On the derivation of the discrete energy levels of the quantum mechanical harmonic oscillator

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Abstract

The aim of this paper will be to provide an alternative derivation of the, crucially discrete, energy levels of the quantum mechanical harmonic oscillator. In line with Ehrenfest's Theorem, an expression will be obtained for the time derivative of the expectation value each power of the position operator X, and each power multiplied by the momentum operator P. These expressions can in turn be written in terms of the expectation values of powers of X, potentially multiplied by the P only. Thus the time derivative can be represented by matrix. The determinant of this matrix vanishes for states satisfying the time–independent Schrödinger Equation and from taking the determinant as a function of the energy of the system an expression for the discrete allowed energies can be obtained.

1 Introduction

1.1 Outline

The remainder of this paper is organised as follows. In section 2 an expression will be obtained for the time derivative of the expectation value of all powers of X, and potentially multiplied by P. In the latter case, the expectation value of a second power of P multiplied with X will appear. This second power of P will then be written as the difference between the Hamiltonian and the potential. In section 3 a vector is defined that contains all of these expectation values. The time derivative can then be represented by a matrix Λ, and its zero eigenvalues correspond to states satisfying the time–independent Schrödinger Equation. In section 4 an expression for the determinant of a reduced version of Λ is obtained by defining submatrices. Finally, in section 5 it will be shown that, using numerical tools, energy levels can be obtained for versions of Λ that are large, but not infinite.

1.2 Preliminaries

We will look at the time derivative of expectation values in quantum mechanics. In the X–basis, we have that

$$\begin{aligned}
\langle A\rangle &= \int d^3\mathbf{x}\bar{\psi}A\psi \\
\frac{\partial}{\partial t}\langle A\rangle &\equiv \frac{\partial}{\partial t}\langle\psi|A|\psi\rangle = \frac{\partial}{\partial t}\int dx\langle\psi|x\rangle\langle x|A|\psi\rangle \\
&= \int d^3\mathbf{x}\left(\frac{\partial}{\partial t}\bar{\psi}\right)A\psi + \bar{\psi}A\left(\frac{\partial}{\partial t}\psi\right) \\
&= \int d^3\mathbf{x}\left(\bar{\psi}\frac{i}{\hbar}HA\psi - \frac{i}{\hbar}\bar{\psi}AH\psi\right) \qquad (1)
\end{aligned}$$

Where we assume ψ of the form $\psi = \exp(\frac{i}{\hbar}Ht)$.

$$\frac{\partial}{\partial t}\langle A\rangle = \frac{i}{\hbar}\langle[H,A]\rangle \qquad (2)$$

2 Position and Moments

2.1 Position

For particular cases this can be worked out:

$$\begin{aligned}
\frac{\partial}{\partial t}\langle X^n\rangle &= \frac{i}{\hbar}\langle[H,X^n]\rangle \\
&= \frac{i}{2m\hbar}\langle[P^2,X^n]\rangle \\
&= \frac{i}{2m\hbar}\langle P[P,X^n]+[P,X^n]P\rangle \qquad (3)
\end{aligned}$$

Here we assume that the Hamiltonian consists in a P–dependence of, generally, the form $\frac{1}{2m}P^2$ and otherwise contains only terms commuting with X. We can elaborate on the commutator:

$$\begin{aligned}
[P,X^n] &= X[P,X^{n-1}] + [P,X]X^{n-1} \\
&= X^{n-1}[P,X^1] + i\hbar(n-1)X^{n-1} \\
&= \left\{\begin{array}{ll} 0 & n=0 \\ -i\hbar nX^{n-1} & n>0 \end{array}\right\} = -i\hbar nX^{n-1} \qquad (4)
\end{aligned}$$

The case $n=0$ will vanish by itself, since n appears as a factor in the expression, so equation 4 is general for nonnegative n. Interestingly, we can see that this expression is exactly $[P,X^n] = -i\hbar\frac{\partial}{\partial X}X^n$.

So for $n > 0$ we can expand equation 3.

$$\begin{aligned}
\frac{\partial}{\partial t}\langle X^n\rangle &= \frac{-i^2\hbar n}{2m\hbar}\langle PX^{n-1} + X^{n-1}P\rangle \\
&= \frac{n}{2m}\langle\{P, X^{n-1}\}\rangle \qquad (5)
\end{aligned}$$

Here the notation for the *anticommutator* of A and B is $\{A, B\} \equiv AB + BA$ and it is not to be confused with the Poisson brackets. We also see the expected result, for $n = 1$, that $\frac{\partial}{\partial t}\langle X\rangle = \frac{1}{2m}\langle 2P\rangle = \frac{\langle P\rangle}{m}$, in line with Ehrenfest's theorem.

We can, in the light of what is to come, elaborate on this anticommutator a bit more:

$$\begin{aligned}
\{P, X^{n-1}\} &= PX^{n-1} + X^{n-1}P = 2PX^{n-1} + [X^{n-1}, P] \\
&= \begin{cases} 2PX^{n-1} = 2P & n = 1 \\ 2PX^{n-1} + i\hbar(n-1)X^{n-2} & n > 1 \end{cases} \\
&= 2PX^{n-1} + i\hbar(n-1)X^{n-2} \qquad (6)
\end{aligned}$$

The case $n = 0$ is irrelevant, since the anticommutator will not appear at all then. The case $n = 1$ simplifies to only the first term appearing, since the second term vanishes due to the factor $(n - 1)$.

Then, for $n > 1$ equation 5 becomes:

$$\frac{\partial}{\partial t}\langle X^n\rangle = \frac{n}{m}\langle PX^{n-1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle X^{n-2}\rangle \qquad (7)$$

In conclusion, the time evolution of $\langle X^n\rangle$ is given by

$$\begin{aligned}
\frac{\partial}{\partial t}\langle X^n\rangle &= \begin{cases} 0 & n = 0 \\ \frac{1}{m}\langle P\rangle & n = 1 \\ \frac{n}{m}\langle PX^{n-1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle X^{n-2}\rangle & n > 1 \end{cases} \\
&= \frac{n}{m}\langle PX^{n-1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle X^{n-2}\rangle \qquad (8)
\end{aligned}$$

2.2 Moments

Likewise, the following can be calculated:

$$\begin{aligned}
\frac{\partial}{\partial t}\langle PX^n\rangle &= \frac{i}{\hbar}\langle[H, PX^n]\rangle \\
&= \frac{i}{\hbar}\langle\frac{1}{2m}[P^2, PX^n] + [V(X), PX^n]\rangle \qquad (9)
\end{aligned}$$

Taking a look at the first term, which is

$$\begin{aligned}
\frac{1}{2m}[P^2, PX^n] &= \frac{1}{2m}(P[P, PX^n] + [P, PX^n]P) \\
&= \frac{-i\hbar n}{2m}(PPX^{n-1} + PX^{n-1}P) \\
&= \frac{-i\hbar n}{2m}P\{P, X^{n-1}\}, \qquad (10)
\end{aligned}$$

where I used that $[P, PX^n] = P[P, X^n] = -i\hbar nPX^{n-1}$

As for the second (potential) term, we assume that it is a polynomial or can be written as one, possibly of infinite degree (as a Taylor Series, for instance). Then

$$V(X) = \sum_{j=0}^{\infty} v_j X^j \qquad (11)$$

Then, since the commutator is linear (i.e. $[A + B, C] = [A, C] + [B, C]$),

$$\begin{aligned}
[V(X), PX^n] &= [V(X), P]X^n = \sum_{j=0}^{\infty} v_j [X^j, P]X^n \\
&= +i\hbar \sum_{j=1}^{\infty} j v_j X^{j+n-1} \qquad (12)
\end{aligned}$$

The case $j = 0$ vanishes from the sum, since X^0 commutes with P.

The expressions 10 and 12 can be substituted in equation 9, under the condition that $n > 0$, and assuming linearity of expectation values $\langle A+B\rangle = \langle A\rangle + \langle B\rangle$:

$$\begin{aligned}
\frac{\partial}{\partial t}\langle PX^n\rangle &= \frac{i}{\hbar}\langle\frac{1}{2m}[P^2, PX^n] + [V(X), PX^n]\rangle \\
&= \frac{i}{\hbar}\langle\frac{1}{2m}[P^2, PX^n]\rangle + \frac{i}{\hbar}\langle[V(X), PX^n]\rangle \\
&= \frac{-i^2\hbar n}{2m\hbar}\langle P\{P, X^{n-1}\}\rangle + \frac{i^2\hbar}{\hbar}\sum_{j=1}^{\infty} j v_j \langle X^{j+n-1}\rangle \\
&= \frac{n}{2m}\langle P\{P, X^{n-1}\}\rangle - \sum_{j=1}^{\infty} j v_j \langle X^{j+n-1}\rangle \qquad (13)
\end{aligned}$$

Where we already see that if we inspect $\frac{\partial}{\partial t}\langle PX^n\rangle$ and take $n = 0$, then we get the derivative $-\frac{\partial}{\partial X}V(X)$ of the potential, which, of course, equals the force,

$$\frac{\partial}{\partial t}\langle P\rangle = -\sum_{j=1}^{\infty} j v_j \langle X^{j-1}\rangle \tag{14}$$

For the harmonic oscillator, we would have that all $v_j = 0$, except for $v_2 = \frac{1}{2}m\omega_0^2$. Then

$$\frac{\partial}{\partial t}\langle P\rangle = -m\omega_0^2\langle X\rangle, \tag{15}$$

which is precisely the force that we would expect.

The anticommutator can again be expanded following equation 6:

$$\frac{\partial}{\partial t}\langle PX^n\rangle = \frac{n}{m}\langle P^2X^{n-1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle PX^{n-2}\rangle - \sum_{j=1}^{\infty} j v_j \langle X^{j+n-1}\rangle \tag{16}$$

The P^2–term is problematic in the light of what is to come, and can consequently be eliminated, since we take the Hamiltonian to be of the form $H = \frac{P^2}{2m} + \sum_{j=0}^{\infty} v_j X^j$. Thus $\frac{P^2}{m} = 2H - 2\sum_{j=0}^{\infty} v_j X^j$. Assuming that only stationary states (i.e. states $|\psi_E\rangle$ that satisfy $H|\psi_E\rangle = E|\psi_E\rangle$) are relevant, we can rewrite the equation 16, using the hermiticity of H, such that $\langle\psi_E|H = \langle\psi_E|H^\dagger = \langle\psi_E|E^\dagger = E\langle\psi_E|$,

$$\begin{aligned}\frac{n}{m}\langle P^2X^{n-1}\rangle &= 2n\langle HX^{n-1}\rangle - 2n\langle\sum_{j=0}^{\infty} v_j X^j X^{n-1}\rangle \\ &= 2nE\langle X^{n-1}\rangle - 2n\sum_{j=0}^{\infty} v_j\langle X^{j+n-1}\rangle \end{aligned}\tag{17}$$

So, most generally, equation 17 can be substituted into 16, so that

$$\begin{aligned}\frac{\partial}{\partial t}\langle PX^n\rangle &= 2nE\langle X^{n-1}\rangle - 2n\sum_{j=0}^{\infty} v_j\langle X^{n+j-1}\rangle \\ &\quad + \frac{i\hbar n(n-1)}{2m}\langle PX^{n-2}\rangle - \sum_{j=1}^{\infty} j v_j\langle X^{j+n-1}\rangle \\ &= 2nE\langle X^{n-1}\rangle - \sum_{j=0}^{\infty}(2n+j)v_j\langle X^{n+j-1}\rangle \\ &\quad + \frac{i\hbar n(n-1)}{2m}\langle PX^{n-2}\rangle \end{aligned}\tag{18}$$

where $j = 0$ term is now included into the sum of the sums, but is cancelled out by its factor j.

In the example of the harmonic oscillator, we have $v_j = 0$ for all $j \neq 2$, and $v_2 = \frac{1}{2}m\omega_0^2$. Then

$$\frac{\partial}{\partial t}\langle PX^n\rangle = 2nE\langle X^{n-1}\rangle - (n+1)m\omega_0^2\langle X^{n+1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle PX^{n-2}\rangle \quad (19)$$

which will also, for $n = 0$, generate the more particular equation 15.

3 Matrix and Vector Formalism

3.1 Definitions

I will define a vector

$$\xi = \begin{bmatrix} \langle X^0\rangle \\ \langle P\rangle \\ \langle X\rangle \\ \langle PX\rangle \\ \langle X^2\rangle \\ \langle PX^2\rangle \\ \vdots \end{bmatrix} = \begin{bmatrix} \xi_{\chi(0)} \\ \xi_{\chi(0)+1} \\ \xi_{\chi(1)} \\ \xi_{\chi(1)+1} \\ \xi_{\chi(2)} \\ \xi_{\chi(2)+1} \\ \vdots \end{bmatrix} \quad (20)$$

It is organised such that the expectation value of X^n ends up in the $(2n+1)$th row, and the expectation value of PX^n in the row after that, the $2(n+1)$th. I define a function $\chi(n)$ that yields the row number of $\langle X^n\rangle$, so that the row number of $\langle PX^n\rangle$ is $\chi(n)+1$,

$$\chi(n) \equiv 2n + 1 \quad (21)$$

Then I hope to find the existence of a matrix Λ such that

$$\frac{\partial}{\partial t}\xi = \Lambda\xi \quad (22)$$

Stationary states then signal the existence of a nullspace, or, more explicitly, zero eigenvalues.

$$\frac{\partial}{\partial t}\xi = \Lambda\xi = 0 = 0\xi \quad (23)$$

The determinant must then equal zero, so that Λ is singular:

$$\det|\Lambda| = 0 \quad (24)$$

3.2 Entries of Λ

The equations for the time evolution of the expectation values then dictate the entries of the matrix Λ and they are given by equation 8,

$$\begin{aligned}\frac{\partial}{\partial t}\langle X^n\rangle = \frac{\partial}{\partial t}\xi_{\chi(n)} &= \frac{n}{m}\langle PX^{n-1}\rangle + \frac{i\hbar n(n-1)}{2m}\langle X^{n-2}\rangle \\ &= \frac{n}{m}\xi_{\chi(n-1)+1} + \frac{i\hbar n(n-1)}{2m}\xi_{\chi(n-2)}, \qquad (25)\end{aligned}$$

and equation 18,

$$\begin{aligned}\frac{\partial}{\partial t}\langle PX^n\rangle = \frac{\partial}{\partial t}\xi_{\chi(n)+1} &= 2nE\langle X^{n-1}\rangle - \sum_{j=0}^{\infty}(2n+j)v_j\langle X^{n+j-1}\rangle \\ &\quad + \frac{i\hbar n(n-1)}{2m}\langle PX^{n-2}\rangle \\ &= 2nE\xi_{\chi(n-1)} - \sum_{j=0}^{\infty}(2n+j)v_j\xi_{\chi(n+j-1)} \\ &\quad + \frac{i\hbar n(n-1)}{2m}\xi_{\chi(n-2)+1} \qquad (26)\end{aligned}$$

Also, the expression $n(n-1)$ will appear regularly, and it seems useful to define $\kappa(n) \equiv i\hbar n(n-1)$, so that

$\kappa(n)$

n	0	1	2	3	4	5	6	7	8	9	10
$\frac{\kappa(n)}{i\hbar}$	0	0	2	6	12	20	30	42	56	72	90

For the harmonic oscillator the case is more simple, equation 25 remaining the same, and expression 26 changing according to equation 19:

$$\begin{aligned}\frac{\partial}{\partial t}\xi_{\chi(n)+1} &= 2nE\xi_{\chi(n-1)} - (n+1)m\omega_0^2\xi_{\chi(n+1)} \\ &\quad + \frac{i\hbar n(n-1)}{2m}\xi_{\chi(n-2)+1} \qquad (27)\end{aligned}$$

I then also define $\mu(n) \equiv (n+1)m\omega_0^2$.

Then, finally, the set of equations corresponding to the harmonic oscillator is:

$$\frac{\partial}{\partial t}\xi_{\chi(n)} = \frac{\kappa(n)}{2m}\xi_{\chi(n-2)} + \frac{n}{m}\xi_{\chi(n-1)+1} \qquad (28)$$

$$\frac{\partial}{\partial t}\xi_{\chi(n)+1} = \frac{\kappa(n)}{2m}\xi_{\chi(n-2)+1} + 2nE\xi_{\chi(n-1)} - \mu(n)\xi_{\chi(n+1)} \qquad (29)$$

3.3 Constructing Λ

Then the first few columns and rows of Λ can be constructed, taking into consideration that each equation above contains only ξ_q with q having only $\chi(n)$ with no other multiples of n than $2n$, and thus the construction shifts regularly diagonally:

$$\Lambda = \begin{bmatrix} \cdot & & & & & & & & & \\ & \cdot & -\mu(0) & & & & & & & \\ & \frac{1}{m} & \cdot & & & & & & & \\ 2E & & & \cdot & -\mu(1) & & & & & \\ \frac{\kappa(2)}{2m} & & & \frac{2}{m} & \cdot & & & & & \\ & \frac{\kappa(2)}{2m} & 4E & & & \cdot & -\mu(2) & & & \\ & & \frac{\kappa(3)}{2m} & & & \frac{3}{m} & \cdot & & & \\ & & & \frac{\kappa(3)}{2m} & 6E & & & \cdot & -\mu(3) & \\ & & & & \frac{\kappa(4)}{2m} & & & \frac{4}{m} & \cdot & \\ & & & & & & & & & \ddots \end{bmatrix} \tag{30}$$

If we define a smaller submatrix containing precisely the content of equations 28 and 29, we can write Λ in terms of it:

$$S_\Lambda(n) = \begin{bmatrix} \frac{\kappa(n)}{2m} & \cdot & \cdot & \frac{n}{m} & \cdot & \cdot & \cdot \\ \cdot & \frac{\kappa(n)}{2m} & 2nE & \cdot & \cdot & \cdot & -\mu(n) \end{bmatrix} \tag{31}$$

We also find that since the first row of Λ is empty, its determinant must already be zero. It will now be interesting to look at the reduced, more correct, problem.

3.4 Reducing Λ

Trivial entries of $\xi_{\lambda=\mathbf{0}}$ can then be eliminated. We observe the following facts about this matrix:

1. All entries move diagonally through the matrix.

2. None of the entries are *a priori* supposed to be allowed to become zero, except for the $2nE$ entry — which we hope will not become zero, but which must formally be allowed to —, since we have taken E, the energy of the system, to be a free parameter. As for the other terms:

   - $\frac{n}{m}$ cannot be zero since for $n = 0$ it is outside of the matrix, and the m is, for the system to be physically meaningful, finite.

- $-\mu(n) = -(n+1)m\omega_0^2$ cannot be zero unless $n = -1$, which falls outside the matrix, or $m = 0$ or $\omega_0^2 = 0$, both of which must on physical grounds be abandoned.
- $\frac{\kappa(n)}{2m}$ cannot be zero, for finite m, unless $\kappa(n) = 0$. Due to its second power of n it is a parabola and takes its only two zeroes at $n = 0$ and $n = 1$, which fall outside the matrix.

   Thus it seems reasonable to assume that all the entries, except for $2nE$, that are currently displayed in the matrix are nonzero.

3. Consequently there can be set down conditions on the eigenvectors $\xi_{\mathbf{\Lambda}}$ for it to satisfy $\Lambda\xi_{\mathbf{\Lambda}} = 0$. The entries $-\mu(0)$ and $\frac{1}{m}$ are the only entries in their rows, due to observation 1. Due to observation 2 this implies that it must be the entries of the vector ξ which become zero: $\xi_{\chi(0)+1} = \xi_{\chi(1)} = 0$.

4. Given the result of observation 3, equation 29 for $n = 2$ dictates that $-\mu(2)\xi_{\chi(3)} = 0$ and equation 28 for $n = 3$ that $\frac{3}{m}\xi_{\chi(2)+1} = 0$. Using observation 2 this implies $\xi_{\chi(2)+1} = \xi_{\chi(3)} = 0$.

5. Observation 4 can be iterated any number of time, to yield that for $s = 0, 1, 2, 3, \ldots$,
$$\xi_{\chi(2s)+1} = \xi_{\chi(2s+1)} = 0. \tag{32}$$

Thus the configuration of the matrix Λ dictates that these entries in the eigenvector corresponding to the zero eigenvalue must be zero whatsoever. Thus it must be the other entries that determine whether a given eigenvector corresponding to the zero eigenvalue is nontrivial. This means that the problem can be reduced to inspecting the determinant of a derived matrix that gives the action of Λ on only the entries of $\xi_{\mathbf{\Lambda}}$ that are not necessarily zero for a zero eigenvalue.

Thus a new, reduced, matrix Λ^- can be constructed, which contains only the elements corresponding to potentially nonzero entries in ξ, and similarly ξ^- contains all entries of ξ except for $\xi_{\chi(0)}$ (for all practical purposes), and $\xi_{\chi(2s)+1}$ and $\xi_{\chi(2s+1)}$ for $s = 0, 1, 2, 3, \ldots$, such that equation 23 becomes:

$$\Lambda^-\xi^- = 0 \tag{33}$$

4 Energy Eigenvalues

4.1 Formal approach

Λ^- is more compact than Λ. For each of the two occurences of n, one is eliminated in the process of reducing Λ, so each row of Λ^- corresponds a unique value of n. Furthermore, Λ^- must take zero eigenvalue for Λ to take a zero eigenvalue.

$$\Lambda^- = \left[\begin{array}{ccccccccc}
2E & & -\mu(1) & & & & & & \\
\frac{\kappa(2)}{2m} & \frac{2}{m} & & & & & & & \\
 & \frac{\kappa(3)}{2m} & 6E & & -\mu(3) & & & & \\
 & & \frac{\kappa(4)}{2m} & \frac{4}{m} & & & & & \\
 & & & \frac{\kappa(5)}{2m} & 10E & & -\mu(5) & & \\
 & & & & \frac{\kappa(6)}{2m} & \frac{6}{m} & & & \\
 & & & & & \frac{\kappa(7)}{2m} & 14E & & \\
 & & & & & & \frac{\kappa(8)}{2m} & \frac{8}{m} & \\
 & & & & & & & \frac{\kappa(9)}{2m} & \\
 & & & & & & & & \ddots
\end{array}\right] \tag{34}$$

I will from now on indicate the components of ξ^- according to the value of n, starting at $n = 1$.

At this point it is clear that for $E = 0$, there can be no nontrivial ξ^- that satisfies $\Lambda^-\xi^- = 0$.

We can now inspect the process of generating an eigenvector. Assuming a particular E, the question here is how an eigenvector can be found, corresponding to an eigenvalue 0. This process, it is hoped, will reveal certain E that can be chosen and others that cannot.

The first component ξ_1^- can be chosen freely. This reflects the freedom of scale in the, at least, one–dimensional eigenspace of Λ^-. However, consequently the equation corresponding to the first row of Λ^- fixes ξ_3^-, since $2E\xi_1^- = \mu(1)\xi_3^-$. Likewise, the equation corresponding to the second row fixes ξ_2^-, since $\frac{\kappa(2)}{2m}\xi_1^- = -\frac{2}{m}\xi_2^-$. The third row, then, determines ξ_5^- and the fourth ξ_4^-. In this manner all entries of ξ^- are completely determined up to a one–dimensional scale once E is set.

4.2 Reconstructing det $|\Lambda^-|$

In a more analytic approach, we can take the expression for the energy levels of the harmonic oscillator as a starting point, and deduce what form the polynomial of the determinant $\det|\Lambda|$ must have.

We write that

$$\det|\Lambda| \equiv y(E) = 0 \tag{35}$$

For a polynomial in E to have a solution E_j such that $y(E_j) = 0$ it must be possible to factor out this particular solution: $y(E) = (E - E_j)y(E)$. Since we should wish $y(E_j) = 0$ for $E_j = (j + \frac{1}{2})\hbar\omega_0 = \frac{(2j+1)\hbar\omega_0}{2}$, we should be able to factor out

$$y(E) = \lim_{n\to\infty} y_0 \prod_{j=0}^{n} (E \pm E_j)^2 \tag{36}$$

But $(E - E_j)(E + E_j) = E^2 - E_j^2$, so

$$y(E) = \lim_{n\to\infty} C \prod_{j=0}^{n} \left(E^2 - E_j^2\right) \tag{37}$$

In the discussion that is to come, the overall factor C will be omitted, since it can be viewed as a scale factor and does not influence the results to come.

We can now evaluate equation 36 starting with $n = 0$. Then $y(E) = E^2 - E_0^2$. It is clear that in spite of repeated multiplication with $(E^2 - E_j^2)$, $y(E)$ will still remain a polynomial in E:

$$y_n(E) = \sum_{i=0}^{m} e_{i,n} E^i \tag{38}$$

From the particular case $y_0(E) = E^2 - E_0$ above we see that $m = 2$ and that all $e_{i,0} = 0$ except for $e_{0,0} = E_0$ and $e_{0,2} = -1$.

Then, when increasing n,

$$\begin{aligned}
y_{n+1}(E) &= \left(\sum_{i=0}^{m(n)} e_{i,n} E^i\right)\left(E^2 - E_{n+1}^2\right) \\
&= \left(\sum_{i=0}^{m(n)} e_{i,n} E^{i+2}\right) - \left(\sum_{i=0}^{m(n)} e_{i,n} E_{n+1}^2 E^i\right) \\
&= \left(\sum_{i=0}^{m(n)+2} e_{(i-2),n} E^i\right) - \left(\sum_{i=0}^{m(n)} (e_{i,n} E_{n+1}^2 E^i\right) \\
&= \sum_{i=0}^{m(n)+2} \left(e_{(i-2),n} - e_{i,n} E_{n+1}^2\right) E^i,
\end{aligned} \tag{39}$$

where we take all $e_{i,n} = 0$ except for $0 \leq i \leq m(n)$.

The order of the polynomial increases by 2 (thus $m(n) = 2(n+1)$), only even powers of the coefficients are observed and the new coefficients are obtained from the old ones via the recursion relation:

$$e_{i,(n+1)} = \underbrace{e_{(i-2),n}}_{\text{shift}} - \underbrace{e_{i,n}E_{n+1}^2}_{\text{manifestation}} \tag{40}$$

The values of $e_{i,n}$ can be found for several n:

	i	0	2	4	6
n	0	$+E_0^2$	-1		
	1	$-E_0^2E_1^2$	$E_0^2 - E_1^2$	-1	
	2	$+E_0^2E_1^2E_2^2$	$-E_0^2E_1^2 - E_0^2E_2^2 + E_1^2E_2^2$	$E_0^2 - E_1^2 + E_2^2$	-1

Thus it is clear from this table that for a particular i, we find the sum of all possible products of squares of $n + 1 - \frac{i}{2}$ different E_j (there are always $n + 1$ different E_j to choose from). In a semi–formal notation:

$$e_{i,n} = \sum_{\text{combinations}}^{\binom{n+1}{n+1-\frac{i}{2}}} \left(\pm \prod_{j\in\{0,1,\ldots,n\}}^{n+1-\frac{i}{2}} E_j^2 \right) \tag{41}$$

It is not difficult to see that the recursion relationship as introduced in equation 40 leaves this structure intact. The reason for 41 to hold, is that (1) in the initial distribution ($e_0 = E_0$ and $e_2 = 1$) equation 41 is already satisfied and (2) in the ith column, the recursion relationship 40 puts all products of $n+1-\frac{i}{2}$ out of E_i, $i \in \{0, 1, 2, \ldots, n-1\}$, (by the *shift term*), which are all possible combinations excluding E_n, and then adds all possible combinations of $n - \frac{i}{2}$ out of E_i (by the *manifestation term*), multiplied by E_n, which thus yields all combinations of $n + 1 - \frac{i}{2}$ out of E_i, $i \in \{0, 1, 2, \ldots, n\}$ that include E_n. The new entry is then the sum of all combinations including E_n and all those excluding E_n, thus *all* possible combinations. Thus equation 41 is proven by induction.

Since $E_j = \left(j + \frac{1}{2}\right)\hbar\omega_0$,

$$e_{i,n} = \left(\sum_{\text{combinations}}^{\binom{n+1}{n+1-\frac{i}{2}}} \left(\pm \prod_{j\in\{0,1,\ldots,n\}}^{n+1-\frac{i}{2}} \left(j + \frac{1}{2}\right)^2 \right) \right) (\hbar\omega_0)^{n+1-\frac{i}{2}} \tag{42}$$

I then define $n!^2_{\frac{1}{2}} \equiv \prod_{j=0}^{n} \left(j+\frac{1}{2}\right)$ so that

$$e_{i,n} = \left(\sum_{\text{combinations}}^{\binom{n+1}{\frac{i}{2}}} \frac{1}{\pm \prod_{j\in\{0,1,\ldots,n\}}^{\frac{i}{2}} \left(j+\frac{1}{2}\right)^2} \right) n!^2_{\frac{1}{2}} \left(\hbar\omega_0\right)^{n+1-\frac{i}{2}} \tag{43}$$

4.3 Submatrices of Λ^-

The repetitive construction of Λ^- allows the definition of submatrices Λ_p^-, which contain all entries Λ_{ij}^- with $i \geq 2p+1$ and $j \geq 2p+1$. Then $\Lambda^- = \Lambda_0^-$ and, generally, for $p' = 2p+1$,

$$\Lambda_p^- \equiv \begin{bmatrix} 2p'E & & -\mu(p') & & & & \\ \frac{\kappa(p'+1)}{2m} & \frac{p'+1}{m} & & & & & \\ & \frac{\kappa(p'+2)}{2m} & 2(p'+2)E & & -\mu(p'+2) & & \\ & & \frac{\kappa(p'+3)}{2m} & \frac{p'+3}{m} & & & \\ & & & \frac{\kappa(p'+4)}{2m} & 2(p'+4)E & & \\ & & & & \frac{\kappa(p'+5)}{2m} & \frac{p'+5}{m} & \\ & & & & & & \ddots \end{bmatrix} \tag{44}$$

By the method of *expansion by minors* we then obtain an expression for the determinant of this submatrix:

$$\begin{aligned} \det\left|\Lambda_p^-\right| &= 2p'E \cdot \det \begin{vmatrix} \frac{p'+1}{m} & & & \\ \frac{\kappa(p'+2)}{2m} & 2(p'+2)E & & -\mu(p'+2) \\ & \frac{\kappa(p'+3)}{2m} & \frac{p'+3}{m} & \\ & & \frac{\kappa(p'+4)}{2m} & \Lambda_{p+2}^- \end{vmatrix} \\ &\quad - \frac{\kappa(p'+1)}{2m} \cdot \det \begin{vmatrix} & -\mu(p') & & \\ \frac{\kappa(p'+2)}{2m} & 2(p'+2)E & & -\mu(p'+2) \\ & \frac{\kappa(p'+3)}{2m} & \frac{p'+3}{m} & \\ & & \frac{\kappa(p'+4)}{2m} & \Lambda_{p+2}^- \end{vmatrix} \\ &= 2p'E\frac{p'+1}{m} \cdot \det \begin{vmatrix} 2(p'+2)E & & -\mu(p'+2) \\ \frac{\kappa(p'+3)}{2m} & \frac{p'+3}{m} & \\ & \frac{\kappa(p'+4)}{2m} & \Lambda_{p+2}^- \end{vmatrix} \\ &\quad - \frac{\kappa(p'+1)}{2m} \cdot +\mu(p') \cdot \det \begin{vmatrix} \frac{\kappa(p'+2)}{2m} & & -\mu(p'+2) \\ & \frac{p'+3}{m} & \\ & \frac{\kappa(p'+4)}{2m} & \Lambda_{p+2}^- \end{vmatrix} \end{aligned}$$

$$
\begin{aligned}
&= 2p'E\frac{p'+1}{m}\cdot\det\left|\Lambda^-_{p+1}\right| \\
&\quad -\frac{\kappa(p'+1)}{2m}\cdot\mu(p')\cdot\frac{\kappa(p'+2)}{2m}\cdot\det\left|\begin{array}{cc}\frac{p'+3}{m} & \\ \frac{\kappa(p'+4)}{2m} & \Lambda^-_{p+2}\end{array}\right| \\
&= 2p'E\frac{p'+1}{m}\cdot\det\left|\Lambda^-_{p+1}\right| \\
&\quad -\frac{\kappa(p'+1)}{2m}\cdot\mu(p')\cdot\frac{\kappa(p'+2)}{2m}\cdot\frac{p'+3}{m}\cdot\det\left|\Lambda^-_{p+2}\right| \qquad (45)
\end{aligned}
$$

4.4 Recursive Relationship

Thus we obtain a recursive relationship with

$$\det\left|\Lambda^-_p\right| = C_1(p)E\cdot\det\left|\Lambda^-_{p+1}\right| + C_2(p)\cdot\det\left|\Lambda^-_{p+2}\right| \qquad (46)$$

where

$$
\begin{aligned}
C_1(p) &= 2p'\frac{p'+1}{m} = \frac{2}{m}(2p+1)(2p+2) \\
C_2(p) &= -\frac{\kappa(p'+1)}{2m}\cdot\mu(p')\cdot\frac{\kappa(p'+2)}{2m}\cdot\frac{p'+3}{m} \\
&= \frac{-i^2\hbar^2\omega_0^2}{2^2m^2}\left((2p+2)(2p+1)(2p+2)(2p+3)(2p+2)(2p+4)\right) \\
&= \frac{+\omega_0^2\hbar^2}{2^2m^2}\Big((2p+1)(2p+2)^3(2p+3)(2p+4)\Big). \qquad (47)
\end{aligned}
$$

The recursion relationship in equation 46 can be evaluated for Λ^-_p and iterated once to yield:

$$
\begin{aligned}
\det\left|\Lambda^-_p\right| &= \Big(C_1(p)C_1(p+1)E^2 + C_2(p)\Big)\det\left|\Lambda^-_{p+2}\right| \\
&\quad +C_2(p+1)\cdot\det\left|\Lambda^-_{p+3}\right| \qquad (48)
\end{aligned}
$$

This last fact will require some checking of argumentation, but if we then set $\det\left|\Lambda^-_{p+3}\right| = 0$ an equation for E is obtained by setting the whole determinant equation (so back to Λ^-_0) to zero:

$$
\begin{aligned}
-E^2 &= \frac{C_2(p)}{C_1(p)C_1(p+1)} \\
&= \frac{\omega_0^2\hbar^2m^2}{2^4m^2}\frac{(2p+1)(2p+2)^3(2p+3)(2p+4)}{(2p+1)(2p+2)(2p+3)(2p+4)} \\
&= \frac{\omega_0^2\hbar^2}{2^2}(p+1)^2 \qquad (49)
\end{aligned}
$$

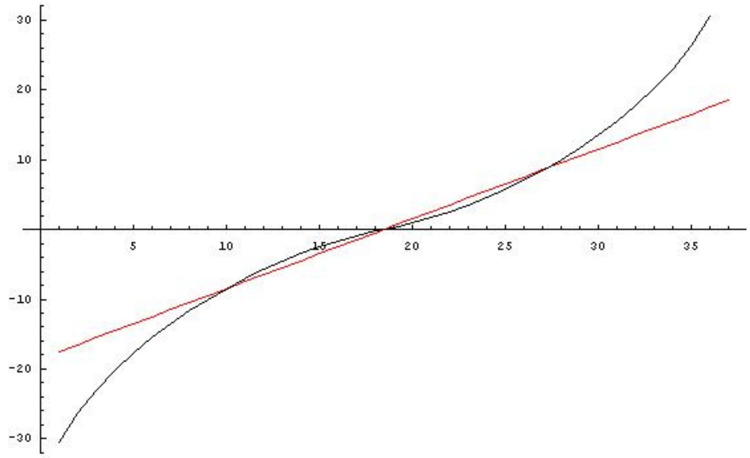

Figure 1: Results of numerical approximation

We had hoped we would get:

$$+E^2 = \frac{\omega_0^2 \hbar^2}{2^2}(2p+1)^2 \tag{50}$$

In fact, we are quite close, but (1) there is a minus sign in front of the energy, which makes all solutions imaginary, (2) there is $(p+1)^2$ instead of $(2p+1)^2$ and (3) the energy levels are allowed to be negative.

5 Numerical Approximation

For purposes of numerical approximation, the determinant of the first 74×74 entries of Λ has been computed and its zero–values solved numerically. The result is depicted below, where the discrete energy levels are connected by a cubic spline, and the straight line indicates the expected energy levels. Again, it is evident that the slope of the line connecting the computed energy levels is exactly half of that of the expected energy levels.

6 References

[1] Random notes by Dr. Frank Witte. The concept of the derivation has been entirely Witte's. The contribution of the author consists in the elaboration of some mathematical details.