{1D} \Rightarrow n_{\max}^{1D} = \frac{2}{\pi} \frac{m\omega L^2}{\hbar} - 1. \quad (10)$$

However, these states are mixed by the harmonic oscillator potential.

Using the ratio of the ground state energies, $E_0^{HO}/E_0^{1D} = 4m\omega L^2/(\hbar\pi^2)$, together with Eq. (9) and Eq. (10), the following spectral situations apply:

- For $(\frac{\pi}{2})^2 < \frac{m\omega L^2}{\hbar}$, there are levels below E_c corresponding to the harmonic oscillator and the particle in a box such that $E_0^{HO} > E_0^{1D}$. The oscillator levels dominate the low energy spectrum.
- For $\frac{\pi}{2} < \frac{m\omega L^2}{\hbar} < (\frac{\pi}{2})^2$, there are only the ground states E_0^{1D} and E_0^{HO} below E_c and $E_0^{1D} > E_0^{HO}$.
- For $1 < \frac{m\omega L^2}{\hbar} < \frac{\pi}{2}$, there is only the ground state of the harmonic oscillator E_0^{HO} below E_c .
- For $0 < \frac{m\omega L^2}{\hbar} < 1$, perturbation theory of a particle in a box should be applicable for all levels.

The dimensionless parameter $\beta = \frac{m\omega L^2}{\hbar}$ thus plays a role similar to the parameter λ in Eq. (1). In our abstract case of Eq. (1), the two limits of H are at $\lambda = 0$ and $\lambda = 1$ with strong mixing at $\lambda = 1/2$. In the case above, the two limits are $\beta = 0$ and $\beta = \infty$ with strong mixing when $1 < \beta < (\pi/2)^2$. In this respect, we can formally relate β to λ using an expression of the form $\lambda = \beta/(\beta + \beta_c)$ where β_c is the value of β in the strong mixing region. For example, one may choose $\beta_c = \pi/2$.

Consider as a numerical illustration of the two-mode spectra the case of $m = \hbar = 1$, $L = \pi/2$ and $\omega = 4$ shown in Fig. 2. With these parameters, Eq. (9) gives $n_{\max}^{HO} = 4.53$. Thus one should see no more than 4 equidistant states. Indeed, in Fig. 2, there are four equidistant energy levels that correspond to a harmonic oscillator spectrum.

With respect to the critical energy E_c , there is a more explicit classification of the spectral structure:

- Perturbed particle in a one-dimensional box spectrum for energies $E \gg E_c$ such that Eq. (7) holds,
- One-dimensional harmonic oscillator spectrum in Eq. (6) for energies $E_c \gg E$ such that Eq. (9) holds,
- Intermediate spectrum for energies $E \approx E_c$.

IV. HILBERT SPACE OF THE BASIS WAVE FUNCTIONS

Before discussing the toy model using an oblique basis, it is instructive to discuss briefly the harmonic oscillator problem in Eq. (5) using the wave functions for a free particle in a one-dimensional box as in Eq. (4); and vice versa, solving the problem of a free particle in a one-dimensional box in Eq. (3) using the wave functions for a particle in the harmonic oscillator potential given in Eq. (6).

Due to the different domains of the wave functions, there are some specific problems that need to be addressed. For example, using wave functions for a free particle in a one-dimensional box to solve the pure harmonic oscillator problem may not be appropriate especially for high energy states $E \gg E_c$. This is because all such functions vanish outside the box (see Fig. 3) unlike the oscillator wave functions, especially as the energy increases. The converse is also problematic because oscillator functions that are non-zero outside the box will lead to infinite energy.

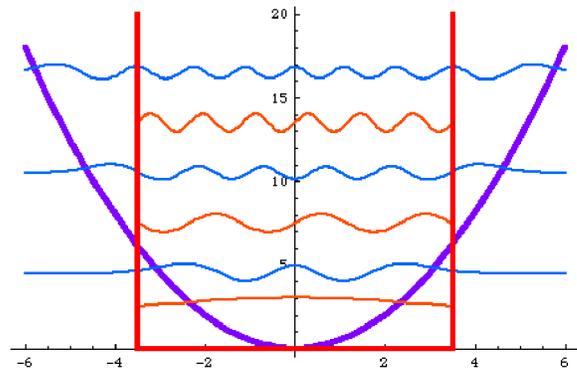


FIG. 3: Spreading of the wave functions: harmonic oscillator wave functions spread outside the harmonic oscillator potential into the classically forbidden region; particle in a box wave functions are zero at and outside of the box boundary.

The influence of the boundary conditions on the properties of a quantum-mechanical system has been recognized from the dawn of quantum mechanics. It is well known that some problems with seemingly separable Hamiltonians may re-couple due to the boundary conditions.²⁴ Some recent studies on the problem of confined one-dimensional systems using equations for relevant cut-off functions have been discussed by Barton, Bray, and Mackane.⁶ Their method has been further developed in a more general setting by Berman.²⁵ Other authors aim at variational procedures using simple cut-off functions^{26,27} or derive asymptotic estimates for multi-particle systems using the Kirkwood-Buckingham varia-

tional method.²⁸ Somewhat different approaches focus on shape-invariant potentials and use supersymmetric partner potentials to derive energy shifts and approximate wave functions,²⁹ as well as dependence of the ground-state energy on sample size.³⁰ In the next few paragraphs, we discuss the structure of the relevant Hilbert spaces when confinement is present.

A. Harmonic Oscillator in the One-Dimensional Box Basis

Consider the harmonic oscillator in Eq. (5) using the wave functions for a free particle in a one-dimensional box in Eq. (4). There are no practical difficulties for energies $E \ll E_c$ as defined in Eq. (8) as long as the turning points of the oscillator are sufficiently deep into the box (sufficiently far from the walls of the box). However, for energies $E \gg E_c$, the basis wave functions are localized only on the interval $[-L, L]$ and thus cannot provide the necessary spread over the width of the potential (Fig. 3). This situation would be appropriate for the toy model in Eq. (2) but not for the pure harmonic oscillator problem in Eq. (5).

One simple solution to the spreading problem is to continue the basis wave functions using periodicity. This way the necessary spread of the basis wave functions can be achieved and the new basis will stay orthogonal but must be re-normalized. If one continues the wave functions to infinity, normalization will require Dirac delta functions but for continuation on a finite interval, the functions can be normalized to unity as usual. However, these basis wave functions do not decay to zero in the classically forbidden zone. This means that a significant number of basis wave functions will be needed to account for the appropriate behavior within the classically forbidden zone.

Another alternative is to change the support domain corresponding to non-zero values of the function by stretching or squeezing, accomplished through a scaling of the argument of the basis wave functions, $x \rightarrow x\alpha_n/L$. This way the support becomes $[-L, L] \rightarrow [-\alpha_n, \alpha_n]$. Here, α_n is a scale factor for the n -th basis wave function in Eq. (4), estimated either from the width of the harmonic oscillator potential, or determined by variational minimization. Either way, the new set of basis functions will be non-orthogonal. In general, there may even be a linear dependence. However, for the basis functions discussed here, linear dependence may not appear due to the different number of nodes for each wave function. The number of nodes (zeros) is not changed under the re-scaling procedure. While the potential width scaling is simpler, its applicability is more limited than the variationally-determined one which can be extended to more general situations.⁵

B. Particle in a Box in the Harmonic-Oscillator Basis

When the choice of the basis is not made with appropriate care, an operator that should be Hermitian may become non-hermitian. In nuclear physics, although this is unlikely for a finite shell-model calculation using an occupation number representation,³¹ it is an obstacle when one wishes to use a hard core potential and a harmonic-oscillator basis.¹⁵

Suppose we want to solve the problem of a free particle in a one-dimensional box $[-L, L]$ as given in Eq. (3) using the harmonic oscillator wave functions in Eq. (6). The first thing to do is to change the inner product of the wave functions:

$$(f, g) = \int_{-\infty}^{\infty} f^*(x) g(x) dx \rightarrow \int_{-L}^L f^*(x) g(x) dx. \quad (11)$$

Then, it is immediately clear that the set of previously orthonormal harmonic oscillator wave functions $\Psi_n(q)$ in Eq. (6) will lose their orthonormality and even their linear independence. The set of functions $\Psi_n(q)$ with support domain restricted to $[-L, L]$ and denoted by $\Psi_n(q; [-L, L])$ become linearly dependent if L is so small that there is more than one function $\Psi_n(q; [-L, L])$ with the same number of nodes within $[-L, L]$. While this linear dependence can be handled, the real problem is the loss of hermiticity of the physically significant operators. Neither the variational nor the potential-width wave function scaling will help to cure the loss of hermiticity of operators, such as those of linear momentum and energy. This non-hermiticity is due to the behavior of the basis states at the boundary, mainly the non-vanishing of the wave functions at $-L$ and L .

To understand the loss of hermiticity, we look at the off-diagonal matrix elements of the momentum operator ($\hat{p} = -i\hbar \frac{\partial}{\partial q}$). After some trivial manipulations, we have:

$$(\Psi_m, \hat{p}\Psi_n) = (\hat{p}\Psi_m, \Psi_n) - i\hbar (\Psi_m^*(q)\Psi_n(q))|_{-L}^L.$$

It is clear from the above expression that *hermiticity will be maintained only when all of the basis functions are zero at the boundary of the interval $[-L, L]$* . Actually, the necessary condition is that the wave functions have the same value at $\pm L$; they need to be zero only for the case of an infinite potential wall.

In our simple example, all operators are built from the momentum operator \hat{p} and position operator \hat{q} . Thus, in order to ensure hermiticity, it is sufficient to make sure that \hat{p} is Hermitian which requires the basis wave functions to vanish at the boundaries $-L$ and L . For this purpose, one can look at the nodes of each basis wave function and scale it so that its outer nodes are at the boundary points. From the nodal structure of the harmonic oscillator wave functions, it is clear that the first two wave functions (Ψ_0 and Ψ_1) cannot be used since they have fewer than two nodes. Since the physical

requirement that the wave functions have to be zero at the boundary is the cornerstone in quantizing the free particle in a one-dimensional box as in Eq. (4), it is not surprising that the nodally adjusted harmonic oscillator wave functions are very close to the exact wave functions for the free particle in a one-dimensional box as shown in Fig. 4.

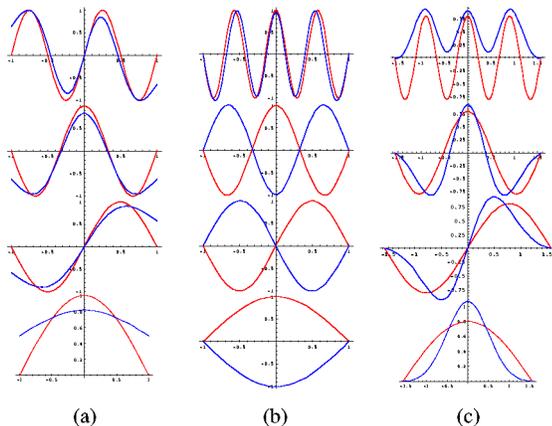


FIG. 4: Harmonic-oscillator trial wave functions (dark gray) adjusted with respect to the one-dimensional box problem: (a) adjusted according to the potential width $E_n^{1D} = \omega_n^2 L^2 / 2 \Rightarrow \omega_n = \frac{\hbar}{L^2} (1 + 2n)$, (b) nodally adjusted (first three are deliberately phase shifted), (c) boundary adjusted using $\Psi(q) \rightarrow \Psi(q) - \Psi(L)(1 + q/L)/2 - \Psi(-L)(1 - q/L)/2$. The exact wave functions (light gray) for a particle in a box are zero at ± 1 , as clearly seen in the (a) graphs.

In general, calculating the nodes of a function may become very complicated. To avoid problems with finding the roots, one can evaluate the wave function at the boundary points, then shift the wave function by a constant to get zeros at the boundary, $\Psi(q) \rightarrow \Psi(q) - \Psi(L)$. This idea works well for even parity wave functions, but has to be generalized for odd parity by adding a linear term, $\Psi(q) \rightarrow \Psi(q) - (\Psi(L)/L)q$. Thus, for a general function, we can have: $\Psi(q) \rightarrow \Psi(q) - (1 + q/L)\Psi(L)/2 - (1 - q/L)\Psi(-L)/2$. In Fig. 4 we have shown some of the resulting wave functions. Notice that this procedure gives a new wave function Ψ that has good behavior inside the interval $[-L, L]$ and grows linearly with q outside the interval $[-L, L]$. This contrasts with the behavior of the cut-off function $f(q)$ obtained by Barton *et al*,⁶ where the function $f(q)$ has an L/q singularity at the origin ($q = 0$). The use of a cut-off function to enforce boundary conditions has been studied by Barton *et al*⁶ and Berman²⁵ and provides an interesting integral equation for the cut-off function. On the other hand, a simple cut-off function supplemented by a variational method seems to be very effective.^{26,27,28}

An alternative, more involved construction can be explored which relies on the Lanczos algorithm. This algorithm is an iterative process that uses the Hamiltonian

of the system to generate a new basis state from the previous state at each iteration. By using the boundary matching process above, one can set up and successfully run a modification of the usual Lanczos algorithm³² to solve for the few lowest eigenvectors of the free particle in a one-dimensional box through an arbitrary, but reasonable, choice of the initial wave function.⁵ The major modification is to project every new function, $\Psi_{n+1} = H\Psi_n$, into the appropriate Hilbert space and subtract the components along any previous basis vectors. Only then should one attempt to evaluate the matrix elements of H related to the new basis vector that is clearly within the correct Hilbert space. This way, one has to double the number of scalar product operations compared to the usual Lanczos algorithm where the matrix elements of H are calculated along with the complete re-orthogonalization of the basis vectors.

C. Oblique Basis for the Two-Mode System

In the previous two subsections we saw that a basis that is appropriate for one mode of our model system, harmonic oscillator in a box, is not appropriate for the other mode. If we desire a description in the critical mixed region characterized by E_c as shown in Fig. 1, a combination of the two basis sets seems appropriate. This is referred to as an oblique basis, stemming from a geometrical analogy. A two-dimensional space is usually described in terms of the Cartesian (x, y) axes or, indeed, in terms of any other orthogonal pair obtained by rotating those axes. While such orthogonal choices are more convenient and familiar, any two axes, as long as they are not linearly dependent, also suffice to describe the space. Such a choice constitutes an ‘‘oblique’’ pair. Similarly, when we mix both harmonic oscillator and particle in a box states, we have an oblique basis.

In using such an oblique basis, there are two main problems to be addressed in order to have a proper Hilbert space of our quantum mechanical system. First, we have to make sure that any set of states that are derived from harmonic oscillator functions satisfies the boundary conditions of the problem. For the particle in a box states the boundary conditions are satisfied by construction. We discussed already a few possible ways to construct states with the correct boundary conditions. An interesting additional method, suggested by one of our referees, would be to use Hermite functions with non-integer index. For such functions with index between n and $n + 1$, the position of the outer node is correspondingly between the outer nodes of the n -th and $(n + 1)$ -th Hermite functions. Second, after the chosen set of functions has been modified to satisfy the boundary conditions, the orthonormality of these functions would most likely be destroyed. Even if the two basis sets are orthonormal by themselves, they would not be orthonormal as a whole and may even be linearly dependent. While this might seem a serious technical problem, it has a well known solution through

re-orthonormalization of the basis or by proceeding with a generalized eigenvalue problem.⁴

Our oblique basis consists of modified harmonic oscillator (MHO) basis states that satisfy the boundary conditions along with basis states of a free particle in a box (BOX). To obtain the wave functions and eigenenergies we solve the generalized eigenvalue problem within this oblique basis. Schematically, these basis vectors and their overlap matrix can be represented in the following way:

$$\begin{aligned} \text{basis vectors} &: \mathcal{E} = \begin{pmatrix} e_\alpha : \text{box} - \text{basis} \\ e_i : \text{mho} - \text{basis} \end{pmatrix}, \\ \text{overlap matrix} &: \Theta = \begin{pmatrix} \mathbf{1} & \Omega \\ \Omega^\dagger & \mu \end{pmatrix} \quad \begin{aligned} \Omega_{\alpha i} &= e_\alpha \cdot e_i, \\ \mu_{ij} &= e_i \cdot e_j, \end{aligned} \\ \text{hamiltonian} &: H = \begin{pmatrix} H_{\alpha\beta} & H_{\alpha j} \\ H_{i\beta} & H_{ij} \end{pmatrix} = \\ &= \begin{pmatrix} H_{\text{box} \times \text{box}} & H_{\text{box} \times \text{mho}} \\ H_{\text{mho} \times \text{box}} & H_{\text{mho} \times \text{mho}} \end{pmatrix}, \end{aligned}$$

where $\alpha = 1, \dots, \dim(\text{box} - \text{basis})$ and $i = 1, \dots, \dim(\text{mho} - \text{basis})$.

In these notation, the eigenvalue problem:

$$Hv = Ev$$

with

$$v = v^\alpha e_\alpha + v^i e_i$$

takes the form:

$$\begin{pmatrix} H_{\alpha\beta} & H_{\alpha j} \\ H_{i\beta} & H_{ij} \end{pmatrix} \begin{pmatrix} v^\beta \\ v^j \end{pmatrix} = E \begin{pmatrix} \mathbf{1} & \Omega \\ \Omega^\dagger & \mu \end{pmatrix} \begin{pmatrix} v^\beta \\ v^j \end{pmatrix}.$$

which is a generalized eigenvalue problem.

V. DISCUSSION OF THE TOY MODEL CALCULATIONS AND RESULTS

Despite the simplicity of the toy model in Eq. (2), the harmonic oscillator in a box exhibits some of the essential characteristics of a more complex system. Some of our interest lies in problems associated with the use of fixed-basis calculations. In particular, one such problem is the slow convergence of the calculations.¹⁹ If one can implement an exact arithmetic, one may not worry too much about the slow convergence when enough time, storage, and other computer resources are provided. However, numerical calculations are plagued with numerical errors so that a calculation that converges slowly may be compromised by accumulated numerical error. Of course, having the correct space of functions is of the utmost importance in any calculation.

Having considered the main problems one may face in studying the simple toy model in Eq. (2), we continue our discussion with the spectrum for the case of $m = \hbar = 2L/\pi = 1$ and $\omega = 4$. As one can see in

Fig. 2, the first three energy levels are equidistant and almost coincide with the harmonic oscillator levels as expected from Eq. (9). For these states, the wave functions are also essentially the harmonic oscillator wave functions. The intermediate spectrum is almost missing. Above E_c , the spectrum is that of a free particle in a one-dimensional box perturbed by the harmonic oscillator potential. We find that an oblique-basis calculation reproduces the lowest eight energy levels using 14 basis functions, seven nodally adjusted harmonic oscillator states and seven states of a free particle in a box. In contrast, a fixed-basis calculation, using only the wave functions of a free particle in a one-dimensional box, requires 18 basis states.

Due to the simplicity of the toy model, it does not appear as if the oblique-basis calculation has a big numerical advantage over calculations using the fixed basis of the box wave functions. There are two main reasons for this: (1) there is a critical energy E_c that separates the two modes, (2) the spectrum above E_c has a nice regular structure.

The regular structure above E_c results in a very favorable situation for the usual fixed-basis calculations since the dimension of the space needed to obtain the n -th eigenvalue grows as $n + \alpha$. The parameter α is relatively small and does not change much in a particular region of interest. For example, the $\omega = 16$ calculations need only $\alpha = 15$ extra basis vectors when calculating any of the eigenvectors up to the hundredth. The relatively constant value of α can be understood by considering the harmonic oscillator potential as an interaction that creates excitations out of the n -th unperturbed box state. Therefore, α is the number of box states with energies in the interval E_n^0 and $E_n^0 + \omega^2/2 \langle \Phi_n | x^2 | \Phi_n \rangle$ where E_n^0 is the n -th unperturbed box state energy. There is a rapid de-coupling of the higher energy states from any finite excitation process that starts out of the n -th state. This de-coupling is due to the increasing energy spacing of the box spectrum which results in a limited number of states mixed by the harmonic oscillator potential. Using the upper limit $E_c/3$ on δE_n^1 , one can estimate $\alpha \approx \frac{1}{\sqrt{3}} n_{\text{max}}^{1D}$.

The sharp separation of the two modes also allows for a safe use of the harmonic oscillator states without any rescaling. This is especially true when ω is very large since then the low energy states are naturally localized within the box. Therefore, instead of diagonalizing the Hamiltonian in a box basis, one can just use the harmonic oscillator wave functions.

Fig. 5 shows the absolute deviation ($\Delta E = E_n^{\text{exact}} - E_n^{\text{estimate}}$) of the calculated energy spectrum for the case of $\omega = 16$, $L = \pi/2$, $\hbar = m = 1$. Here, E_n^{estimate} stands for one of the three energy estimates one can make: the harmonic oscillator E_n^{HO} , particle in a one-dimensional box E_n^{1D} , and the first order perturbation theory estimate considering the harmonic oscillator potential as a perturbation, ($E_n^{1D} + \omega^2/2 \langle \Phi_n | x^2 | \Phi_n \rangle$). There are about 19 states that match the harmonic oscillator spectrum which is consistent with the expected value from Eq. (9).

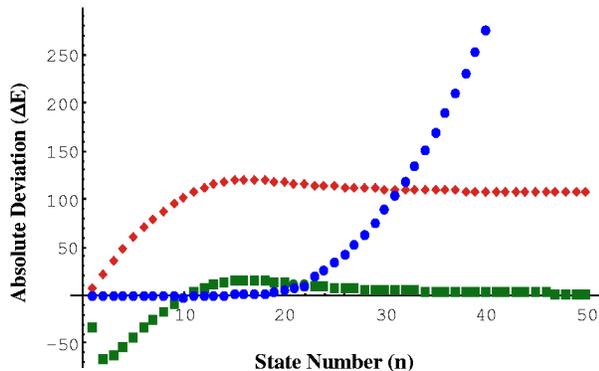


FIG. 5: Absolute deviations of variously calculated energies from the exact energy eigenvalues for $\omega = 16$, $L = \pi/2$, $\hbar = m = 1$ as a function of n . Circles represent deviation of the exact energy eigenvalue from the corresponding harmonic oscillator eigenvalue ($\Delta E = E_n^{exact} - E_n^{HO}$), the diamonds are the corresponding deviation from the energy spectrum of a particle in a box ($\Delta E = E_n^{exact} - E_n^{1D}$), and the squares are the first-order perturbation theory estimates.

After the $n = 20$ level, perturbation theory gives increasingly better results for the energy eigenvalues. Fig. 6 shows the relative deviation $(1 - E_n^{estimate}/E_n^{exact})$.

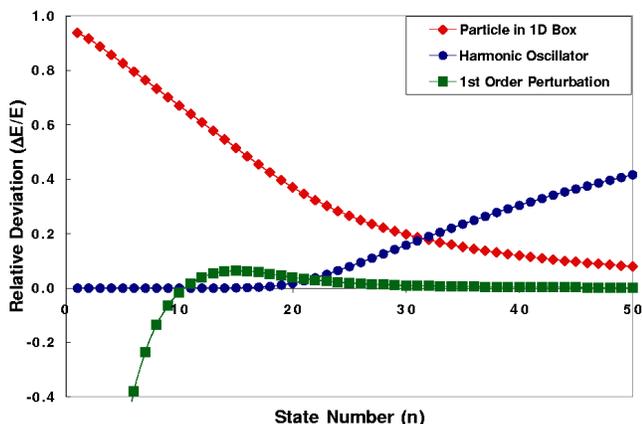


FIG. 6: As in Fig. 5 but for relative deviations from the exact energy eigenvalues of the three calculations.

Note that perturbation theory is valid, as expected, for high energy states determined by Eq. (7). For the high energy spectrum, the harmonic oscillator potential acts as a small perturbation. Thus the first-order corrections in the energy and the wave function are small. Fig. 7 shows that the main component of the 105th exact wave function comes from the 105th box wave function, as it should in a region of small perturbations.

For low energy states, perturbation theory around

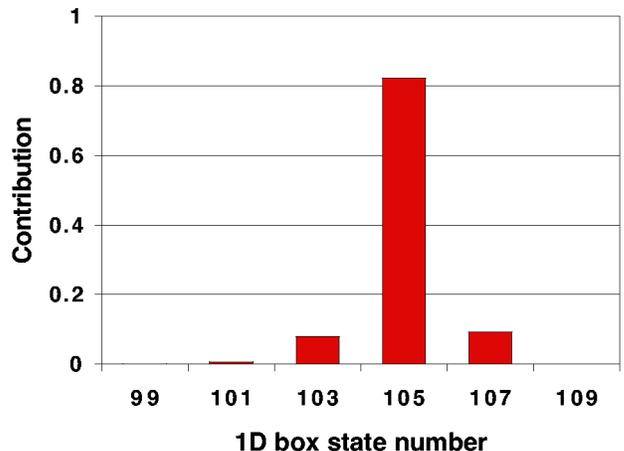


FIG. 7: Non-zero components of the 105th exact eigenvector in the basis of a free particle in a one-dimensional box. Parameters of the Hamiltonian are $\omega = 16$, $L = \pi/2$, $\hbar = m = 1$.

the box states is not appropriate, the harmonic oscillator states being closer to the true states in this region. Specifically, for $m = \hbar = 2L/\pi = 1$ and $\omega = 16$, the first ten states are essentially the harmonic oscillator states to a very high accuracy. The next ten states have still high overlaps with the corresponding harmonic oscillator wave functions. For example, starting from 0.999999 at the tenth state, the overlaps go down to 0.880755 at the twentieth state. After that the overlaps get small very quickly. Fig. 8 shows the structure of the third exact eigenvector when expanded in the box basis. Notice that the third box wave function is almost missing. An explanation lies in the structure of the harmonic oscillator functions, which are essentially exact in this region. Upon projecting these functions in Eq. (6) onto the box functions in Eq. (4), the results can be obtained in closed analytical form. The integrand consists of three factors, an even power of q , a Gaussian and a cosine. While the oscillations of the Hermite polynomial are of varying amplitude, the cosine has evenly spaced nodes and antinodes of equal amplitude. As a result, cancellations can take place between successive terms in the integrand. For the third oscillator function (second of even parity), its one pair of nodes is reflected in the dip seen at $n = 3$ in Fig. 8. Higher oscillator functions with more pairs of nodes can display correspondingly more such dips in the projected squared amplitudes.

This pattern of having a small projection of the exact wave function along the corresponding box wave function continues to persist into the transition region. This may seem unexpected considering the fact that the first order estimates of the energy levels are relatively good. Notice that in our two examples of $\omega = 4$ (Fig. 2) and $\omega = 16$ (Fig. 5), the first order corrections in the transition region are already close to the limiting constant value of $\frac{1}{6}m\omega^2L^2$, even though the corresponding box wave func-

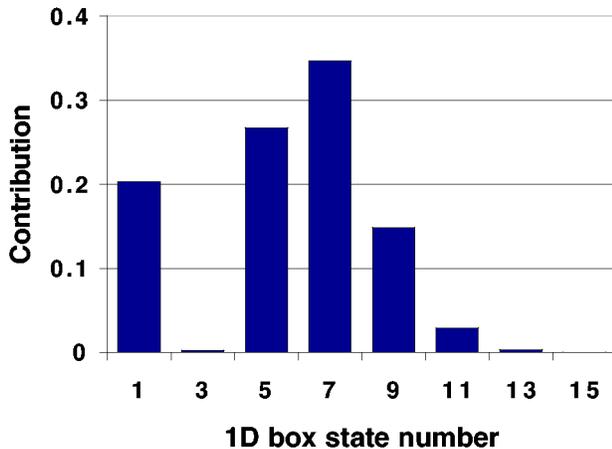


FIG. 8: Non-zero components of the third harmonic oscillator (even parity) eigenvector as expanded in the basis of a free particle in a one-dimensional box. Parameters of the Hamiltonian are $\omega = 16$, $L = \pi/2$, $\hbar = m = 1$.

tions are not present at all in the exact wave function as shown in Fig. 9.

From the results in these graphs, it seems that the transition region is absent since first-order perturbation theory becomes valid immediately after the breakdown of the harmonic oscillator spectrum. That first-order perturbation theory gives good estimates for the energy levels in this transition region is a manifestation of coherent behavior. What actually happens in this region is a coherent mixing of box states by the harmonic oscillator potential in the sense of a quasi-symmetry.^{5,33,34} This coherent mixing is illustrated in Fig. 9, where one can see that the histograms for a few consecutive states are very similar. In this sense we say that the corresponding particle in a box states are coherently mixed. A more precise and detailed discussion of coherent structure, behavior, and quasi-structures can be found elsewhere.⁵

VI. CONCLUSIONS

In summary, we have studied the simplest two-mode system consisting of a one dimensional harmonic oscillator in a one-dimensional box. Depending on the parameters of the two exactly solvable limits, one observes various spectral structures. There is a clear coherent mixing in the transition region. It is remarkable that such a simple system can exhibit coherent behavior similar to the one observed in nuclei. There is clear advantage to using an oblique-basis set which includes both oscillator and particle in a box states. This allows one to use the correct wave functions in the relevant low and high energy regimes relative to E_c . Taking into account the importance of the relevant energy scale of a problem and the wave function localization with respect to

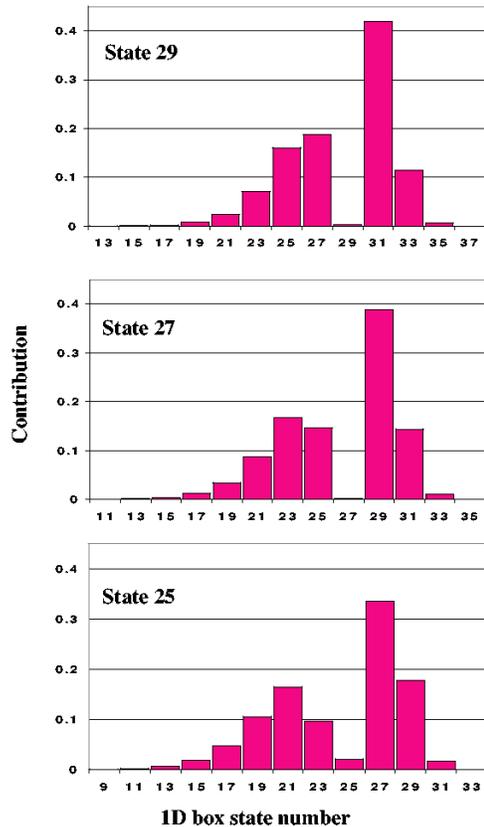


FIG. 9: Coherent structure with respect to the non-zero components of the 25th, 27th and 29th exact eigenvector in the basis of a free particle in a one-dimensional box. Parameters of the Hamiltonian are $\omega = 16$, $L = \pi/2$, $\hbar = m = 1$.

the range of the potential, the oblique-basis method can be extended beyond the idea of using two or more orthonormal basis sets. Specifically, one can consider a variationally-improved basis set by starting with some initially guessed basis states. In the occupation number representation (Fock space), which is often used in the nuclear shell model,³¹ this variationally-improved basis method seems inapplicable. But the method is of general interest because of its possible relevance to multi-shell *ab-initio* nuclear physics, atomic physics, and general quantum mechanical calculations. The method may also be related to renormalization-type techniques.⁵

VII. STUDENT EXERCISES

1. Section II views the two Hamiltonians in Eq. (3) and Eq. (5) as limits of Eq. (2) for suitable choices of parameters. Express this feature instead in the form of Eq. (1) with suitable definition and choice of λ and appropriate modification of ω in Eq. (5).
2. Treating the harmonic oscillator potential as a per-

turbation, work out the first order correction to the energies of particle in a box states. Hence, verify Eq. (7).

3. Project the third harmonic oscillator wave function (second even parity state with two nodes) onto the wave functions of a particle in a box to verify the structure shown in Fig. 8. Integrals involved have products of powers of q , a Gaussian and a cosine in q , and you may take integration limits to $\pm\infty$.
4. As a variational counterpart of the oblique basis concept in this paper, the product of the ground state functions of a particle in a box and an oscillator may be chosen as a trial wave function. With such a form, calculate through the Rayleigh-Ritz variational principle the ground state energy of the

system.

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