Dialling up Energy Point Spectra in Polynomial Quantum Harmonic Oscillators and Violation of the Sturm-Liouville Nodal Ordering Theorem

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Harmonic quantum oscillators are building blocks of quantum theory, particularly field theory. Here I show that a polynomial of degree $N$ of a harmonic oscillator Hamiltonian allows us to devise a fully solvable continuous quantum system for which the first $N$ discrete energy eigenvalues can be chosen at will. In general such a choice leads to a re-ordering of the associated energy eigenfunctions such that the number of their nodes does not increase monotonically with increasing level number.

For continuous quantum systems it is generally hard to work out their energy spectrum, and given an energy spectrum, it is generally hard to write down a Hamiltonian of a continuous system with that spectrum.

It is therefore noteworthy that a finite arbitrary point spectrum of $N$ real values can always be assigned a continuous one-dimensional quantum system’s Hamiltonian $\hat{H}(\hat{x}, \hat{p})$, with this spectrum as its first $N$ energy eigenvalues. This is shown here by explicit construction of a Hamiltonian using real polynomials $\mathcal{P}(\hat{h})$ of $N$-th degree of the harmonic quantum oscillator Hamiltonian $\hat{h}(\hat{x}, \hat{p})$.

Hamiltonians of this or similar form arise as effective descriptions of fields [1], oscillating beams [2], nano-oscillators [3] and Kerr-oscillators [4–6].

Interestingly, Hamiltonians of the form $\mathcal{P}(\hat{h})$ violate the Sturm-Liouville rule for regular quantum mechanical Hamiltonians $[\hat{H}_{reg} = \frac{\hat{p}^2}{2m} + V(\hat{x})]$ of one-dimensional bound state systems according to which the ground state $\phi_0$ has no node and excited states $\phi_n$ have $n$ nodes.

The dimensionless harmonic oscillator Hamiltonian is

$$\hat{h} = \hat{b}^\dagger \hat{b} + \frac{1}{2} = \hat{n} + \frac{1}{2} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}, \quad (1)$$

where I set Planck’s reduced constant $\hbar$, the spring constant and mass of the oscillator all equal to ‘1’. The bosonic creation operator $\hat{b}^\dagger$ and annihilation operator $\hat{b}$ in Eq. (1) fulfill the commutation relation $[\hat{b}, \hat{b}^\dagger] = 1$ and form the number operator $\hat{b}^\dagger \hat{b} = \hat{n}$. The associated position and momentum operators are, respectively, $\hat{x} = \frac{1}{\sqrt{2}} (\hat{b}^\dagger + \hat{b})$ and $\hat{p} = \frac{i}{\sqrt{2}} (\hat{b}^\dagger - \hat{b})$.

The harmonic oscillator eigenfunctions are

$$\phi_n(x) = \langle x|n \rangle = \langle x| (\frac{\hat{b}^\dagger)^n}{\sqrt{n!}} |0\rangle = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{x^2}{2}} \eta_n(x), \quad (2)$$

where $\eta_n$ are the Hermite polynomials.

Now, form the Hamiltonian $\hat{H}$ using a polynomial $\mathcal{P}$ with real coefficients $a_j$ of the form

$$\hat{H} \equiv \mathcal{P}(\hat{h}) = \sum_{j=1}^{N} a_j \hat{h}^j. \quad (3)$$

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FIG. 1. Spectrum and energy eigenstates. (a), the first nine energy eigenvalues of the harmonic oscillator $h_n = n + \frac{1}{2}$ for $n = 0, 1, 2, \ldots, 8$ are mapped via the polynomial $\mathcal{P}(\xi) = \xi^2 - \frac{\xi}{2}$ to $E_n = \mathcal{P}(h_n)$. This map changes the order of the values $E_n$ such that the state with index $n = 3$ has the lowest eigen-energy $E_3 = -\frac{5}{2}$. (b), the corresponding states are displayed together with the cross-section $\mathcal{P}(\frac{1}{2}x^2) = H(x, 0)$ of the Hamiltonian and with their ordinate off-set by $E_n$.

The associated classical Hamiltonian $H(x, p) = \mathcal{P}(\frac{r^2}{2})$ is a function of $r = \sqrt{x^2 + p^2}$ alone.

Since $\hat{H}$ and $\hat{h}$ commute they share the eigenfunctions $\phi_n$, but their energy spectra, $h_n = n + \frac{1}{2}$ of $\hat{h}$, and

$$E_n \equiv \langle \phi_n | \hat{H} | \phi_n \rangle = \mathcal{P}(h_n) \quad (4)$$

of $\hat{H}$, differ from each other in magnitude and can additionally be out of order:

$E_n$ can be greater than or equal to $E_{n+1}$.

Such a violation of the Sturm-Liouville ordering rule for wavefunction nodes seems not to have been reported before (Berry and Mondragon did however notice that degeneracies can occur for 1D-systems which are quartic in momentum [2]).

For $H = -\frac{\hbar^2}{2m} \hat{h} + \hat{h}^2$, this ordering violation is demonstrated in Fig. 1; although this case is discussed in Ref. [5] the reordering is not mentioned there either.

I now show that we can dial up an arbitrary real point spectrum for the $N$ first energy eigenstates of $\hat{H}$. By ‘first’ I mean the entries of the column-vector $E = [E_0, E_1, \ldots, E_{N-1}]^T$ of Eq. (4). These are in general not the lowest lying energy values.

Rewriting Eq. (3) in a suitable matrix form is achieved by casting the energy values of $\hat{h}^j$ into the form of a
square $N \times N$ ‘energy-matrix’ $[\epsilon^{(N)}]_{n,j} = (h_n)^j$. The coefficient column-vector $\mathbf{a} = [a_1, a_2, ..., a_N]^\top$ then, according to Eq. (3), obeys $\mathbf{E} = \epsilon \cdot \mathbf{a}$ where the dot stands for matrix multiplication.

For instance, $\epsilon^{(5)}$ has the form

$$\epsilon^{(5)} = \begin{bmatrix}
1 & 1/4 & 1/8 & 1/16 & 1/32 \\
3 & 27 & 81 & 243 & 125 \\
5 & 125 & 625 & 3125 & 50 \\
7 & 343 & 2401 & 6561 & 500 \\
9 & 729 & 6561 & 59049 & 500 \\
\end{bmatrix}. \tag{5}$$

The determinant $|\epsilon^{(N)}| = \prod_{g=1}^{N-1} [g!(2g + 1)]/2^N$ is non-zero, hence, $\epsilon^{(N)}$ can always be inverted.

In other words, the column vector $\mathbf{E}$, containing $N$ desired energy values, does uniquely specify the polynomial’s coefficient vector $\mathbf{a}$ and thus the Hamiltonian $\hat{H}$, with this spectrum for its first $N$ eigenfunctions.

One is free to generalise this approach, for example, by assigning energy values to only some eigenfunctions $\phi_n$. To this end one can strip out the $m$-th entry in $\mathbf{E}$ together with the $m$-th row in $\epsilon$ thus removing an assignment for an ‘unwanted’ state $\phi_m$ [whose value would still be assigned implicitly through Eq. (4)]. One then also has to strip out one column of $\epsilon$ (together with the associated entry in $\mathbf{a}$) to keep $\epsilon$ invertible. This column could, e.g., be the last $(N$-th) column in which case the polynomial $P$ would be reduced by one order.

Hamiltonians of the form $\hat{H} = \mathcal{P}(\hat{h})$ have special dynamical features. Their phase space current follows circles concentric to the phase space origin; for a proof see the Appendix of Ref. [6].

To conclude, I have identified a class of one-dimensional continuous quantum systems that feature energy point spectra which can be dialled up at will. Owing to the occurrence of high orders in momenta, the eigenfunctions of these point spectra are out of order with respect to the number of nodes associated with level numbers (Sturm-Liouville ordering).

It will be interesting to see whether the approach presented here can be generalised to systems with continuous spectra.

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