TECHNISCHE UNIVERSITÄT CHEMNITZ

Do equidistant energy levels necessitate a harmonic potential?

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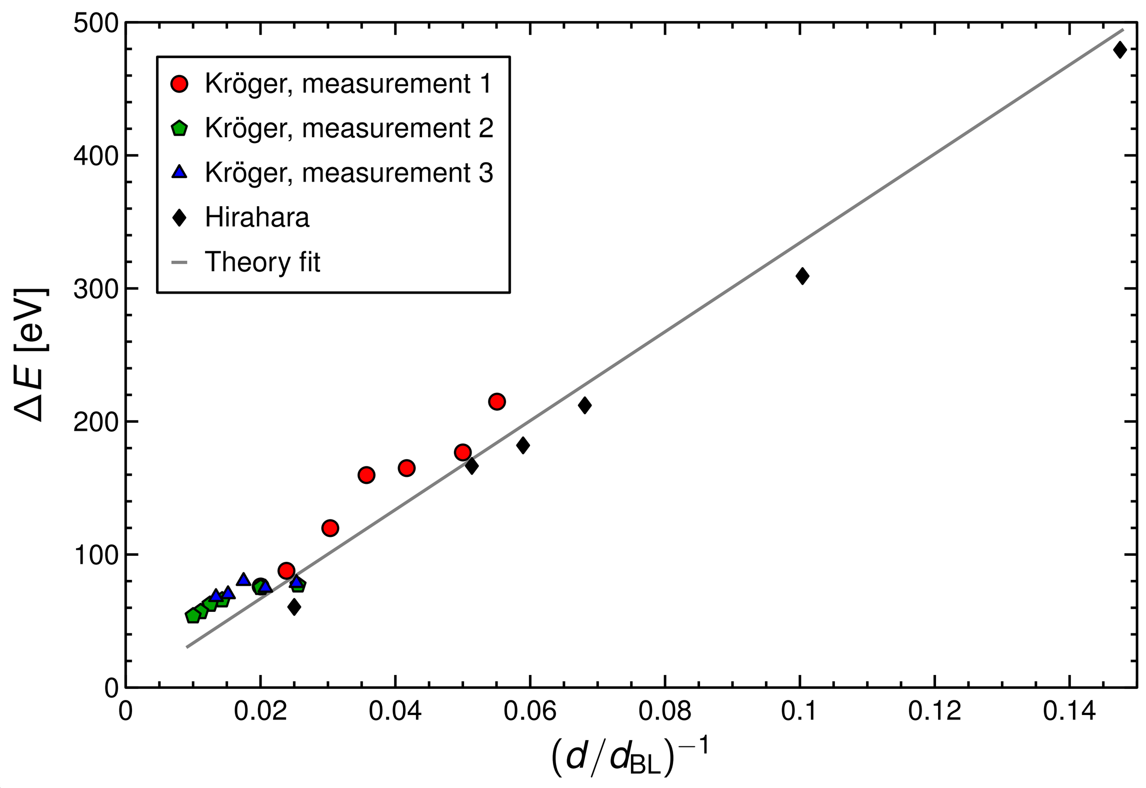
Experimental results and harmonic oscillator model

[1] T. Hirahara et al.: *Quantum well states in ultrathin Bi films: Angle-resolved photoemission spectroscopy and first-principles calculations study*, Physical Review B 75 (2007), 035422

[2] P. Kröger, C. Tegenkamp et al.: *Controlling conductivity by quantum well states in ultrathin Bi(111) films*, Physical Review B 97 (2018), 045403



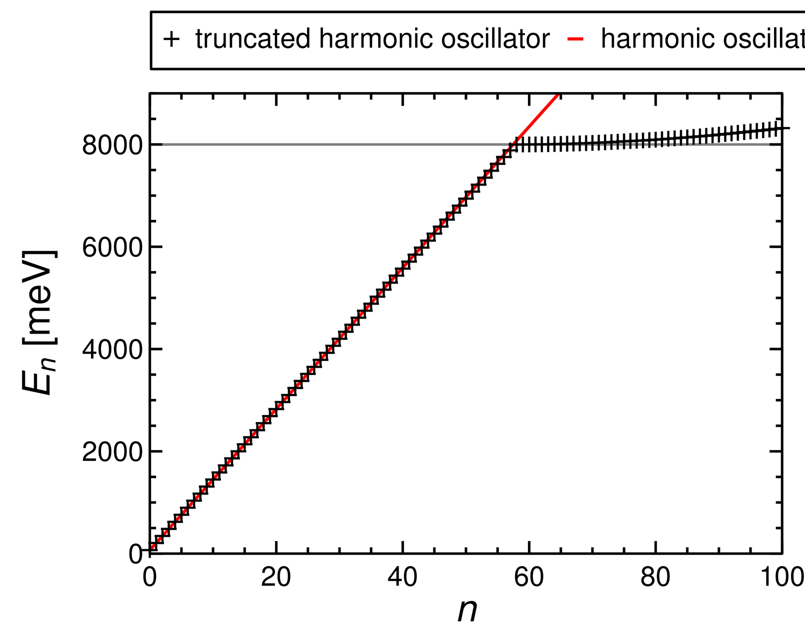
- Quantum well states in Bi films:
  bandgap E_g measured
  $1/d$-dependence found (d ...film thickness)
- Typical models:
  Square well potential: $\Delta E \sim 1/d^2$
  Quadratic potential: $\Delta E \sim 1/d$

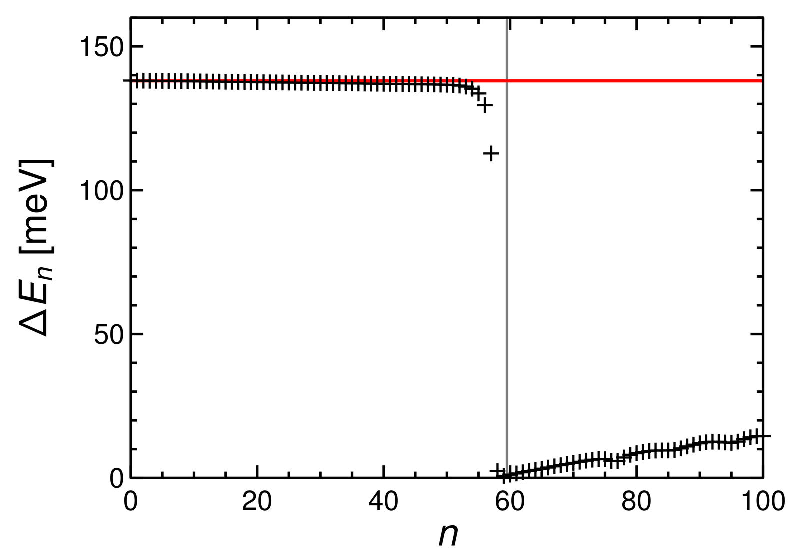
- Simple model: truncated harmonic oscillator

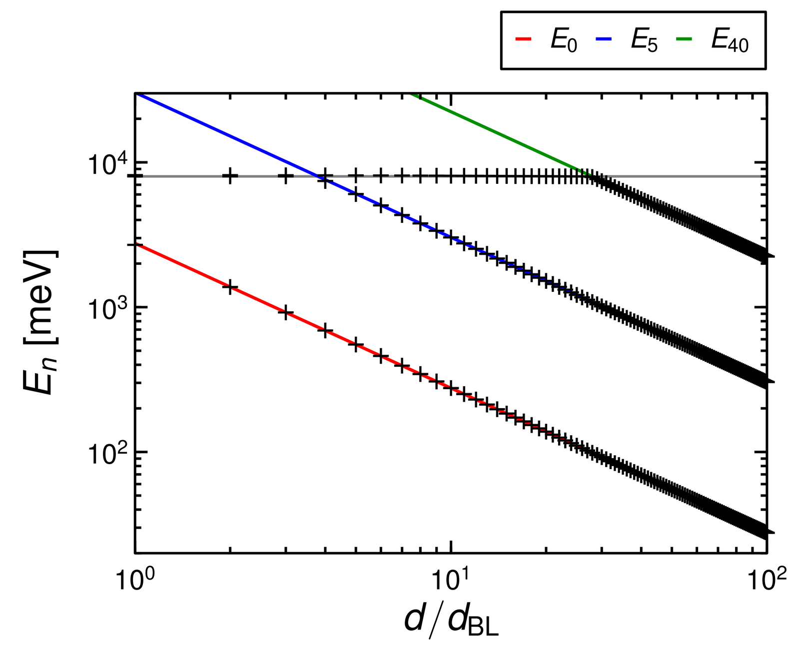
$$V(x) = E_g \begin{cases} 1 & |x| \geq d/2 \\ (2x/d)^2 & |x| \leq d/2 \end{cases}$$

$$\rightarrow \quad \Delta E = \frac{2\hbar}{d}\sqrt{\frac{2E_g}{m^*}}$$

- Example: $E_g/m^* = 8\,\mathrm{eV}/m_e$, $d = 16\,\mathrm{nm}$ (fig. below)







Approaches for calculating potentials with equidistant spectra

Shift operator approach

[3] Dubov et al.: *Equidistant spectra of anharmonic oscillators*, Journal of Experimental and Theoretical Physics 75 (1992), p. 446–451

[4] S. Dubov et al.: *Equidistant spectra of anharmonic oscillators*, Chaos 4 (1994), p. 47–53

Factorization method

[5] B. Mielnik: *Factorization method and new potentials with the oscillator spectrum*, Journal of Mathematical Physics 25 (1984), p. 3387–3389

[6] D. J. Fernández C et al.: *A simple generation of exactly solvable anharmonic oscillators*, Physics Letters A 244 (1998), p. 309–316

Conclusion

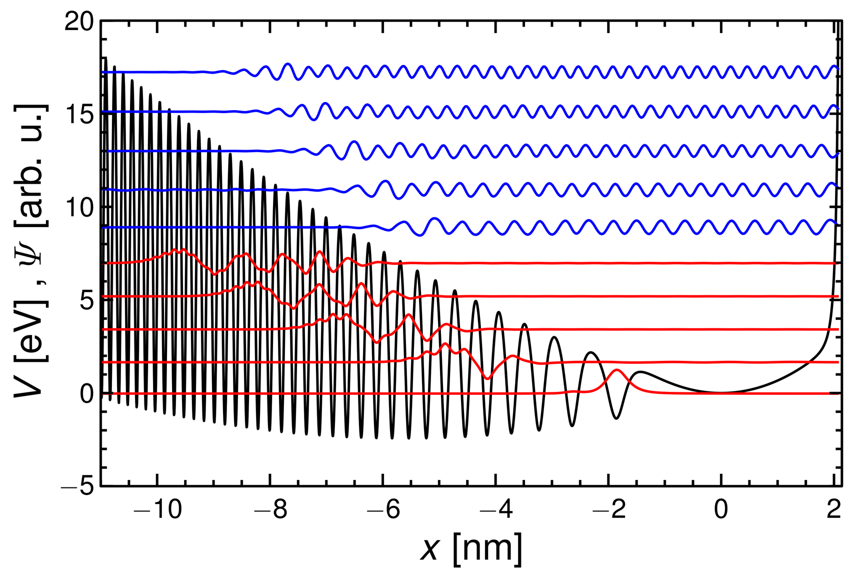
- **Energy levels of thin films cannot provide all information about the underlying confinement potentials**
- **Many different oscillating and diverging potential shapes with equidistant energy levels are possible**
- Different spectra are constructable with factorization method choosing appropriate ϵ_{k_i}
- Different potential shapes for given spectrum are adjustable by choosing appropriate A_{k_i}

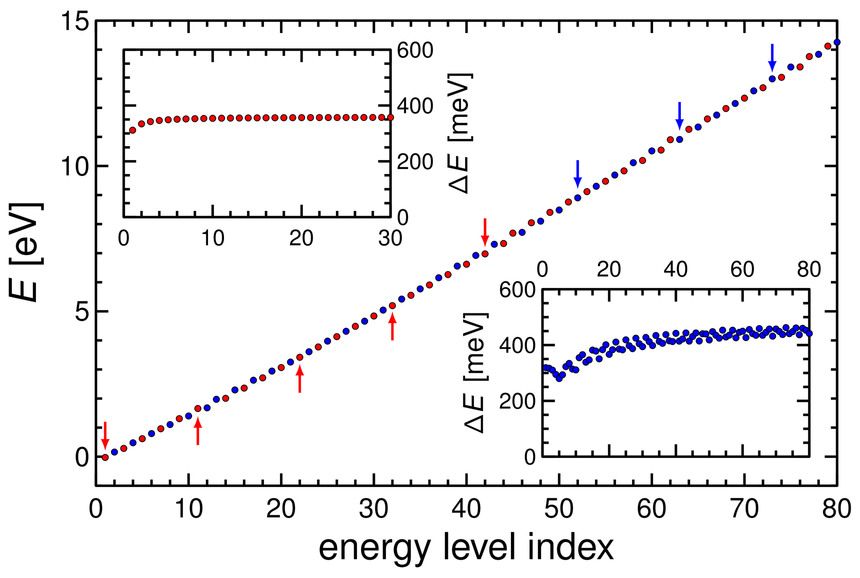
Shift operator approach [3,4]

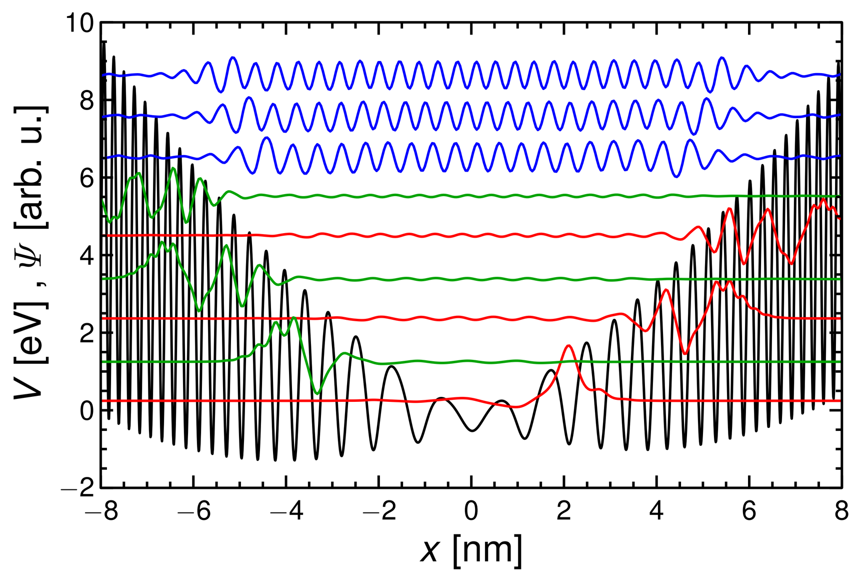
- Solving $[\mathcal{H}, \mathcal{L}] = \mathcal{L}$, $\mathcal{L}$ ...shift operator (generalized creation operator)
- Expansion $\mathcal{L} = \sum_{k=0}^{K} \alpha_k(\xi)(\mathrm{i}\mathcal{P})^k$, $\mathcal{P}$ ...momentum operator
- Solving $k+1$ differential equations for unknowns $\alpha_k(\xi)$ and unknown potential $U(\xi)$
- 1st order: $\mathcal{L} = \alpha_0(\xi) + \alpha_1(\xi)\mathrm{i}\mathcal{P} \rightarrow$ creation operator $\rightarrow$ harmonic potential $U(\xi) = \frac{1}{2}\xi^2$
- 2nd order: isotonic potential $U(\xi) = \frac{1}{8}\xi^2 + \frac{A}{\xi^2}$
- 3rd order: Solving $\frac{3}{2}[W(\xi)^2]'' - \frac{1}{4}W''''(\xi) - \xi^2 W''(\xi) + 3\xi W'(\xi) = 0$ with $U(\xi) = \frac{1}{2}\xi^2 + W(\xi)$
- Darboux transformation yields some solutions:

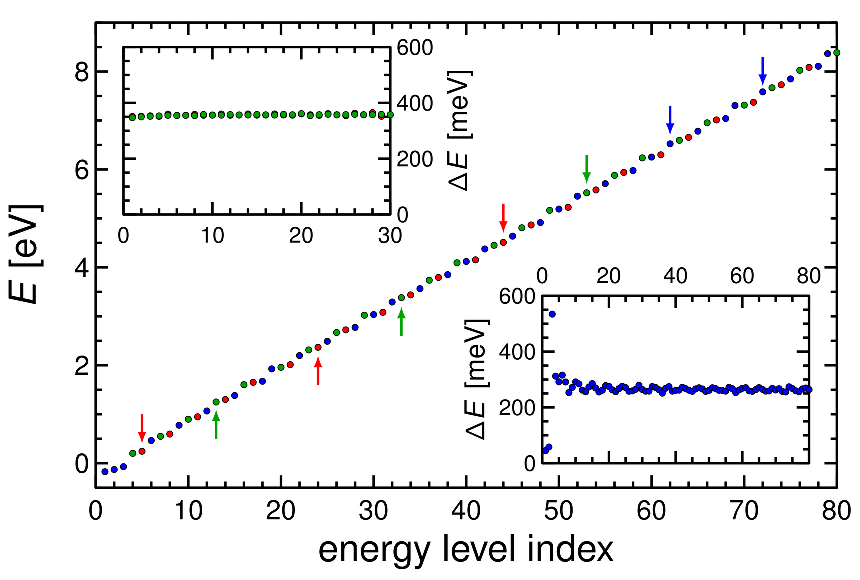
$$U_m(\xi) = -\frac{1}{2}\xi^2 + \left(\frac{P_m'(\xi)}{P_m(\xi)} + \xi\right)^2 \quad , \quad P_{2m+\delta} = \sum_{k=0}^{m} \frac{4^k}{(m-k)!(2k+\delta)!}\xi^{2k+\delta} \quad , \quad \delta \in \{0,1\}$$

Exemplary numeric solutions:









Factorization method [5,6]

- Operator $a^\dagger = \frac{1}{\sqrt{2}}\left[-\frac{\mathrm{d}}{\mathrm{d}\xi} + \alpha(\xi)\right]$ transforms $\mathcal{H}_1$ into $\mathcal{H}_2$: $\mathcal{H}_2 a^\dagger = a^\dagger \mathcal{H}_1$ with $\mathcal{H}_i = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + V_i(\xi)$
- $V_2(\xi) = V_1(\xi) - \alpha'(\xi)$ with $\alpha'(\xi) + \alpha(\xi)^2 = 2[V_1(\xi) - \epsilon]$
- $V_2(\xi)$ has same spectrum as $V_1(\xi)$, except an additional energy level at ϵ
- Analytically solvable for $V_1(\xi) = \frac{1}{2}\xi^2$ for $\epsilon = -\left(k + \frac{1}{2}\right) \rightarrow \alpha_k(\xi),\ V_k(\xi)$

$$\alpha_k(\xi) = \xi + \frac{\mathrm{d}}{\mathrm{d}\xi}\log\left\{[1 + A_k\,\mathrm{erf}(\xi)]h_k(\xi) + A_k\frac{2}{\sqrt{\pi}}\mathrm{e}^{-\xi^2}p_k(\xi)\right\} \text{ with } h_k(\xi) = (-\mathrm{i})^k H_k(\xi) \quad ,$$

$$p_{2k+\delta}(\xi) = \sum_{m=0}^{k} 2^m \frac{(2k-m-\delta)!}{(2k-2m-\delta)!}h_{2k-2m-\delta}(\xi) \quad , \quad \delta \in \{0,1\} \quad , \quad A_k \text{ ...constant}$$

- Multiple transformations with different ϵ_{k_i}: additional energy levels at every ϵ_{k_i}

$$V_{k_1 \ldots k_n}(\xi) = V_{k_1 \ldots k_{n-1}}(\xi) - \alpha'_{k_1 \ldots k_n}(\xi) \quad , \quad \alpha_{k_1 \ldots k_n}(\xi) = -\alpha_{k_1 \ldots k_{n-1}}(\xi) - 2\frac{k_n - k_{n-1}}{\alpha_{k_1 \ldots k_{n-1}}(\xi) - \alpha_{k_1 \ldots k_{n-2}k_n}(\xi)}$$

Exemplary solutions: