Two Unrelated Topics of Interest for the Purpose of Demonstration

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This paper offers a demonstration of the appearance and general document features of the Physical Review style sheet as adapted from the American Physical Society specifications for journal submissions. Although the topics in this paper were written specifically for *Publicon*, it is hoped they will nonetheless be regarded with interest by the physics community.

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I. HIGH-PRECISION VALUE FOR THE QUARTIC ANHARMONIC OSCILLATOR GROUND STATE

A. Introduction

As is well known, only a very limited number of one–dimensional potentials allow for an exact solution of the Schrödinger equation. This means that for many model potentials one has to resort to numerical solution methods. For judging their accuracy, reliability, and speed it is important to have high–precision values of certain nonexactly solvable potentials. The most investigated of such potentials is the quartic anharmonic oscillator [1-19] described by

$$-\psi_k''(z) + z^4\, \psi_k(z) = \varepsilon_k\, \psi_k(z) \tag{1}$$

The eigenfunctions to the eigenvalues ε_k decay exponentially for $z \to \pm\infty$.

B. The Hill Determinant Method

A classical method to solve Sturm–Liouville problems of type 1 is to calculate the eigenvalues of a truncated version of the corresponding Hill determinant. Using the harmonic oscillator basis $\phi_n(z)$ we write $\psi_0(z) = \sum_{k=0}^{\infty} \alpha_k\, \phi_k(z)$ where

$$-\phi_k''(z) + z^2\, \phi_k(z) = \epsilon_k\, \phi_k(z) \tag{2}$$

$$\phi_n(z) = \frac{1}{\sqrt{\sqrt{\pi}\, 2^n\, n!}}\, e^{\frac{-z^2}{2}}\, H_n(z) \tag{3}$$

Forming the matrix elements $\hbar_{m,n} = \int_{-\infty}^{\infty} \phi_m(z)\, (-\phi_n''(z) + z^4\, \phi_n(z))\, dz$. For $n \geq m$ we obtain

$$\hbar_{m,n} = \begin{cases} 0 & n - m > 4 \\ 2^{\frac{m-n}{2}-4} \sqrt{\frac{m!}{n!}} \big(32\, n\, \delta_{m,n-2}\, (n-1)^2 + 16\, (n-3)\, (n-2)\, n\, \delta_{m,n-4}\, (n-1) + \\ \quad 4\, (2\, n\, (3\, n+5)+5)\, \delta_{m,n} + 8\, (n+1)\, \delta_{m,n+2} + \delta_{m,n+4}\big) & \text{else} \end{cases} \tag{4}$$

A rough estimation shows that one obtains about 0.2 digits per harmonic oscillator state. So by taking into account the first 500 eigenstates and carrying out the calculation with about five thousand digits one obtains about 120 reliable digits for ε_0. (This calculation takes about 20 minutes on a 2000 vintage workstation using *Mathematica* 4 [20].)

$$\varepsilon_0 = 1.06036209048418289964704601669266354551520872852897793321624524169594356304434442112689629913467170351054624435858252558098276 3829 \ldots$$

The Hill determinant approach allows in addition to the calculation of the eigenvalues, the calculation of the eigenvectors. The following graphic visualizes the matrix of eigenvectors of $(h_{m,n})_{1 \leq n,m \leq 100}$. The graphic shows that the lowest eigenfunctions are quite similar to the harmonic oscillator eigenfunctions. Higher states are complicated mixtures of harmonic oscillator states. The overall "checkerboard"–like structure results from the fact that the contribution of the antisymmetric (symmetric) harmonic oscillator states to the symmetric (antisymmetric) anharmonic oscillator states is identical zero. The very high states are dominated by truncation effects and do not correctly mimic the anharmonic oscillator states.

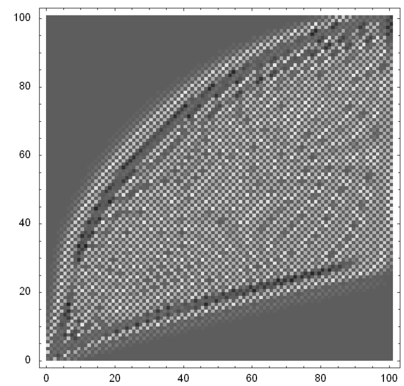

Figure 1: The matrix of eigenvectors of $(h_{m,n})_{1 \leq n,m \leq 100}$.

C. The New Algorithm

To get a very high–precision approximation of

$$-\psi''(x) + z^4\, \psi(x) = \lambda\, \psi(x) \tag{5}$$

we start with the series expansion

$$\psi(x) = y_n(x) = \sum_{k=0}^{n} a_k(\lambda)\, x^k \tag{6}$$

For the ground state we choose (ignoring normalization) $\psi(0) = 1$, $\psi'(0) = 0$. For "suitable chosen" x^* we then find high–precision approximations for the zeros of $y_n(x^*)$ and $y_n'(x^*)$. These zeros then bound λ_0 from below and above.

Using the differential equation one obtains the following recursion relation for the $a_k(\lambda)$:

$$a_k(\lambda) = \frac{a_{m-6}(\lambda) - \lambda\, a_{m-2}(\lambda)}{m^2 - m} \tag{7}$$

For large n ($n \to \infty$) we want the function $y_n(x)$ to vanish as $x \to \infty$. For a λ smaller than the smallest possible λ, the function $y_n(x^*)$ will not have a zero, but the function $y_n'(x^*)$ will have a zero for a certain x^*. For a λ larger than the smallest possible λ, the function $y_n(x^*)$ will have a zero, but the function $y_n'(x^*)$ will not have a zero for a certain x^*. This allows to find a bounding interval for λ_0. The next two graphics show $y_{80}(x)$ and $y_{80}'(x)$ for 10 equidistant values for λ from the interval $[1.05, 1.08]$ to visualize this bounding process. (For more details, see [21].)

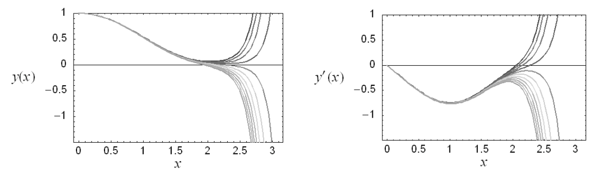

Figure 2: $y_{80}(x)$ and $y'_{80}(x)$ for 10 equidistant values for λ from the interval [1.05, 1.08].

It is straightforward to implement the calculation of the bounding interval for λ_0 in *Mathematica* in a three–line program (see [22]). Using `FindRoot` we calculate high–precision values for the zeros of $y_n(\xi)$ and $y'_n(\xi)$.

```
λBounds[n_, ξ_, opts___] :=
   Function[f, λ /. FindRoot[f[n, λ, ξ] == 0,
       {λ, 106/100, 107/100}, opts]] /@ {y, yPrime};
```

The calculation of $y_n(\xi)$ and $y'_n(\xi)$ is also straightforward based on a recursive calculations of the $a_k(\lambda)$.

```
y[n_, λ_Real, ξ_] := Module[{a6, a4, a2, ak, σ},
   {a6, a4, a2} = {1, -λ/2, λ^2/24};
    σ = a6 + a4*ξ^2 + a2*ξ^4;
    Do[ak = a6 - λ*(a2/(k*(k - 1)));
      {a6, a4, a2} = {a4, a2, ak};
      σ = σ + ak*ξ^k, {k, 6, n, 2}]; σ]

y[n_, λ_Real, ξ_] := Module[{a6, a4, a2, ak, σ},
   {a6, a4, a2} = {1, -λ/2, λ^2/24};
    σ = a6 + 2*ξ*a4 + 4*ξ^3*a2;
    Do[ak = a6 - λ*(a2/(k*(k - 1)));
      {a6, a4, a2} = {a4, a2, ak};
      σ = σ + k*ak*ξ^(k - 1), {k, 6, n, 2}]; σ]
```

Calculating now `λBounds[16000, 16,` *startingValues*`, WorkingPrecision→6000, AccuracyGoal→600, MaxIterations→100]` (where *startingValues* has been obtained from a call to `λBounds` recursively, one gets in a few minutes a 1184 digit approximation to the ground state energy of the quartic anharmonic oscillator.

ε_0 = 1.06036209048418289964704601669266354551520872852897793321624524169594356
30443444211268962991346717035105462443585825525580879808210293147013176836373
82493578922624600470817544696014163748841728225690593575779088806178879026360
15493956902751961489009429348735844094426948979012139714642909519233545338283
47033505757615112025703988852372024022184110308657373109139891545365841031116
79405833548600092274400696311267023886229714296996105921558322667137693550867
36100008318300275179262335739139061361807764985969618149941279280927284070795
61060440722946809949136275729273872791368902798424722261716944488954751370438
06840543918778772953234245874372543178323190603810687416044034374530146847278
13918612940470431034013510716071103530089298232754276615189869505650471602527
56089526262191025688200964410287815640052705292932405076382650282591124773625
38471854714402572285438485297450458570978840249066999570476844587709176202912
43752732549071164334402302947306923981908956853745359884460160023132919330593
95869304916644281633946163324287004261461237743009952234204208597735690153565
41685030894185134879573410658547971946759646679661346768858643795265451956056
82867159583388847434670120424207149192900487 32 …

Statistical analysis of the number does not show any regularity.

D. Summary

A power series based approach to the high–precision calculation of the ground state of the anharmonic oscillator was presented. *Mathematica* code to carry out the calculation, as well as results were given. The method can straightforwardly be used to calculate ten thousands of digits of the quartic anharmonic, as well as other anharmonic oscillators. Work concerning the application of the method to higher states is in progress.

All calculations and visualizations have been carried out in *Mathematica* 4.

E. Local Density of States for the Harmonic Oscillator

The next graphic shows the local density of states $\mathcal{D}_E(x) = \left\langle x \,\middle|\, \theta\big(E - \hat{H}\big) \,\middle|\, x \right\rangle$ for the harmonic oscillator [21].

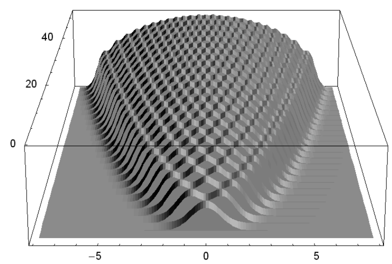

Figure 3: The local density of states $\mathcal{D}_E(x) = \left\langle x \,\middle|\, \theta\big(E - \hat{H}\big) \,\middle|\, x \right\rangle$ for the harmonic oscillator.

F. Acknowledgments

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II. ARE BRILLOUIN ZONES OF HIGH ORDER FRACTAL?

A. Introduction

Brillouin zones are among the most popular objects a solid state physicists deals with [24-27]. Despite the fundamental importance for the explanation of most properties of crystalline solids, Brillouin zones as an own subject have rarely been investigated (the only ones we are aware of are [28-31]). For electronic properties, mostly the low order Brillouin zones matter, as an ownstanding subject the high order Brillouin zones are interesting. Mathematically, the $(n + 1)$th Brillouin zone is the set of points that a line to them crosses exactly n bisector planes. In computational geometry a nth order Brillouin zones is also called nth degree Voronoi region or nth nearest point Voronoi diagrams. The most important fact for high order Brillouin zones is that their shape approaches that of a thin spherical shell and their volume is a constant. Here, for the first time we report on some computational results of higher order Brillouin zones. All calculations and visualizations were done with *Mathematica* 4 [20].

Recursive definition of Brillouin zones: Given a lattice Λ in $\mathbb{R}^d$ with lattice points $\boldsymbol{h}_i$ (i being a multiindex) the first Brillouin zone $\mathcal{BZ}_1$ is the closure of the set of all points $\boldsymbol{x}$ such that $|\boldsymbol{x} - \boldsymbol{0}| \leq |\boldsymbol{x} - \boldsymbol{h}_i|$ for all $\boldsymbol{h}_i \neq \boldsymbol{0}$. The nth order Brillouin zones is the closure of the set of all points $\boldsymbol{x}$ such that $|\boldsymbol{x} - \boldsymbol{0}| \leq |\boldsymbol{x} - \boldsymbol{h}_i|$ for all $\boldsymbol{h}_i \neq \boldsymbol{0}$ and $\boldsymbol{x} \notin \mathcal{BZ}_{n-1}$.

B. 2D Hexagonal lattice

Figure 4 shows the first twenty Brillouin zones of a 2D hexagonal lattice. It is interesting to observe that the first, third, and fourth Brillouin zones have the shape of an hexagon. For higher orders the shape becomes much more complicated.

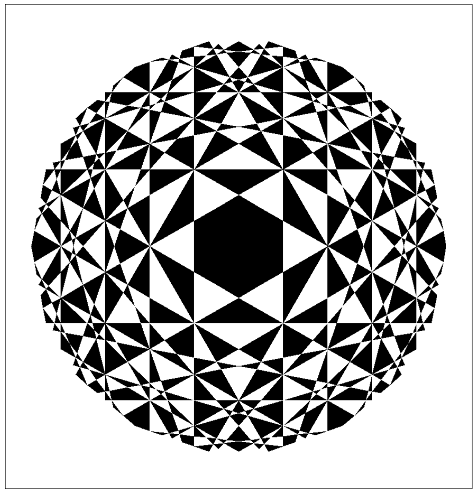

Figure 4: The first twenty Brillouin zones of a 2D hexagonal lattice.

Figure 5 shows the 200th Brillouin zone in one symmetry unit (inside an angle of 30°). One sees many small and a few quite large Landsberg zones. The distribution $p(A)$ of the area of the Landsberg zones in the limit $n \to \infty$ might be an interesting subject to study.

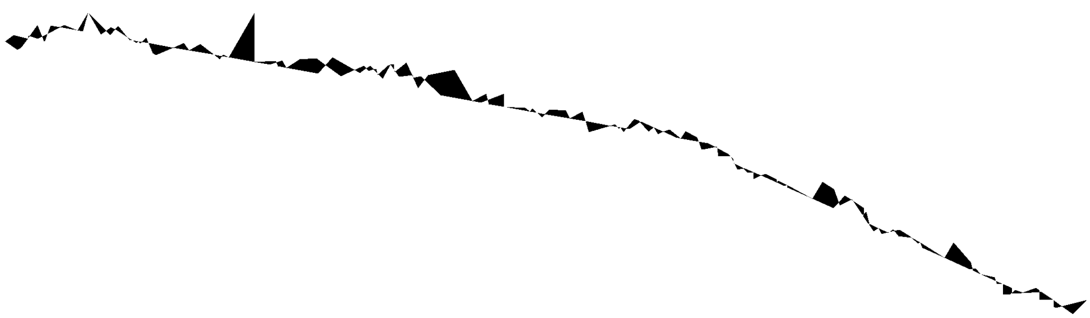

Figure 5: The 200th Brillouin zone in one symmetry unit (inside an angle of 30°).

A good numerical fit to number of faces (line segments) $\sharp_n$ of the nth Brillouin zone is $\sharp_n \propto n^{1.15}$. Figure 6 shows the circumference of the Brillouin zones normalized to the circumference of a circle with the same radius. Does the ratio approach a finite value in the limit $n \to \infty$?

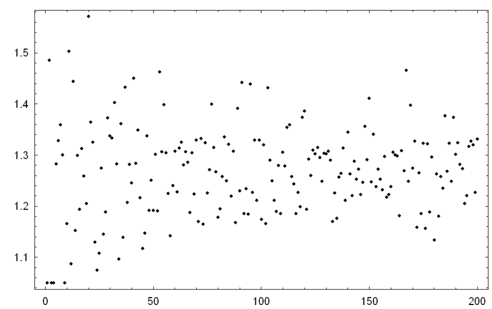

Figure 6: The circumference of the Brillouin zones normalized to the circumference of a circle with the same radius.

C. 3D Cubic Lattices

In [32] we gave a complete implementation for the effective calculation of higher order Brillouin zones of the three cubic lattice in $\mathbb{R}^3$. Figure 7 shows the (outside of) 15th Brillouin zone for the simple cubic, Figure 8 shows the 18th for the face–centered cubic and Figure 9 shows the 10th for the body–centered cubic lattice. The higher order Brillouin zones show quite complicated behavior. Large faces alternate with small ones, relatively plane regions alternate with quite structured ones. The appearance of the $n+1$th Brillouin zone is typically completely independent of the appearance of the nth Brillouin zone.

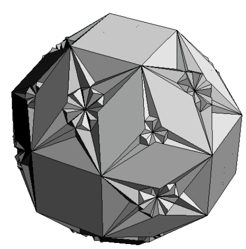

Figure 7: The (outside of) 15th Brillouin zone for the simple cubic.

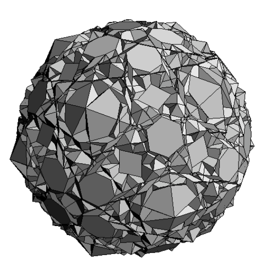

Figure 8: The (outside of) 18th Brillouin zone for the face–centered cubic.

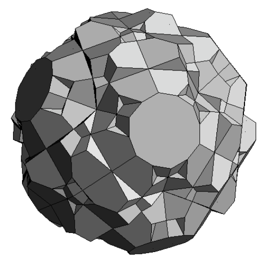

Figure 9: The (outside of) 10th Brillouin zone for the body–centered cubic lattice.

Using this implementation we analysed various properties of higher order Brillouin zones. Figure 10 shows the area of the Brillouin zones normalized to the area of a sphere of the same volume. The order of the three curves from the bottom is sc, fcc, bcc.

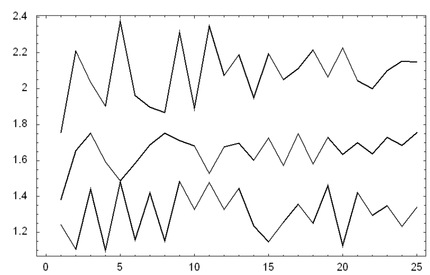

Figure 10: The area of the Brillouin zones normalized to the area of a sphere of the same volume.

The last result to be given here is the number of faces of the Brillouin zones. By a face we mean any connected planar part of the outside facing side of a Brillouin zone (point contacts separate faces). Table I gives the results for the first 25 Brillouin zones.

Table I. The results for the first 25 Brillouin zones.

n	*sc*	*fcc*	*bcc*
1	6	14	12
2	12	72	48
3	72	96	30

Table II. The results for the first 25 Brillouin zones.

n	*sc*
1	6

Table III. The results for the first 25 Brillouin zones.

n	*sc*	*fcc*
1	6	14
2	12	72

Table IV. The results for the first 25 Brillouin zones.

n	*sc*	*fcc*	*bcc*	*bcc*
1	6	14	12	12
2	12	72	48	48
3	72	96	30	30

D. Summary

Preliminary results about some computational results about higher order Brillouin zones have been presented. Further work is in progress and will be published elsewhere.

All calculations and visualizations have been carried out in *Mathematica* 4.

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