Do equidistant energy levels necessitate a harmonic potential?

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Abstract: In this supplementary material, the shift-operator approach [Chaos 4 (1994), 47] is derived and a few resulting potentials and states are depicted. Furthermore, The solution of the harmonic oscillator and its perturbation with different monomials is derived. A few examplary results are shown.

1 Shift-operator approach

1.1 Definition and basic operator equation

The Schrödinger equation in dimensionless coordinates

$$\xi=\sqrt{\frac{m\omega}{\hbar}}x \quad , \quad \epsilon_n=\frac{E_n}{\hbar\omega} \quad , \quad \psi(\xi)=\sqrt[4]{\frac{\hbar}{m\omega}}\Psi(x) \quad , \quad U(\xi)=\frac{V(x)}{\hbar\omega} \tag{1}$$

is

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial\xi^2}+U(\xi)\right]\psi_n(\xi)=\epsilon_n\psi_n(\xi) \quad . \tag{2}$$

The shift operator

$$\mathcal{L}\psi(\xi,\epsilon)=\psi(\xi,\epsilon+1) \quad , \quad \mathcal{L}^\dagger\psi(\xi,\epsilon)=\psi(\xi,\epsilon-1) \tag{3}$$

shifts each state in energy by $\hbar\omega$. Applying the Hamiltonian operator gives

$$\begin{aligned}&\mathcal{H}\mathcal{L}\psi(\xi,\epsilon)=(\epsilon+1)\psi(\xi,\epsilon+1) \quad , && \mathcal{H}\mathcal{L}^\dagger\psi(\xi,\epsilon)=(\epsilon-1)\psi(\xi,\epsilon-1) \quad ,\\ &\mathcal{L}\mathcal{H}\psi(\xi,\epsilon)=\epsilon\psi(\xi,\epsilon+1) \quad , && \mathcal{L}^\dagger\mathcal{H}\psi(\xi,\epsilon)=\epsilon\psi(\xi,\epsilon-1) \quad .\end{aligned} \tag{4}$$

For an equidistant spectrum $\epsilon_{n+1}=\epsilon_n+1$ this gets

$$\begin{aligned}&\mathcal{H}\mathcal{L}\psi_n(\xi)=\epsilon_{n+1}\psi_{n+1}(\xi) \quad , && \mathcal{H}\mathcal{L}^\dagger\psi_n(\xi)=\epsilon_{n-1}\psi_{n-1}(\xi) \quad ,\\ &\mathcal{L}\mathcal{H}\psi_n(\xi)=\epsilon_n\psi_{n+1}(\xi) \quad , && \mathcal{L}^\dagger\mathcal{H}\psi_n(\xi)=\epsilon_n\psi_{n-1}(\xi) \quad .\end{aligned} \tag{5}$$

With this, a resulting operator equation can be set up using commutators:

$$[\mathcal{H},\mathcal{L}]=\mathcal{L} \quad , \quad [\mathcal{H},\mathcal{L}^\dagger]=-\mathcal{L}^\dagger \quad . \tag{6}$$

It follows $[\mathcal{H},\mathcal{L}\mathcal{L}^\dagger]=[\mathcal{H},\mathcal{L}^\dagger\mathcal{L}]=0$. Consequently, $\mathcal{L}\mathcal{L}^\dagger$, $\mathcal{L}^\dagger\mathcal{L}$, and $[\mathcal{L},\mathcal{L}^\dagger]$ are functions of $\mathcal{H}$. Thus, $\mathcal{L}$ can be written as a polynomial of the dimensionless momentum operator $\mathcal{P}=-\mathrm{i}\frac{\partial}{\partial\xi}$:

$$\mathcal{L}=\sum_{k=0}^{K}\alpha_k(\xi)(\mathrm{i}\mathcal{P})^k \quad . \tag{7}$$

K is the order of the shift operator. $\alpha_k(\xi)$ are free parameters. Inserting Eq. (7) into Eq. (6) and comparing the coefficients yields $K+2$ differential equations for $K+1$ unknown functions $\alpha_k(\xi)$ and the additional unknown function $U(\xi)$.

1.2 First-order shift operator

Inserting the first-order shift operator

$$\mathcal{L}=\alpha_0(\xi)+\alpha_1(\xi)\mathrm{i}\mathcal{P} \tag{8}$$

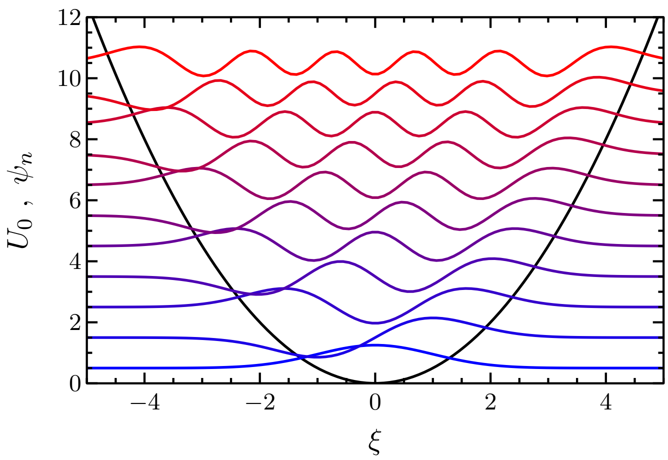

Figure 1: Potential and lowest states of the first-order shift operator.

into Eq. (6) yields

$$\begin{aligned} 0 &= \alpha_0 + \frac{1}{2}\alpha_0'' + U'\alpha_1 \quad , \\ 0 &= \alpha_0' + \alpha_1 + \frac{1}{2}\alpha_1'' \quad , \\ 0 &= \alpha_1' \quad . \end{aligned} \tag{9}$$

The solution for the α_k yields the condition

$$U' = \xi \quad . \tag{10}$$

Integrating this yields the harmonic oscillator potential

$$U_0 = \frac{1}{2}\xi^2 \quad . \tag{11}$$

The corresponding shift operator

$$\mathcal{L} = -\xi + \mathrm{i}\mathcal{P} \quad , \quad \mathcal{L}^\dagger = \xi + \mathrm{i}\mathcal{P} \tag{12}$$

is the creation resp. the annihilation operator. The corresponding solution of the Schrödinger equation is

$$\epsilon_n = \frac{1}{2} + n \quad , \quad \psi_n(\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(\xi) \exp\left(-\frac{1}{2}\xi^2\right) \quad , \tag{13}$$

where $H_n(\xi)$ are the Hermite polynomials. The potential and the states of the first-order shift operator are depicted in Fig. 1.

1.3 Second-order shift operator

Inserting the second-order shift operator

$$\mathcal{L} = \alpha_0(\xi) + \alpha_1(\xi)\mathrm{i}\mathcal{P} + \alpha_2(\xi)(\mathrm{i}\mathcal{P})^2 \tag{14}$$

into Eq. (6) yields

$$\begin{aligned} 0 &= \alpha_0 + \frac{1}{2}\alpha_0'' + U'\alpha_1 + U''\alpha_2 = 0 \quad , \\ 0 &= \alpha_0' + \alpha_1 + \frac{1}{2}\alpha_1'' + 2U'\alpha_2 \quad , \\ 0 &= \alpha_1' + \alpha_2 + \frac{1}{2}\alpha_2'' \quad , \\ 0 &= \alpha_2' \quad . \end{aligned} \tag{15}$$

The solution for the α_k yields the condition

$$\xi U' + 2U = \frac{1}{2}\xi^2 \quad . \tag{16}$$

Multiplying with ξ and summarizing using the product rule yields

$$(\xi^2 U)' = \frac{1}{2}\xi^3 \quad . \tag{17}$$

Integrating and dividing by ξ^2 yields

$$U_1 = \frac{1}{8}\xi^2 + \frac{A}{\xi^2} \quad . \tag{18}$$

The shift operator is

$$\mathcal{L} = \frac{1}{4}\xi^2 - \frac{2A}{\xi^2} - \frac{1}{2} - \xi \mathrm{i}\mathcal{P} - (\mathrm{i}\mathcal{P})^2 \quad , \quad \mathcal{L}^\dagger = \frac{1}{4}\xi^2 - \frac{2A}{\xi^2} + \frac{1}{2} + \xi \mathrm{i}\mathcal{P} - (\mathrm{i}\mathcal{P})^2 \quad . \tag{19}$$

The solution of the Schrödinger equation can be achieved with the asymptotic behaviour

$$\xi \to \infty : \qquad \psi''_\infty - \frac{1}{2}\xi^2 \psi_\infty = 0 \quad , \qquad \psi_\infty \sim \exp\left(-\frac{1}{4}\xi^2\right) \quad , \tag{20}$$

$$\xi \to 0 : \qquad \psi''_0 - \frac{4A}{\xi^2}\psi_0 = 0 \quad , \qquad \psi_0 \sim \xi^{(1+\sqrt{1+8A})/2} \tag{21}$$

and the consequential approach

$$\psi_n(\xi) = \xi^{(1+\sqrt{1+8A})/2} \sum_{k=0}^{n} a_k \xi^k \exp\left(-\frac{1}{4}\xi^2\right) \quad . \tag{22}$$

It follows

$$\epsilon_n = \frac{1}{2} + n + \frac{1}{4}\sqrt{1+8A} \quad , \tag{23}$$

$$\psi_n(\xi) = C_n J_n(\xi) \left(\frac{\xi^2}{2}\right)^{(1+\sqrt{1+8A})/4} \exp\left(-\frac{1}{4}\xi^2\right) \quad , \tag{24}$$

$$J_n(\xi) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{\Gamma\left(\frac{\sqrt{1+8A}}{2}+1\right)}{\Gamma\left(\frac{\sqrt{1+8A}}{2}+1+k\right)} \left(\frac{\xi^2}{2}\right)^k \quad , \tag{25}$$

$$C_n = \sqrt{\frac{\sqrt{2}\Gamma\left(\frac{\sqrt{1+8A}}{2}+1+n\right)}{n!\Gamma^2\left(\frac{\sqrt{1+8A}}{2}+1\right)}} \quad . \tag{26}$$

The potential and the states of the second-order shift operator are depicted in Fig. 2.

1.4 Third-order shift operator

Inserting the thirt-order shift operator

$$\mathcal{L} = \alpha_0(\xi) + \alpha_1(\xi)\mathrm{i}\mathcal{P} + \alpha_2(\xi)(\mathrm{i}\mathcal{P})^2 + \alpha_3(\xi)(\mathrm{i}\mathcal{P})^3 \tag{27}$$

into Eq. (6) yields

$$0 = \alpha_0 + \frac{1}{2}\alpha''_0 + U'\alpha_1 + U''\alpha_2 + U'''\alpha_3 \quad , \tag{28}$$

$$0 = \alpha'_0 + \alpha_1 + \frac{1}{2}\alpha''_1 + 2U'\alpha_2 + 3U''\alpha_3 \quad , \tag{29}$$

$$0 = \alpha'_1 + \alpha_2 + \frac{1}{2}\alpha''_2 + 3U'\alpha_3 \quad , \tag{30}$$

$$0 = \alpha'_2 + \alpha_3 + \frac{1}{2}\alpha''_3 \quad , \tag{31}$$

$$0 = \alpha'_3 \quad . \tag{32}$$

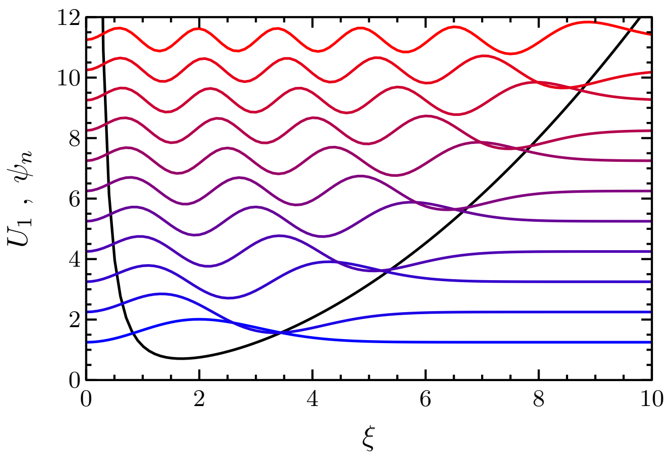

Figure 2: Potential and lowest states of the second-order shift operator.

The solution for the α_k yields the shift operator

$$\mathcal{L} = \left(\frac{3}{2}\left(U^2\right)' - \frac{1}{4}U''' - \frac{\xi^2+3}{2}U' + \frac{1}{2}\xi\right) + \left(\frac{1}{2}\xi^2 - 3U - 1\right)\mathrm{i}\mathcal{P} - \xi(\mathrm{i}\mathcal{P})^2 + (\mathrm{i}\mathcal{P})^3 \quad , \tag{33}$$

$$\mathcal{L}^\dagger = -\left(\frac{3}{2}\left(U^2\right)' - \frac{1}{4}U''' - \frac{\xi^2+3}{2}U' - \frac{1}{2}\xi\right) + \left(\frac{1}{2}\xi^2 - 3U + 1\right)\mathrm{i}\mathcal{P} + \xi(\mathrm{i}\mathcal{P})^2 + (\mathrm{i}\mathcal{P})^3 \tag{34}$$

and the condition

$$\frac{3}{2}\left(W^2\right)'' - \frac{1}{4}W'''' + \xi^2 W'' + 3\xi W' = 0 \tag{35}$$

with $U = W + \frac{1}{2}\xi^2$. Multiplying with ξ and summarizing using the product rule yields the first integral

$$\frac{3}{2}\xi\left(W^2\right)' - \frac{3}{2}W^2 - \frac{1}{4}\xi W''' + \frac{1}{4}W'' + \xi^3 W' = A \quad . \tag{36}$$

Multiplying with W', using the identities of Eq. (36)

$$\frac{3}{2}\xi\left(W^2\right)' - \frac{1}{4}\xi W''' + \xi^3 W' = A + \frac{3}{2}W^2 - \frac{1}{4}W'' \quad , \tag{37}$$

$$\xi^3 W' = -\xi^2\left(\frac{A + \frac{3}{2}W^2 - \frac{1}{4}W''}{\xi}\right)' \quad , \tag{38}$$

and summarizing using the chain rule yields another first integral

$$-\frac{1}{2}\left(\frac{A + \frac{3}{2}W^2 - \frac{1}{4}W''}{\xi}\right)^2 - \frac{1}{2}W^3 + \frac{1}{8}\left(W'\right)^2 = AW + B \quad . \tag{39}$$

Using a Darboux transformation, a possible solution can be written in the form

$$W = -\xi^2 + \frac{4}{3}\mu + \left(\frac{\chi_\mu'}{\chi_\mu}\right)^2 \tag{40}$$

with

$$-\frac{1}{2}\chi_\mu'' + \frac{1}{2}\xi^2\chi_\mu = \mu\chi_\mu \quad . \tag{41}$$

With $\mu = -\left(m + \frac{1}{2}\right)$ two possible classes of solutions are

$$U_m = -\frac{1}{2}\xi^2 - \frac{2}{3}(2m+1) + \left(\frac{P_m'(\xi)}{P_m(\xi)} + \xi\right)^2 \quad , \tag{42}$$

$$P_{2m} = \sum_{k=0}^{m} \frac{4^k}{(m-k)!(2k)!}\xi^{2k} \quad , \tag{43}$$

$$P_{2m+1} = \sum_{k=0}^{m} \frac{4^k}{(m-k)!(2k+1)!}\xi^{2k+1} \quad . \tag{44}$$

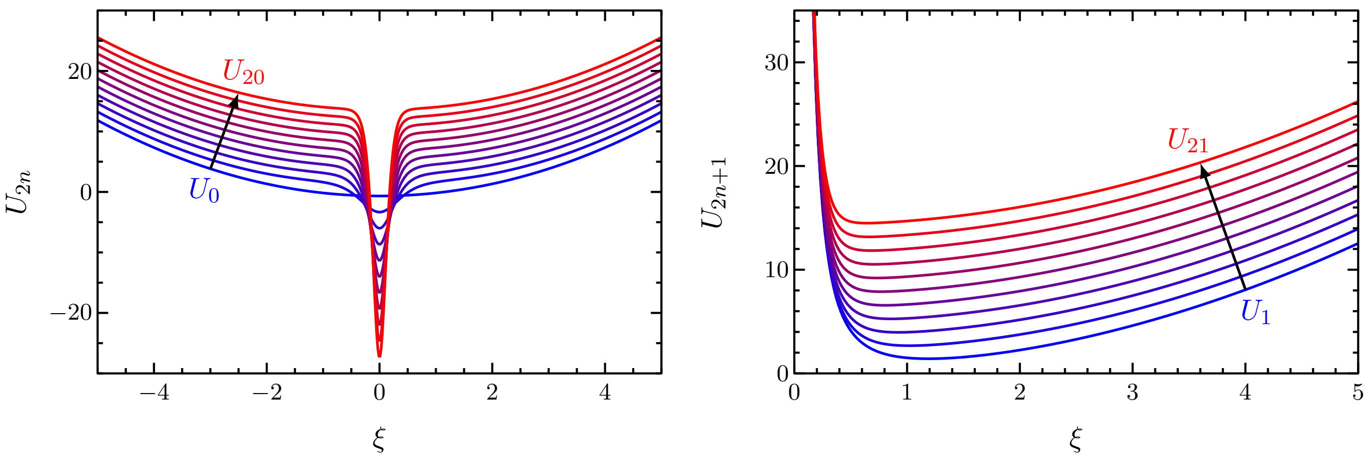

Figure 3: Potentials of the third-order shift operator obtained by a Darboux transformation.

U_{2n} are quadratic potentials with a dip at the minimum. U_0 is the harmonic potential. The corresponding energy levels are equidistant with $\Delta\epsilon = 1$. The ground state of potential U_{2n} is additionally lowered by $2n$. U_{2n+1} are singular potentials at $\xi = 0$. U_1 is the one of the second-order shift operator. The corresponding energy levels are equidistant with $\Delta\epsilon = 2$ ($\Delta\epsilon = 1$ can be achieved by rescaling $\xi = \xi'/2$). The potentials of the third-order shift operator are depicted in Fig. 3. The potentials U_2 and U_4 and corresponding lowest states are shown in Fig. 4 and Fig. 5.

2 Perturbed 1D harmonic oscillator

The Schrödinger equation for the 1D harmonic oscillator is

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2\right]\Psi_n(x) = E_n^{(0)}\Psi_n(x) \quad . \tag{45}$$

Substituting with the dimensionless variables

$$x = \sqrt{\frac{\hbar}{m\omega}}\xi \quad , \quad E_n^{(0)} = \hbar\omega\epsilon_n^{(0)} \quad , \quad \Psi(x) = \sqrt[4]{\frac{m\omega}{\hbar}}\psi(\xi) \tag{46}$$

yields the dimensionless formula

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial \xi^2} + \frac{1}{2}\xi^2\right]\psi_n(\xi) = \epsilon_n^{(0)}\psi_n(\xi) \quad . \tag{47}$$

Its solution is

$$\epsilon_n^{(0)} = n + \frac{1}{2} \quad , \quad \psi_n(\xi) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\exp\left(-\frac{1}{2}\xi^2\right)H_n(\xi) \quad , \tag{48}$$

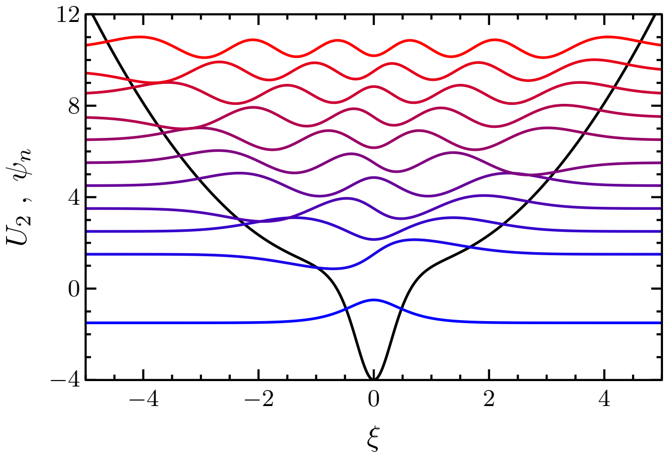

Figure 4: Potential U_2 and corresponding lowest states of the third-order shift operator.

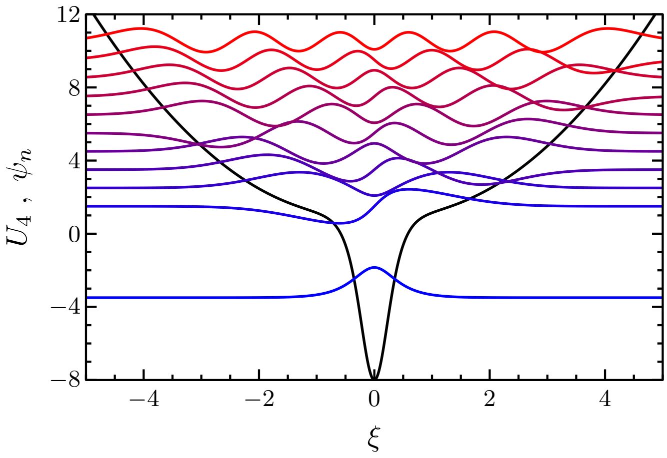

Figure 5: Potential U_4 and corresponding lowest states of the third-order shift operator.

where H_n are the Hermite polynomials. They can be expressed the following:

$$H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(n-1)H_{n-2}(\xi) \quad . \tag{49}$$

The Schrödinger equation of a system, which is perturbed with the perturbation potential $v(x) = \frac{1}{2}\hbar\omega u(\xi)$, respective the corresponding dimensionless perturbation potential $u(\xi)$, is

$$\left[\mathcal{H}_0 + \lambda u(\xi)\right]\phi_k(\xi) = \epsilon_k \phi_k(\xi) \quad . \tag{50}$$

Transforming the eigenstates into the basis of unperturbed eigenstates and expanding the eigenenergies and coefficients in Taylor series in λ,

$$\phi_k = \sum_n c_{kn}\psi_n \quad , \quad \epsilon_k = \sum_p \lambda^p \epsilon_k^{(p)} \quad , \quad c_{km} = \sum_p \lambda^p c_{km}^{(p)} \quad , \quad u_{mn} = \int\limits_{-\infty}^{\infty} \psi_m^*(\xi) u(\xi) \psi_n(\xi)\,\mathrm{d}\xi \quad , \tag{51}$$

yields

$$\left(\epsilon_m^{(0)} - \epsilon_k^{(0)}\right) c_{km}^{(0)} + \sum_{p=1}^{\infty} \left[\left(\epsilon_m^{(0)} - \epsilon_k^{(0)}\right) c_{km}^{(p)} - \epsilon_k^{(p)} \delta_{km} - \sum_{q=1}^{p-1} \epsilon_k^{(q)} c_{km}^{(p-q)} + \sum_n c_{kn}^{(p-1)} u_{mn} \right] \lambda^p = 0 \quad . \tag{52}$$

This gives recursion equations for the pth order corrections:

$$\epsilon_k^{(p)} = \sum_{n \neq k} u_{kn} c_{kn}^{(p-1)} - \sum_{q=2}^{p-1} \epsilon_k^{(q)} c_{kk}^{(p-q)} \tag{53}$$

$$c_{km}^{(p)} = \frac{1}{\epsilon_k^{(0)} - \epsilon_m^{(0)}} \left(\sum_n u_{mn} c_{kn}^{(p-1)} - u_{kk} c_{km}^{(p-1)} - \sum_{q=2}^{p-1} \epsilon_k^{(q)} c_{km}^{(p-q)} \right) \quad . \tag{54}$$

Especially for the 1st, 2nd, and 3rd order corrections, one gets

$$\epsilon_k^{(1)} = u_{kk} \quad , \tag{55}$$

$$\epsilon_k^{(2)} = -\sum_{n \neq k} \frac{u_{nk} u_{kn}}{\epsilon_n^{(0)} - \epsilon_k^{(0)}} \quad , \tag{56}$$

$$\epsilon_k^{(3)} = -\sum_{n \neq k} \frac{u_{nk} u_{kk} u_{kn}}{\left(\epsilon_n^{(0)} - \epsilon_k^{(0)}\right)^2} + \sum_{n \neq k} \sum_{l \neq k} \frac{u_{kn} u_{nl} u_{lk}}{\left(\epsilon_n^{(0)} - \epsilon_k^{(0)}\right)\left(\epsilon_l^{(0)} - \epsilon_k^{(0)}\right)} \quad . \tag{57}$$

Expanding $u(\xi)$ in a Taylor series in ξ,

$$u(\xi) = \sum_j u_j \xi^j \quad , \tag{58}$$

gives

$$u_{mn} = \sum_j u_j u_{mn}^{(j)} \quad , \tag{59}$$

$$u_{mn}^{(j)} = \frac{1}{\sqrt{2^{m+n} m! n!}\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \xi^j \mathrm{e}^{-\xi^2} H_m(\xi) H_n(\xi)\,\mathrm{d}\xi \quad . \tag{60}$$

Inserting Eq. (49) gives the recursion

$$u_{mn}^{(j)} = \sqrt{\frac{n+1}{2}} u_{m,n+1}^{(j-1)} + \sqrt{\frac{n}{2}} u_{m,n-1}^{(j-1)} \quad . \tag{61}$$

The diagonal elements $u_{kk}^{(j)}$ are polynomials in k of order $j/2$. For the smallest j one gets

$$u_{kk}^{(0)} = 1 \quad , \tag{62}$$

$$u_{kk}^{(2)} = \frac{1}{2} + k \quad , \tag{63}$$

$$u_{kk}^{(4)} = \frac{3}{4} + \frac{3}{2}k + \frac{3}{2}k^2 \quad , \tag{64}$$

$$u_{kk}^{(6)} = \frac{15}{8} + 5k + \frac{15}{4}k^2 + \frac{5}{2}k^3 \quad , \tag{65}$$

$$u_{kk}^{(8)} = \frac{105}{16} + \frac{35}{2}k + \frac{175}{8}k^2 + \frac{35}{4}k^3 + \frac{35}{8}k^4 \quad . \tag{66}$$

The nondiagonal elements can be written as

$$u^{(j)}_{k,k-l} = \sqrt{\frac{k!}{2^l(k-l)!}} p^{(j)}_{kl} \quad , \tag{67}$$

where $p^{(j)}_{kl}$ is a polynomial in k of order $(j-l)/2$. Thus, $(u^{(j)}_{k,k-l})^2$ is a polynomial in k of order j for all l. For the smallest j and l one gets

$$p^{(1)}_{k,1} = 1 \quad , \tag{68}$$

$$p^{(3)}_{k,1} = \frac{3}{2}k \quad , \tag{69}$$

$$p^{(5)}_{k,1} = \frac{5}{4}(1+2k^2) \quad , \tag{70}$$

$$p^{(7)}_{k,1} = \frac{35}{8}k(2+k^2) \quad , \tag{71}$$

$$p^{(2)}_{k,2} = 1 \quad , \tag{72}$$

$$p^{(4)}_{k,2} = -1+2k \quad , \tag{73}$$

$$p^{(6)}_{k,2} = \frac{15}{4}(1-k+k^2) \quad , \tag{74}$$

$$p^{(8)}_{k,2} = \frac{7}{2}(-1+2k)(3-k+k^2) \quad , \tag{75}$$

$$p^{(3)}_{k,3} = 1 \quad , \tag{76}$$

$$p^{(5)}_{k,3} = \frac{5}{2}(-1+k) \quad , \tag{77}$$

$$p^{(7)}_{k,3} = \frac{21}{4}(2-2k+k^2) \quad , \tag{78}$$

$$p^{(9)}_{k,3} = \frac{21}{4}(-1+k)(9-4k+2k^2) \quad , \tag{79}$$

$$p^{(4)}_{k,4} = 1 \quad , \tag{80}$$

$$p^{(6)}_{k,4} = \frac{3}{2}(-3+2k) \quad , \tag{81}$$

$$p^{(8)}_{k,4} = \frac{7}{2}(7-6k+2k^2) \quad , \tag{82}$$

$$p^{(10)}_{k,4} = \frac{15}{4}(-3+2k)(13-6k+2k^2) \quad . \tag{83}$$

The results are shown in Fig. 6.

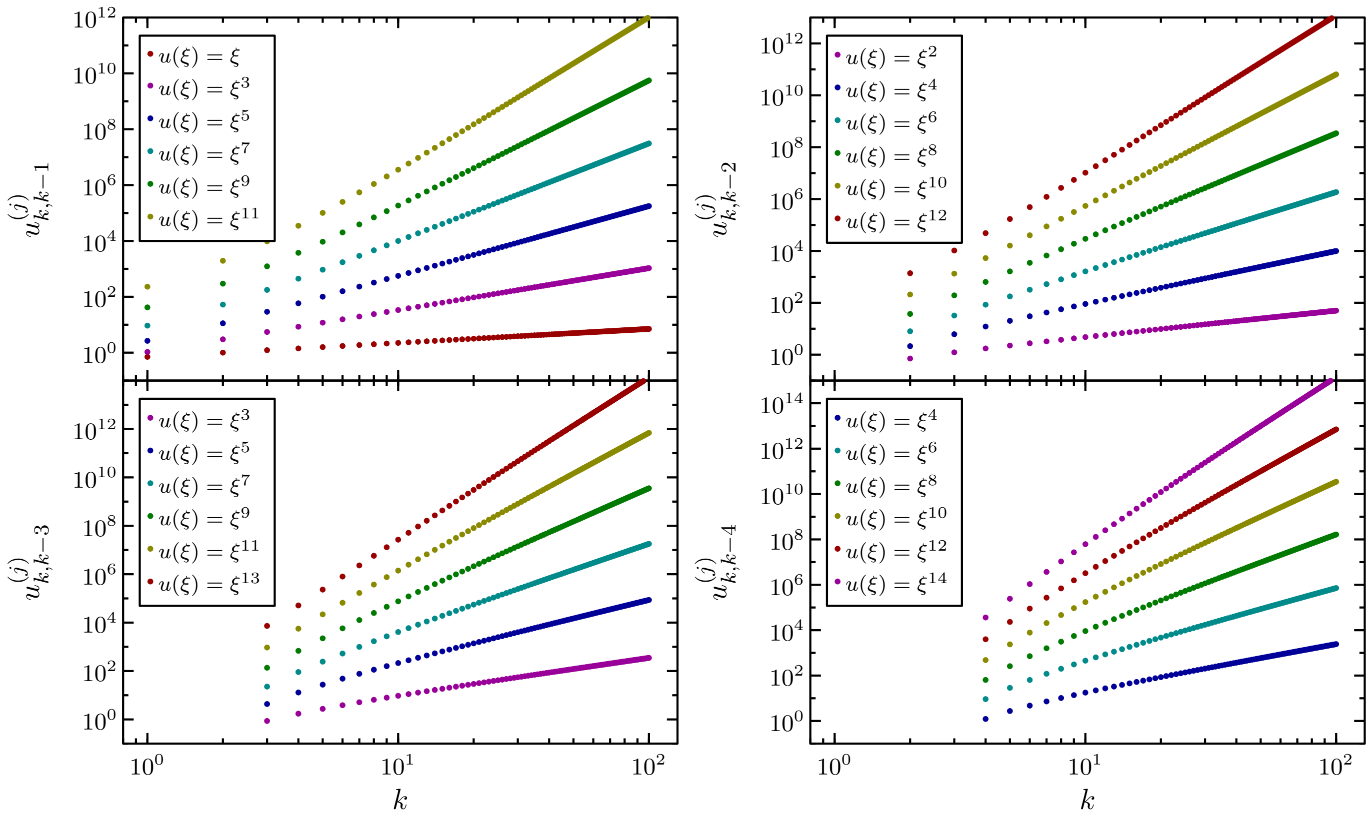

Figure 6: $u^{(j)}_{k,k-l}$ for different l and for different perturbation potentials $u(\xi) = \xi^j$.