A Bi quantum film potential as an inverse problem

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***Abstract*—Experiments generally only offer access to certain output parameters or spectra. When performing device simulations, we often assume that agreement of theoretical and experimental output means that the model describes the device well. However, this conclusion is by no means mandatory. Here, we show an example of a Bi quantum film where measurements show equidistant energy levels. Though this suggests a harmonic oscillator potential, a variety of alternative potentials with equidistant spectra may also describe the structure, especially considering the finite measurement accuracy and range.**

***Index Terms*—quantum well lasers, physics computing, laser theory**

I. Introduction

Comparing theory and experiment in semiconductor heterostructures offers insight into many physical mechanisms. This is the basis of a whole branch of theoretical physics where the output of numerical experiments is compared to measurements. Generally, for matching results it is assumed that the theory applies. Yet we must not forget that we only compare a very limited output. Only physical observables may be measured, and here, the observation is limited by measurement possibilities as well as limitations in time and other resources. However, agreement of a single measurement may not mean that the structure or device is realistically modelled. This is illustrated by the case discussed here: On observing an equidistant spectrum, it is often assumed that the underlying potential must be a harmonic oscillator. Yet this is a classical inverse problem: Although a harmonic oscillator mandates a harmonic potential, the reverse is not true and there is no easy way to derive a potential from its spectrum. We therefore pose the question whether there are other potentials with the same spectral characteristics, especially considering that measurements have a limited range and accuracy, i.e. the spectrum is only known to be approximately equidistant in a certain range.

II. Experiment vs theory – Status quo

In this section, we introduce experimental results from a Bi film structure grown on a Si surface and showing a harmonic-oscillator like spectrum. The experimental results of Kröger et al. [1] and Hirahara et al. [2], i.e. the energy level spacings ΔE as a function of the Bi film thickness, are depicted in Fig. 1 (colored symbols). For the Kröger data, the measured bandgap E_{g} is interpreted as energy spacing ΔE. The inverse thickness dependence can be clearly seen. The solid line shows a fit with a d^{-1} thickness dependence.

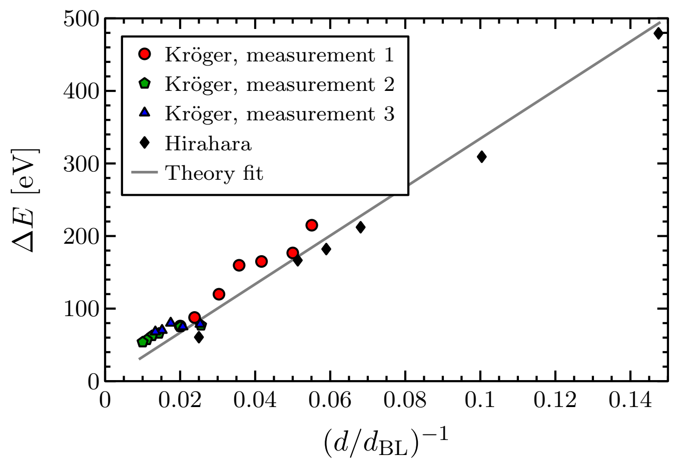

Fig. 1. Experimental data of Kröger et al. [1] (3 different Bi films) and Hirahara et al. [2] in comparison with a fit to the harmonic oscillator.

Customarily, a harmonic oscillator potential is assumed for the spectrum in Fig. 1. However, the Bi quantum well being confined by vacuum on one side and by Si on the other side, a symmetric potential seems improbable. The alternative would be a harmonic oscillator only covering one half-space and bordered by an infinite potential at the origin, allowing the odd states of the symmetric structure and therefore also resulting in equidistant states. However, the question remains what other possibilities are available for an isospectral potential.

III. Alternative isospectral potentials

Using perturbation theory, it may be shown that there is no anharmonic polynomial potential displaying an equidistant spectrum. However, non-polynomial potentials may well be isospectral, see Ref. [3]–[6]. Two approaches have been used: The shift operator approach and the factorisation method.

Briefly speaking, the shift operator approach is based on the definition of an operator which shifts the eigenstates in energy. This shift operator may be expanded in terms of the momentum operator, and solutions for an isospectral potential can be found for the different orders.

The factorisation method uses a generalisation of the creation operator to transform the Hamiltonian into another isospectral one, but with a different potential and an additional

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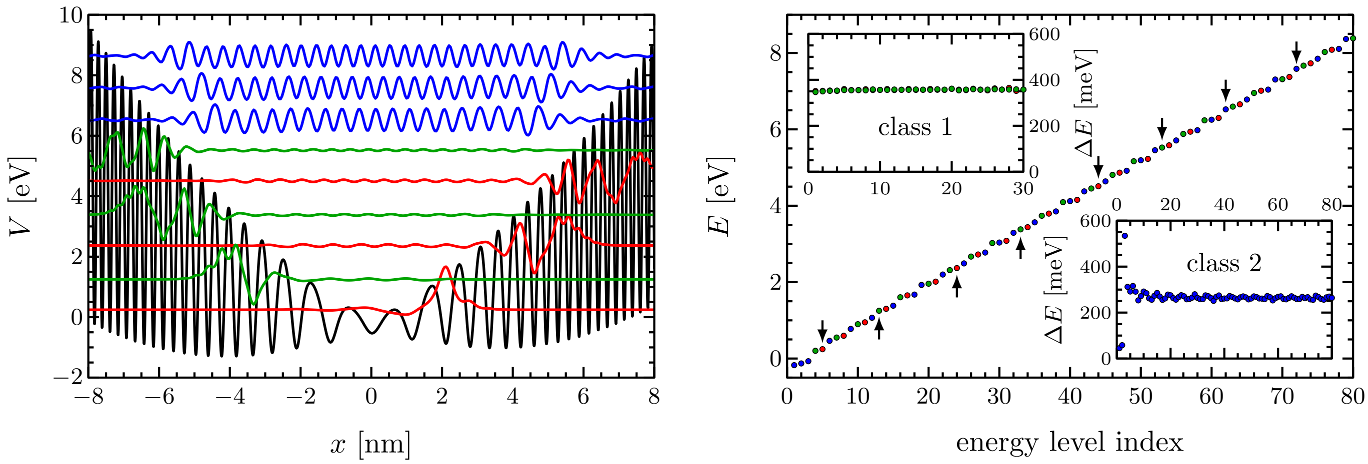

Fig. 2. Left: Example of a non-harmonic potential (black), obtained by the shift operator approach. Coloured curves show some selected eigenstates, shifted by their energy. Right: Corresponding spectrum.

lowest energy level. The latter one can be chosen arbitrarily within some restrictions. Using multiple transformations the additional energy levels can be used to construct a new spectrum, which is equidistant within the measurement range, but with some freedom in modelling the potential.

An example of a potential obtained by the shift operator approach is shown in Fig. 2. The left part depicts the exemplary potential (black) with realistic spatial slab dimensions. Also some selected states are shown (colored), shifted by their respective energies. The right part shows the corresponding spectrum. The potential results in two distinct sets of equidistant states which are spaced in a way of giving a nearly equidistant overall spectrum. The term “nearly equidistant” is mathematically incorrect, but describes a situation which can well be fitted with the performed experiments and translated into “equidistant within the given measurement accuracy”. This is shown by the energy level spacings in the insets, which are in agreement with the measurement results in Fig. 1.

Shift operator approach and factorisation method allow the calculation of a wide variety of potential structures, either with spatial oscillations of different size and period lengths or even showing singularities on one side. Thus, the mere knowledge of the spectrum allows few conclusions about the underlying potential. Further structural knowledge has to enter the analysis: an oscillating potential may model the atomic structure and a singularity could be a model of a slab–vacuum surface.

IV. Atomistic potential calculations

The above results mandate a more direct way of gaining access to the potential structure at hand. To tackle this task, we perform ab initio calculations for Bi slabs of different thicknesses and extract the underlying potential. However, atomistic calculations are also subject to a number of constraints, largely limiting these to the consideration of free-standing Bi slabs surrounded by vacuum, i.e. symmetrical structures. Therefore, the analysis has to take into account both results of the atomistic calculations and conclusions from the above-presented considerations of all isospectral potentials.

V. Conclusion

Starting with multiple measurements of equidistant spectra, we illustrate that these cannot be used to prove the existence of an underlying harmonic oscillator potential. Even assuming measurement of an infinite spectrum with perfect accuracy, a multitude of corresponding anharmonic potentials may be found. Even more potentials must be considered when talking about a finite accuracy and finite range measurement. We conclude that energy levels do not provide all the information about the underlying confinement potential. Further insight may be achieved by combining our analysis with atomistic calculations.

Considering device simulations, it may be argued that even using an incorrect potential may yield the proper output by inputting correct energy spacings. Yet it must be stressed that in this case the electron-hole overlap as well as the selection rules will be unrealistic and good experiment–theory agreement would have to be considered a mere coincidence.

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