



# Solving the two-dimensional Schrödinger equation using basis truncation: A hands-on review and a controversial case

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**Abstract.** Solutions of the Schrödinger equation by spanning the wave function in a complete basis is a common practice in many-body interacting systems. We shall study the case of a two-dimensional quantum system composed of two interacting spinless electrons and see that the correctness of the matrix approach depends inexplicably on the type of interaction existing between particles. Also, we shall extend the present study to other systems of special interest in order to illustrate the method.

**Keywords.** Matrix mechanics; quantum rings; coupled harmonic oscillators.

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## 1. Introduction

A common textbook quantum physics/chemistry approach to solve the Schrödinger equation in those cases where no analytical solution is available is to utilize matrix mechanics [1]. In atomic and molecular electronic structure calculations, it is often important to go beyond the independent-particle approximation, and thus some numerical machinery is required. Many quantum mechanical research problems that are amenable to solution have been solved using matrix mechanics, one good example being, for instance, the study of electrons on a small lattice [2]. Unfortunately, this approach is very unlikely to be found in textbooks, even in books addressed to specialists. The standard procedure for 1D-basis may still be found in some academic books. However, to the best of our knowledge, the equivalent solution of the Schrödinger in 2D using a basis-expansion is virtually not available.

One decomposes the wave function into a complete set of well-known basis states

$$|\psi\rangle = \sum_{i=1}^{\infty} a_i |\psi_i\rangle, \quad (1)$$

where  $a_i$ 's are the unknown coefficients. Inserting this into the time-independent Schrödinger equation, and

performing inner products with the same basis states yields the eigenvalue equation

$$\sum_{j=1}^{\infty} H_{ij} a_j = E a_i, \quad (2)$$

where the matrix elements are given by

$$H_{ij} = \langle \psi_i | H | \psi_j \rangle. \quad (3)$$

Usually, one simply truncates the expansion to include only the low-lying bound states. If the basis is reasonably chosen, a few states are required to provide satisfactory results. We have to mention that some studies [1] have shown that basis set truncation error is of more importance than truncation of the corresponding perturbation series. However, we shall not be dealing with such situation here. One of the goals in the present endeavor will be to extend the previous approach to more basis elements.

In the present contribution we shall tackle the unexplained behaviour of the matrix formalism depending on the Hamiltonian of a problem, as well as illustrating the matrix formalism in 2D for several systems. In §1 we introduce a quasisolvable model Hamiltonian in two dimensions, where two equally charged particles confined in two concentric rings interact via Coulomb

repulsion. In §3 we present the corresponding numerical approach, where the matrix formalism works perfectly well. The introduction of a brand new system possessing analytical solution is done in §4, which constitutes a terrible unexplained failure of the method of basis expansion. The successful extension of the matrix formalism to two interacting quantum harmonic oscillators is illustrated in detail in §5. Finally, some conclusions are drawn in §6.

## 2. The model

We shall provide here a simple system of two interacting spinless electrons. Let us suppose that we have two concentric rings. Electron 1 is located on the inner ring of radius  $R_1$  and electron 2 is located on the outer ring of radius  $R_2$ . Positions are determined by  $\phi_1$  and  $\phi_2$ , respectively. We shall assume  $R_1 \leq R_2$ . The distance between them is given by

$$d(\phi_1, \phi_2) = \sqrt{R_1^2 + R_2^2 - 2R_1R_2 \cos(\phi_1 - \phi_2)}.$$

The corresponding Schrödinger equation with electrons interacting via Coulomb potential reads as

$$-\frac{1}{2R_1^2} \frac{\partial^2}{\partial \phi_1^2} \Psi(\phi_1, \phi_2) - \frac{1}{2R_2^2} \frac{\partial^2}{\partial \phi_2^2} \Psi(\phi_1, \phi_2) + \frac{1}{d(\phi_1, \phi_2)} \Psi(\phi_1, \phi_2) = E \Psi(\phi_1, \phi_2), \quad (4)$$

where  $\phi_i \in [0, 2\pi)$ . The solution is obviously periodic  $\Psi(0, \phi_2) = \Psi(2\pi, \phi_2)$ ,  $\Psi(\phi_1, 0) = \Psi(\phi_1, 2\pi)$ , with  $R_1R_2 \int_0^{2\pi} \int_0^{2\pi} d\phi_1 d\phi_2 |\Psi(\phi_1, \phi_2)|^2 = 1$ . This case is quasi-exactly solvable by using the distance between particles as a new variable [3]. We shall test our numerical procedure with one exact case in order to check the validity of our approach to the problem.

## 3. Numerical approach

One easy way of preserving periodicity is to span the solution  $\Psi(\phi_1, \phi_2)$  on the basis of two non-interacting particles, one in each ring, and then truncate the expansion to  $N + 1$  terms,  $N$  even. That is,

$$\Psi(\phi_1, \phi_2) = \sum_{m=-\frac{N}{2}}^{\frac{N}{2}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} c_{m,n} \frac{1}{2\pi\sqrt{R_1R_2}} e^{im\phi_1} e^{in\phi_2}. \quad (5)$$

Had we considered concentric spheres, we should be dealing with spherical harmonics. Plugging (5) into

(4), multiplying by  $\frac{1}{2\pi\sqrt{R_1R_2}} e^{-ik\phi_1} e^{-il\phi_2}$  and integrating over  $\{\phi_1, \phi_2\}$  gives

$$\sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{l=-\frac{N}{2}}^{\frac{N}{2}} \left[ \left( \frac{m^2}{2R_1^2} + \frac{n^2}{2R_2^2} \right) \delta_{k,m} \delta_{l,n} + \left\langle kl \left| \frac{1}{d} \right| mn \right\rangle - E \delta_{k,m} \delta_{l,n} \right] c_{k,l} = 0, \quad (6)$$

for  $m, n = -\frac{N}{2}, \dots, \frac{N}{2}$ . Let us regard  $H_{klmn}$  the first line in (6). Solving (6) for  $c_{k,l}$  is tantamount to providing an approximate solution to (4) for the ground or excited states, increasing the accuracy when augmenting the number of terms in the expansion  $N + 1$ .

The matrix element in (6) reads explicitly as

$$\left\langle kl \left| \frac{1}{d} \right| mn \right\rangle = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} d\phi_1 d\phi_2 e^{i(m-k)\phi_1} e^{i(n-l)\phi_2} \times \frac{1}{d(\phi_1, \phi_2)}. \quad (7)$$

The set of eqs (6) for  $c_{k,l}$  does not read yet as a standard eigenvalue problem. Usual approaches to matrix quantum mechanics deal with only one quantum number, either because the instances addressed are one-dimensional problems or physical scenarios with higher spatial dimensions but characterized with only one principal quantum number. We have to point out that when this is not the case, not a single textbook explains, to our knowledge, how to proceed.

In order to tackle the problem given by (6), we shall transform  $H_{klmn} \rightarrow A_{ij}$  and  $c_{k,l} \rightarrow g_j$ ,  $i, j = 1, \dots, (N + 1)^2$  using

- $i = (m + \frac{N}{2})(N + 1) + (n + \frac{N}{2}) + 1$ ,
- $j = (k + \frac{N}{2})(N + 1) + (l + \frac{N}{2}) + 1$ ,

$\forall (k, l, m, n)$ . Note that by doing so, the problem significantly increases the effective total dimension of the ensuing eigenvalue problem. Also, it is straightforward to extend the previous linear mapping of indexes to more quantum numbers if required. However, if that was the case, the final computational problem becomes quite involved (the dimension of the final matrix scales with  $(N + 1)^d$ , where  $d$  is the dimension of the problem).

With the previous transformation, we have the usual eigenvalue and eigenvector problem

$$\sum_{j=1}^{(N+1)^2} (A_{ij} - E\delta_{ij}) g_j = 0, \quad (8)$$

and  $i = 1, 2, \dots, (N + 1)^2$ . Finding the corresponding eigenvalues will give the energy spectrum of the system.

**Table 1.** Solution coefficients  $c_{k,l}$  for the analytic case  $R_1 = \frac{13}{7}\sqrt{3(13 - \sqrt{78})}$ ,  $R_2 = \frac{13}{7}\sqrt{3(13 + \sqrt{78})}$ . The numerical ground energy is virtually ‘equal’ to exact energy  $\frac{28}{507}$  (in atomic units). Notice the symmetry in the indexes  $k, l$  and in the numerical value of  $c_{k,l}$ . As we can appreciate, only 11 coefficients  $c_{k,l}$  in the expansion suffice to find the right solution. See text for details.

$k$	$l$	$c_{k,l}$
-5	5	4.52937008E - 005
-4	4	0.000210684568
-3	3	0.00133573123
-2	2	0.0393656555
-1	1	-0.401700424
0	0	0.821078904
1	-1	-0.401700424
2	-2	0.0393656555
3	-3	0.00133573123
4	-4	0.000210684568
5	-5	4.52937008E - 005

In order to find the eigenvectors, the inverse transformation  $g_j \rightarrow c_{k,l}$  can be proved to be unique. In other words, given  $j$  and  $N$ , we find a unique couple  $(k, l)$ . In practice, we have to solve a linear diophantine equation.

In order to validate our numerical results, we can compare them with the analytic case of two concentric rings [3]. Results are shown in table 1. The matching is perfect.

The symmetry in the coefficients has a two-fold meaning: on the one hand, the total truncated state is real, whereas on the other hand, the system depends only on the difference of angles  $|\phi_1 - \phi_2|$ .

The method of spanning the function in a suitable basis proves to be very much convenient. Although numerical, it becomes an exact eigenvalue problem when the number of truncated elements  $N$  tends to infinity.

#### 4. An analytical (and pathological) counterexample

Let us suppose now that our system is not interacting via Coulomb repulsion, but under the action of a harmonic potential between particles. The corresponding Schrödinger equation to solve is thus given by

$$\begin{aligned}
 & -\frac{1}{2R_1^2} \frac{\partial^2}{\partial \phi_1^2} \Psi(\phi_1, \phi_2) - \frac{1}{2R_2^2} \frac{\partial^2}{\partial \phi_2^2} \Psi(\phi_1, \phi_2) \\
 & + \frac{1}{2} \Omega^2 [R_1^2 + R_2^2 - 2R_1 R_2 \cos(\phi_1 - \phi_2)] \Psi(\phi_1, \phi_2) \\
 & = E \Psi(\phi_1, \phi_2). \tag{9}
 \end{aligned}$$

In order to solve (9) analytically, we have to be able to introduce new variables and solve the problem by the method of separation of variables. Let us introduce the variables  $\{\alpha = \phi_1 - \phi_2, \beta = \frac{1}{2}(\phi_1 + \phi_2)\}$ . Furthermore, we shall seek solutions of the form  $\Psi(\phi_1, \phi_2) = u(\alpha)v(\beta)$ . After some calculations, the new Schrödinger equation with respect to variables  $(\alpha, \beta)$  will look like

$$\begin{aligned}
 & -\frac{1}{2} \left( \frac{1}{R_1^2} + \frac{1}{R_2^2} \right) \frac{u''(\alpha)}{u(\alpha)} - \frac{1}{8} \left( \frac{1}{R_1^2} + \frac{1}{R_2^2} \right) \frac{v''(\beta)}{v(\beta)} \\
 & - \Omega^2 R_1 R_2 \cos(\alpha) - \frac{1}{2} \left( \frac{1}{R_1^2} - \frac{1}{R_2^2} \right) \frac{u'(\alpha)}{u(\alpha)} \frac{v'(\beta)}{v(\beta)} \\
 & = \left[ E - \frac{1}{2} \Omega^2 (R_1^2 + R_2^2) \right]. \tag{10}
 \end{aligned}$$

It is plain that the fact of having different radii prevents us from solving the corresponding Schrödinger equation analytically. Nevertheless, we have attempted the matrix solution of the previous problem, although with no analytic result to compare with.

Proceeding as previously, that is, substituting (5) in (9), multiplying by  $\frac{1}{2\pi\sqrt{R_1 R_2}} e^{-ik\phi_1} e^{-il\phi_2}$  and integrating over  $\{\phi_1, \phi_2\}$ , we obtain

$$\begin{aligned}
 & \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{l=-\frac{N}{2}}^{\frac{N}{2}} \left[ \left( \frac{m^2}{2R_1^2} + \frac{n^2}{2R_2^2} \right) \delta_{k,m} \delta_{l,n} \right. \\
 & + \frac{1}{2} \Omega^2 \langle kl | [R_1^2 + R_2^2 - 2R_1 R_2 \cos(\phi_1 - \phi_2)] | mn \rangle \\
 & \left. - E \delta_{k,m} \delta_{l,n} \right] c_{k,l} = 0, \tag{11}
 \end{aligned}$$

which further simplifies into

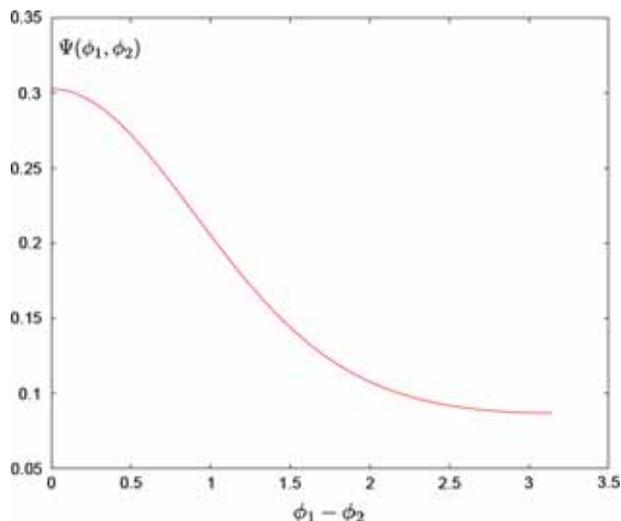
$$\begin{aligned}
 & \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{l=-\frac{N}{2}}^{\frac{N}{2}} \left[ \left( \frac{m^2}{2R_1^2} + \frac{n^2}{2R_2^2} \right) \delta_{k,m} \delta_{l,n} \right. \\
 & - R_1 R_2 \Omega^2 \langle kl | \cos(\phi_1 - \phi_2) | mn \rangle \\
 & \left. - \Lambda_E \delta_{k,m} \delta_{l,n} \right] c_{k,l} = 0, \tag{12}
 \end{aligned}$$

with  $\Lambda_E \equiv E - \frac{1}{2} \Omega^2 (R_1^2 + R_2^2)$ . Matrix elements  $\langle kl | \cos(\phi_1 - \phi_2) | mn \rangle$  are different from zero for special values of the indexes. The ensuing solution via basis truncation has real coefficients, which is tantamount to saying that it depends on  $\phi_1 - \phi_2$ , as is the case. The set of values for the ground state is given in table 2.

The corresponding wave function is depicted in figure 1. We can appreciate that no nodes are attained. The only way of obtaining these nodes by spanning the wave function on the basis of free particles in a quantum ring is when coefficients are such that the sum of the product plane waves returns purely imaginary terms, the sin

**Table 2.** Solution coefficients  $c_{k,l}$  when  $R_1 = 1, R_2 = 2$  for two particles interacting via Hooke's law. See text for details.

$k$	$l$	$c_{k,l}$
-7	7	1.32216148E-007
-6	6	4.21453413E-006
-5	5	9.99675725E-005
-4	4	0.00168284744
-3	3	0.0188339041
-2	2	0.127820814
-1	1	0.460633757
0	0	0.736370591
1	-1	0.460633757
2	-2	0.127820814
3	-3	0.0188339041
4	-4	0.00168284744
5	-5	9.99675725E-005
6	-6	4.21453413E-006
7	-7	1.32216148E-007



**Figure 1.** Ground-state wave function solution to (9) using plane waves. Notice that there are no nodes at 0 or  $\pi$ . See text for details.

circular functions. However, this instance is not reached for some unknown reason.

Let us now return to eq. (10) and solve the equation when both radii are equal, that is,  $R_1 = R_2 = R$ . This makes possible the separation of variables, returning  $v(\beta) = e^{iL\beta}$ , where  $L$  is the angular momentum number ( $L = 0, \pm 1, \pm 2, \dots$ ). After some algebra, the equation for  $u(\alpha)$  reads as

$$u''(\alpha) + \Omega^2 R^4 \cos(\alpha) u(\alpha) + R^2 \left[ E - \Omega^2 R^2 - \frac{L^2}{4R^2} \right] u(\alpha) = 0, \quad (13)$$

with  $\alpha \in [0, \pi]$ . Introducing

$$A = \Omega^2 R^4$$

and

$$B = R^2 \left[ E - \Omega^2 R^2 - \frac{L^2}{4R^2} \right],$$

we obtain an analytic solution, given by

$$u(\alpha) = S\left(4B, -2A, \frac{\alpha}{2}\right), \quad (14)$$

where  $S$  is the sine elliptic odd Mathieu function. For non-zero  $-2A$ , the Mathieu functions are only periodic in  $\alpha$  for certain values of  $4B$ , and this is how the energy is quantized. Such characteristic values are expressed as  $b_{2(n-1)}$ ,  $n$  being a natural number (actually it is the number of nodes in the wave function between 0 and  $\pi$ ). The values of  $b_{2(n-1)}$  depend on  $-2A$ . The final quantized energies for (9)  $E_{n,L}$  will depend, up to the additive constant  $\Omega^2 R^2 + \frac{L^2}{4R^2}$ , linearly on  $b_{2(n-1)}$ . However, because the values of  $b_{2(n-1)}$  for the Mathieu function are not uniquely defined in the literature, we shall, instead, solve the Schrödinger equation (13) numerically, and use the corresponding eigenenergies.

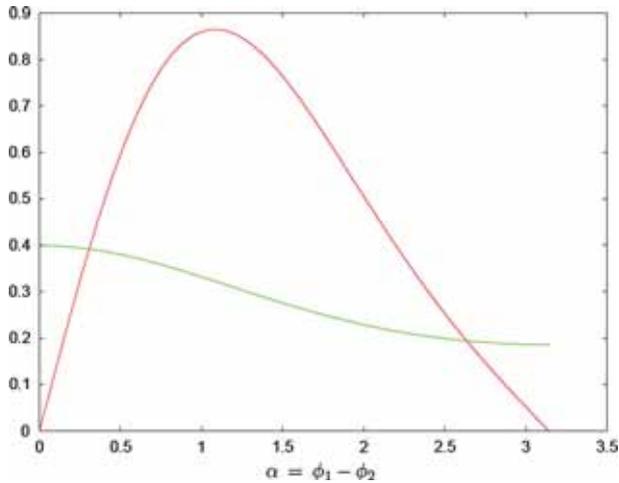
Let us recall that this exact system was considered in the past, and reduces to the case studied in [4], although one can find an equivalent problem in [5].

For the sake of concreteness, let us assume  $R = 1$  and  $\Omega = 1$ . This set of values correspond to the eigenenergies  $E_{n,L} = 1 + \frac{L^2}{4} + \lambda_n$ , where  $\lambda_n$  are the eigenvalues of (13) for that particular choice of parameters. Considering  $L = 0$ -values, we obtain  $E_{n=0,L=0} = 1.3433698\dots$  (atomic units).

Let us suppose now that we want to use our approach using plane waves, which seems to be the most natural choice. As a matter of fact, we just have to replace the Coulomb potential by that of the harmonic oscillator. However, as we shall see now, this approach fails quite dramatically.

First of all, the ground-state energy obtained in this fashion (0.62151077...) does not coincide with the expected one (1.3433698). What is certainly serious is that the matrix approach returns a wave function that has no resemblance whatsoever with the exact one. These features are shown in figure 2. Thus, when  $R_1 = R_2 = R$ , and most certainly in the general case  $R_1 \neq R_2$ , the matrix approach fails in the case of two particles confined in two or the same ring interacting via Hooke's Law.

Thus, having seen how well the truncation basis method works for electrons interacting via Coulomb repulsion as opposed to particles under Hooke's law, it is tantalizing to conclude that spanning the solution to the Schrödinger equation in the natural basis of the concomitant non-interacting system is not enough to ensure the correctness of that solution. However, if we



**Figure 2.** Exact ground-state wave function solution to (13) (upper curve) for  $\Omega = R = 1$ , and closest approach using plane waves (lower curve). Notice the nodes at 0 and  $\pi$ . See text for details.

compare the ground-state wave function obtained via basis truncation ‘and’ the exact one for the hypersphere when  $R_1 = R_2 = R$ , which is analytic [4] as well, they have exactly the same behaviour, with no nodes at either  $\alpha = 0$  or  $\pi$ . In other words, the matrix approach indeed works for a specific dimension of the problem (see ref. [4]), but not for others.

Therefore, we can appreciate an anomaly as far as matrix quantum mechanics is concerned when regarding systems interacting via Hooke’s law. The plane-wave approximation seems to be valid only for Coulomb interaction, but not for the harmonic oscillator unless we go to a specific dimension (concentric hyperspheres), where the approach becomes exact.

### 5. Two models for two coupled quantum harmonic oscillators

We have seen that the case of two charges confined in two concentric rings, and interacting via a harmonic potential, is not amenable to be solved analytically. There, our matrix approach provided a result that could not be compared with the analytic ones. However, when we considered the two rings to be the same, we were providing a framework where results were known exactly, yet our matrix approach failed again. This is a serious failure, as opposed to the case where the two particles interacted via Coulomb repulsion, where analytical and numerical results greatly coincide.

In order to get a better understanding of the situation, we shall now consider how well the matrix approach works when we have a system of two coupled quantum

harmonic oscillators, while at the same time using the set of basis states of two independent harmonic oscillators (in the following, and for all the cases, we shall use 15 terms in the concomitant expansion).

#### 5.1 Real coupling $\gamma xy$

The Hamiltonian under consideration shall be given by

$$H^\gamma(x, y) = -\frac{1}{2}\partial_x^2 + \frac{1}{2}x^2 - \frac{1}{2}\partial_y^2 + \frac{1}{2}y^2 + \gamma xy, \tag{15}$$

where  $\gamma$  is a real-valued coupling constant. We can convert Hamiltonian into a sum of two independent terms if we perform the usual map  $\{X \rightarrow \frac{x+y}{\sqrt{2}}, Y \rightarrow \frac{x-y}{\sqrt{2}}\}$ . In these new variables, the Hamiltonian now reads as

$$H^\gamma(X, Y) = -\frac{1}{2}\partial_X^2 + \frac{1}{2}(1+\gamma)X^2 - \frac{1}{2}\partial_Y^2 + \frac{1}{2}(1-\gamma)Y^2. \tag{16}$$

Obviously, the system now looks like two different quantum harmonic oscillators with different frequencies,  $\omega_X = \sqrt{1+\gamma}$  and  $\omega_Y = \sqrt{1-\gamma}$ . The solution of the Schrödinger equation will return a set of eigenvalues given by

$$E^\gamma(m, n) = \sqrt{1+\gamma} \left(m + \frac{1}{2}\right) + \sqrt{1-\gamma} \left(m + \frac{1}{2}\right), \tag{17}$$

corresponding to the following eigenstates:

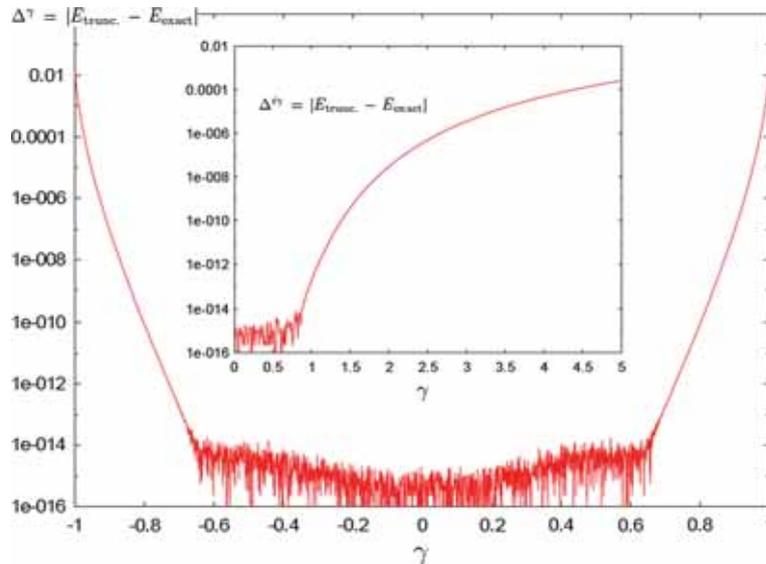
$$\begin{aligned} \Psi(X, Y)_{m,n} &= (2^m m! 2^n n! \pi)^{-\frac{1}{2}} (\omega_X \omega_Y)^{\frac{1}{4}} \\ &\times e^{-\frac{1}{2}\omega_X X^2} e^{-\frac{1}{2}\omega_Y Y^2} \\ &\times H_m(\sqrt{\omega_X} X) H_n(\sqrt{\omega_Y} Y), \end{aligned} \tag{18}$$

where  $H_u(\cdot)$  are the usual Hermite polynomials. In the original coordinates  $(x, y)$ , the eigenfunctions will read as

$$\begin{aligned} \Psi(x, y)_{m,n} &= (2^m m! 2^n n! \pi)^{-\frac{1}{2}} (1-\gamma^2)^{\frac{1}{4}} \\ &\times e^{-\frac{1}{4}\Delta_1(x^2+y^2)} e^{-\frac{1}{2}\Delta_2 xy} \\ &\times H_m(\sqrt{1+\gamma}(x+y)/\sqrt{2}) \\ &\times H_n(\sqrt{1-\gamma}(x-y)/\sqrt{2}), \end{aligned} \tag{19}$$

with  $\Delta_1 \equiv \sqrt{1+\gamma} + \sqrt{1-\gamma}$  and  $\Delta_2 \equiv \sqrt{1+\gamma} - \sqrt{1-\gamma}$ . Obviously, the system will possess real energies for the range  $\gamma \in [-1, 1]$ , but still for  $\gamma > 1$ , although having complex energies, the states (19) will be normalizable (as opposed to  $\gamma < -1$ ).

In this fashion, we can apply the matrix approach to the Hamiltonian  $H^\gamma(x, y)$  (15) for the interval  $\gamma \in [-1, 1]$ , where everything will be real and for  $\gamma > 1$ , where we shall deal with complex numbers.



**Figure 3.** Plot of the difference between the exact and matrix approach ground-state energies, in absolute value, vs. the coupling parameter  $\gamma$ , that is,  $\Delta^\gamma = |E_{\text{trunc.}} - E_{\text{exact}}|$ . The inset depicts the equivalent quantity for the complex interaction, that is,  $\Delta^{i\gamma} = |E_{\text{trunc.}} - E_{\text{exact}}|$ . In both cases, the irregular regions are due to numeric precision. See text for details.

The trial function we shall use will be given by  $|\psi(x, y)\rangle = \sum_{m,n} c_{m,n} |\phi_m(x)\rangle |\phi_n(y)\rangle$ , where  $\{\phi_u(z)\}$  are the usual normalized basis of the one-dimensional quantum harmonic oscillator (with  $\omega = 1$ ). As mentioned, we expect coefficients  $c_{m,n}$  to be real for  $\gamma \in [-1, 1]$ , and complex for  $\gamma > 1$ .

It is mandatory to compute the matrix elements  $H_{klmn}^\gamma \equiv \langle k l | H^\gamma(x, y) | m n \rangle$  in the normalized basis of the one-dimensional quantum harmonic oscillator. After some algebra, we obtain

$$H_{klmn}^\gamma = (m + n + 1) \delta_{k,m} \delta_{l,n} + \gamma \frac{1}{4} \sqrt{m+k+1} \sqrt{n+l+1} \delta_{|m-k|,1} \delta_{|n-l|,1}. \quad (20)$$

The matrix solution to Hamiltonian (15) now proceeds as follows. Because the indices in the quantum harmonic oscillator basis start from 0, we have to solve the following equation:

$$\sum_{k=0}^N \sum_{l=0}^N [H_{klmn}^\gamma - E \delta_{k,m} \delta_{l,n}] c_{k,l} = 0, \quad (21)$$

for  $m, n = 0, \dots, N$ , that is, a total of  $N + 1$  terms.

In order to tackle the solution as an eigenvalue problem, we shall transform  $H_{klmn} \rightarrow A_{ij}$  and  $c_{k,l} \rightarrow g_j$ ,  $i, j = 1, \dots, (N + 1)^2$  using

- $i = m(N + 1) + n + 1$ ,
- $j = k(N + 1) + l + 1$ ,

$\forall (k, l, m, n)$ . Notice that the transformation of indices slightly differs from that of the problem tackled in §3.

With the previous transformation, we have the usual eigenvalue and eigenvector problem

$$\sum_{j=1}^{(N+1)^2} (A_{ij} - E \delta_{ij}) g_j = 0, \quad (22)$$

and  $i = 1, 2, \dots, (N + 1)^2$ . Again, finding the corresponding eigenvalues will give the energy spectrum of the system. Also, in order to find the eigenvectors, we apply the inverse transformation  $g_j \rightarrow c_{k,l}$ .

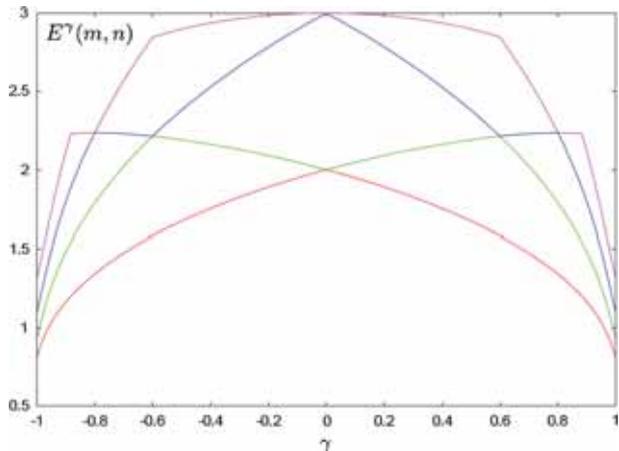
*Ground-state energy vs.  $\gamma$*

The corresponding results match completely with the analytic exact ones. In figure 3 we depict the difference between the exact and matrix approach ground-state energies, in absolute value, vs. the coupling parameter  $\gamma$ , that is,  $\Delta^\gamma = |E_{\text{trunc.}} - E_{\text{exact}}|$ . In most of the region  $\gamma \in [-1, 1]$ , a total of 15 terms suffices to reproduce the exact values. The approach may require two terms in the vicinity of  $|\gamma| = 1$ . Although the wave functions are not shown, the coincidence is also perfect.

*Excited-state energies vs.  $\gamma$*

Obviously, the matrix approach to quantum physics also provides, in the same procedure, those excited states and their energies. The first four excited states are depicted in figure 4. The changing nature either horizontally or vertically is due to two reasons: (i) for a fixed value of  $\gamma$ , the spectrum depends on the two principal quantum numbers  $(m, n)$  and (ii) the variation of the parameter  $\gamma$  itself.

Summing up, we have seen that the matrix approach in the case of two interacting quantum harmonic oscillators



**Figure 4.** Plot of the first four computed excited state energies vs. the coupling parameter  $\gamma$  for the Hamiltonian (15). The coincidence with exact results is perfect. See text for details.

works perfectly well. Recall that in this case, we are no longer using plane waves, because a more obvious basis set is mandatory.

In order to illustrate the accuracy of our results, we can extend the previous two interacting quantum harmonic oscillators study by just mapping the coupling constant to the set of complex numbers, that is,  $\gamma \rightarrow i\gamma$ . The ensuing Hamiltonian will no longer be Hermitian, though. However, very interesting features will appear, as we shall see.

The new Hamiltonian shall read as

$$H^{i\gamma}(x, y) = -\frac{1}{2}\partial_x^2 + \frac{1}{2}x^2 - \frac{1}{2}\partial_y^2 + \frac{1}{2}y^2 + i\gamma xy. \tag{23}$$

### 5.2 Complex coupling $i\gamma xy$

If we allow the original model to hold for a purely complex interaction, we simply have to replace  $\gamma$  by  $i\gamma$  in the original results for the wave function and energy spectrum, and expand. Let us consider the new set of eigenenergies

$$E^{i\gamma}(m, n) = \sqrt{1+i\gamma} \left(m + \frac{1}{2}\right) + \sqrt{1-i\gamma} \left(n + \frac{1}{2}\right). \tag{24}$$

Now, taking into account the following relations

$$\begin{aligned} \sqrt{1+i\gamma} &= \sqrt{1+\gamma^2} \cos \frac{\tan \gamma}{2} \\ &\quad + i\sqrt{1+\gamma^2} \sin \frac{\tan \gamma}{2}, \\ \sqrt{1-i\gamma} &= \sqrt{1+\gamma^2} \cos \frac{\tan \gamma}{2} \end{aligned}$$

$$\begin{aligned} &-i\sqrt{1+\gamma^2} \sin \frac{\tan \gamma}{2}, \\ \cos \frac{\tan \gamma}{2} &= \left(\frac{1}{2} + \frac{1}{2}\sqrt{1+\gamma^2}\right)^{\frac{1}{2}} / \sqrt{1+\gamma^2}, \\ \sin \frac{\tan \gamma}{2} &= \left(-\frac{1}{2} + \frac{1}{2}\sqrt{1+\gamma^2}\right)^{\frac{1}{2}} / \sqrt{1+\gamma^2}, \end{aligned} \tag{25}$$

and collecting all terms, we can express the spectrum (24) as a real and complex contribution

$$\begin{aligned} E^{i\gamma}(m, n) &= \left(\frac{1}{2} + \frac{1}{2}\sqrt{1+\gamma^2}\right)^{\frac{1}{2}} (m + n + 1) \\ &\quad + i \left(-\frac{1}{2} + \frac{1}{2}\sqrt{1+\gamma^2}\right)^{\frac{1}{2}} (m - n). \end{aligned} \tag{26}$$

Remarkably, we expect the system represented by the Hamiltonian (23) to have *real* eigenenergies whenever  $m = n$ . As a matter of fact, Hamiltonian  $H^{i\gamma}(x, y)$  (23) has been recently studied in [6] in the context of several coupled quantum harmonic oscillators. It is a system that possesses partial  $\mathcal{PT}$  symmetry, that is, it is invariant under  $i \rightarrow -i$  (time reversal),  $x_j \rightarrow -x_j$  ( $j$  odd) and  $x_j \rightarrow x_j$  ( $j$  even). What is interesting is that with the same analytic effort in studying the real case with  $\gamma xy$ -interaction, we obtain ‘exactly’ the same results as in ref. [23] for the extension to  $i\gamma xy$ .

Knowing the previous results analytically, we can now proceed to compute the eigenstates and eigenvalues using the matrix approach, bearing in mind that the coefficients in the expansion of the state on the basis of two independent quantum harmonic oscillators will now be complex, as well as the eigenenergies themselves in some particular instances.

#### Ground-state energy vs. $\gamma$

In the case of the ground state, the energy is real. The corresponding results match completely with the analytic exact ones in the complex case  $H^{i\gamma}$ . In figure 3 we depict in the inset the difference between the exact and matrix approach ground-state energies, in absolute value, vs. the coupling parameter  $\gamma$ , that is,  $\Delta^{i\gamma} = |E_{\text{trunc.}} - E_{\text{exact}}|$ . In most of the region  $\gamma \in [0, 1]$ , a total of 15 terms suffices to reproduce the exact values. The approach may require more terms as  $|\gamma|$  becomes large. Also, although the wave functions are not shown, the coincidence is indeed remarkable.

## 6. Conclusions

We have presented two simple yet non-trivial quantum physics systems where the nature of the Hamiltonian defines whether the matrix formalism is correct or not.

By definition, spanning the solution of the Schrödinger equation in a complete basis is an exact problem, regardless of the Hamiltonian involved. In the present contribution we provide an example of a system where the correctness of the formalism works well for a Coulomb interaction, whereas for a harmonic oscillator type it does not reach any satisfactory solution. This problem has interesting echoes not only in unveiling the details of the matrix formalism in quantum physics with more than one particle, but also in the fact that there exists an inconsistency which cannot be accounted for. Incidentally, the counterexample provided constitutes a new system not considered previously in the past. It is imperative to stress the fact that no errors due to truncation have to be considered because the approximation is extremely accurate.

In order to illustrate the matrix formalism, two additional exactly-solvable Hamiltonians have been considered, where a coupling between two particles can be real or complex. We have shown that the matrix formalism works perfectly well in the chosen natural basis of two independent quantum harmonic oscillators.

In the light of the results obtained, there is no way to explain why a system of two particles confined in concentric circles, where the choice of plane waves for the set of basis is not suspicious at all, is not amenable to be tackled using the matrix approach. That is, the approximation fails when they interact via Hooke's Law, while it works perfectly well for the Coulomb interaction.

We believe that the present contribution, besides providing a thorough study of the matrix approach in 2D problems, sheds new light on the potential constraints that the aforementioned formalism may have, which arise depending on the nature of the interaction.

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