Physics

We are investigating a one-dimensional problem, namely a particle of mass m in the quadratic potential $V(q) = m\omega^2 q^2/2$. Here, q is the spatial coordinate of the particle. In dimensionless form, the Hamiltonian of the system is

$$H_0 = \frac{1}{2}\left(p^2 + q^2\right) \ . \tag{2.1}$$

Here, the energies are measured in units of $\hbar\omega$, momenta in units of $\sqrt{\hbar m\omega}$, and lengths in units of $\sqrt{\hbar/(m\omega)}$. The eigenstates $|j\rangle$ of H_0 can be found in any quantum mechanics textbook. In the coordinate representation, they are

$$\varphi_j(q) = \left(2^j j!\sqrt{\pi}\right)^{-1/2} \mathrm{e}^{-q^2/2} \mathcal{H}_j(q) \ ,$$

where $\mathcal{H}_j(q)$ are the Hermite polynomials. We have

$$H_0 |j\rangle = \varepsilon_j^0 |j\rangle \ , \quad \text{where} \quad \varepsilon_j^0 = j + \frac{1}{2} \quad \text{and} \quad j = 0, 1, 2, \ldots \ . \tag{2.2}$$

The ε_j^0 are the energies of the eigenstates of H_0, and the matrix $\langle j|H_0|k\rangle$ is diagonal because the eigenvalues are not degenerate.

We now add an anharmonic potential to H_0,

$$H = H_0 + \lambda q^4 \ , \tag{2.3}$$

and try to determine the matrix $\langle j|H|k\rangle$. To do this, it is useful to write q as a sum of creation and annihilation operators $a^\dagger$ and a,

$$q = \frac{1}{\sqrt{2}}\left(a^\dagger + a\right) \ , \tag{2.4}$$

where a and $a^\dagger$ have the following properties:

$$a^\dagger |j\rangle = \sqrt{j+1}\,|j+1\rangle \ ,$$
$$a|0\rangle = 0 \quad \text{and} \quad a|j\rangle = \sqrt{j}\,|j-1\rangle \quad \text{for} \quad j > 0 \ . \tag{2.5}$$

Consequently, the matrix representation of q in the space of the unperturbed states $|j\rangle$ yields the tridiagonal matrix

$$\begin{aligned} Q_{jk} &= \langle j\,|q|\,k\rangle \\ &= \frac{1}{\sqrt{2}}\sqrt{k+1}\,\delta_{j,k+1} + \frac{1}{\sqrt{2}}\sqrt{k}\,\delta_{j,k-1} = \frac{1}{2}\sqrt{j+k+1}\,\delta_{|k-j|,1} \ . \end{aligned} \tag{2.6}$$

The approximation that we will now use consists of defining this infinite-dimensional matrix for $j, k = 0, 1, \ldots, n-1$ only. The Hamiltonian $H = H_0 + \lambda q^4$, or more precisely its matrix representation, is to be approximated by an $n \times n$ matrix as well, where H_0 is represented by the diagonal matrix with the elements $j + 1/2$, and q^4 by the fourfold matrix product of Q_{jk} with itself. The error of the approximation can be estimated by comparing the eigenvalues of H for different values of n.

Algorithm

The above matrices can be defined in a particularly compact way in *Mathematica*. According to (2.6), $\langle j|q|k\rangle$ is

```
q[j_,k_]:= Sqrt[(j+k+1)]/2 /; Abs[j-k]==1
q[j_,k_]:= 0 /; Abs[j-k] != 1
```

The construct `lhs := rhs /; test` means that the definition is to be used only if the expression on the right hand side has the logical value `True`. The matrix `q` is defined as a list of lists

```
q[n_]:= Table[q[j,k], {j,0,n-1}, {k,0,n-1}]
```

and according to (2.2) H_0 is calculated as

```
h0[n_]:= DiagonalMatrix[Table[j+1/2, {j,0,n-1}]]
```

With this, H can be written as

```
h[n_]:= h0[n] + lambda q[n].q[n].q[n].q[n]
```

One can calculate the eigenvalues of H with `Eigenvalues[...]`, either algebraically (which only works for small values of n) or numerically with `Eigenvalues[N[h[n]]]`, where `lambda` has to be assigned a numerical value beforehand.

Results

The call `h[4] // MatrixForm` yields the Hamiltonian matrix

$$\begin{pmatrix} \frac{1}{2}+\frac{3}{4}\lambda & 0 & \frac{3}{\sqrt{2}}\lambda & 0 \\ 0 & \frac{3}{2}+\frac{15}{4}\lambda & 0 & 3\sqrt{\frac{3}{2}}\lambda \\ \frac{3}{\sqrt{2}}\lambda & 0 & \frac{5}{2}+\frac{27}{4}\lambda & 0 \\ 0 & 3\sqrt{\frac{3}{2}}\lambda & 0 & \frac{7}{2}+\frac{15}{4}\lambda \end{pmatrix} . \tag{2.7}$$

Its eigenvalues are

$$\frac{6+15\lambda \pm 2\sqrt{2}\sqrt{2+12\lambda+27\lambda^2}}{4} \quad \text{and} \quad \frac{10+15\lambda \pm 2\sqrt{2}\,\sqrt{2+27\lambda^2}}{4} . \tag{2.8}$$

These four eigenvalues can be seen in Fig. 2.1 as functions of λ. Without perturbation ($\lambda = 0$) we get the energies $1/2$, $3/2$, $5/2$, and $7/2$ of the harmonic oscillator. As the perturbation λ increases, the upper two eigenvalues separate markedly from the lower ones. This is an effect of the finite size of the matrices. The operator q^4 connects the state $|j\rangle$ with $|j \pm 4\rangle$, and therefore the matrix elements $\langle j|q^4|j \pm 4\rangle$ should be contained in the Hamiltonian matrix `h[n]`, if the energy ε_j is to be calculated more or less correctly. In any case, it is no surprise if the eigenvalues ε_{n-1}, ε_{n-2}, and ε_{n-3} exhibit large discrepancies from the exact result.

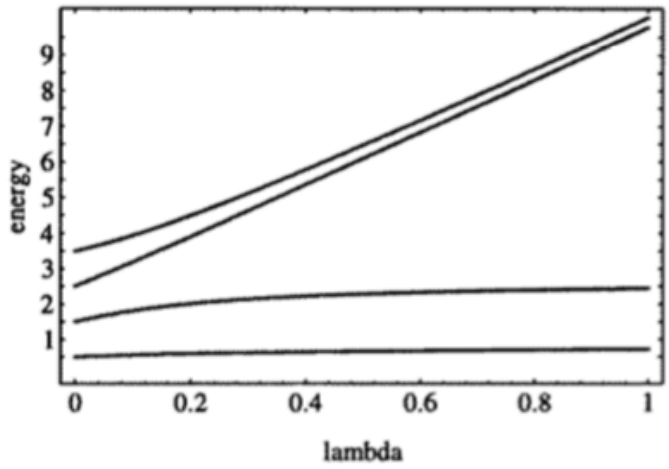

Fig. 2.1. Approximate values for the lowest four energy eigenvalues of the quantum oscillator with the anharmonicity λq^4, as a function of λ

How accurate is the approximation? This can be seen in Fig. 2.2 for the example of the ground state energy ε_0. For an anharmonicity parameter $\lambda = 0.1$, ε_0 is plotted as a function of $1/n$, for $n = 7, \ldots, 20$. Obviously this function is not monotonic. Although we do not know its asymptotic behavior, the value for $n \to \infty$ can be specified very precisely. By using the commands

```
mat = N[h[n] /. lambda -> 1/10, 20];
 li = Sort[Eigenvalues[mat]]; li[[1]]
```

we obtain the following values for $n = 20$ and $n = 40$:

$$\varepsilon_0\,(20) = 0.559146327396\ldots\,,$$
$$\varepsilon_0\,(40) = 0.559146327183\ldots\,.$$

Therefore, for $n = 20$ we have an accuracy of about nine significant figures. Higher energies can only be determined with less accuracy. We obtain

$$\varepsilon_{10}\,(20) = 17.333\ldots\,,$$
$$\varepsilon_{10}\,(40) = 17.351\ldots\,,$$

i.e., an accuracy of only three significant figures.

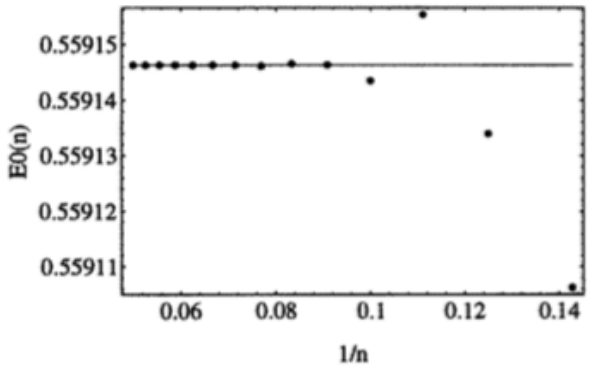

Fig. 2.2. Approximate values for the ground state energy of the anharmonic oscillator as a function of the inverse matrix dimension $1/n$ for $n = 7, 8, \ldots, 20$

In Fig. 2.1 we only considered four levels for our approximation. Therefore, the two upper energies are represented in an entirely incorrect manner. In Fig. 2.3, on the other hand, we have included twenty levels. In this case, the numerical solution of the eigenvalue equation yields a very precise result for the five lowest energies. The energies, as well as their separations, increase as the anharmonicity parameter λ increases.

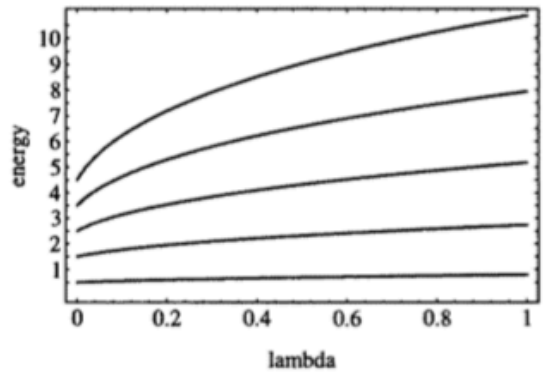

Fig. 2.3. The five lowest energy eigenvalues as a function of the anharmonicity parameter λ