Numerical Mathematics of Quasicrystals

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Joint work with Kai Jiang
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Outline

◆ Background

◆ Quasicrystals
  ➢ Mathematics
  ➢ Experiment
  ➢ Physics
  ➢ Numerical Methods

◆ Discussion
Tilings

Tiling: covering the plane without gaps or overlaps
Tilings

Tiling: covering the plane without gaps or overlaps

Equilateral polygons: Periodic tilings
Tilings

Tiling: covering the plane without gaps or overlaps

Equilateral polygons: Periodic tilings

Pentagon
Penrose Tiling

Aperiodic tiling: no invariance by translation

R. Penrose (1974)
Penrose Tiling

Aperiodic tiling: no invariance by translation

R. Penrose (1974)

A negative example to the Hilbert’s 18th problem
Penrose Tiling

Aperiodic tiling: no invariance by translation

R. Penrose (1974)

Building up of space from congruent polyhedra

A negative example to the Hilbert’s 18th problem
Quasicrystals

The Nobel Prize in Chemistry 2011 was awarded to Shechtman "for the discovery of quasicrystals".

Quasicrystals

The role of quasicrystals

Complete Order: Periodic Crystals

Complete Disorder: Non-Crystalline
Quasicrystals

The role of quasicrystals

Complete Order: Periodic Crystals

What’s More?

Complete Disorder: Non-Crystalline
Quasicrystals

The role of quasicrystals

Complete Order: Periodic Crystals

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Quasicrystals

What’s More?
Quasicrystals

The role of quasicrystals

Complete Order: Periodic Crystals

Quasicrystals

What’s More?

Complete Disorder: Non-Crystalline

Glass
Quasicrystals

The role of quasicrystals

What’s More?

Complete Order:
Periodic Crystals

Quasicrystals

What’s More?

Complete Disorder:
Non-Crystalline

unknown

Glas
Outline

Quasicrystals

> Mathematics
> Physics
> Experiment
> Numerical Methods
Almost Periodic Function

Periodicity

\[ \cos(2\pi x) \]
Almost Periodic Function

Periodicity
Almost Periodic Function

Periodicity

\[
\cos\left(2\pi \sqrt{2} x\right)
\]
Almost Periodic Function

Periodicity

$$\cos(2\pi \sqrt{2} x)$$
Almost Periodic Function

Periodicity

$$\cos(2\pi x) + \cos(2\pi \sqrt{2}x)$$
Almost Periodic Function

Periodicity

\[ \cos(2\pi x) + \cos(2\pi \sqrt{2}x) \]
Almost Periodic Function

Periodicity $\rightarrow$ Quasi-Periodicity

\[ \cos(2\pi x) + \cos(2\pi \sqrt{2}x) \]
Almost Periodic Function

Periodicity $\rightarrow$ Quasi-Periodicity

$\cos(2\pi x) + \cos(2\pi \sqrt{2}x)$

In general, Almost Periodic Function

$$f(x) = \sum_{\lambda_n \in \Lambda} c_n e^{\lambda_n x}, \quad \Lambda \subset \mathbb{R}^d \text{ is a countable set.}$$
Yves Meyer

Meyer’s work:

✓ 1964-1973 QCs from Harmonic Analysis and Number Theory
✓ 1974-1984 Calderón-Zygmund operator theory
✓ 1983-1993 Wavelet
✓ 1994-1999 Navier-Stokes equation
✓ 2000-now QCs and Applications

2010 Gauss Prize
2017 Able Prize
Meyer’s work

Starting point: the local controls the global

\[ \sup_{x \in \mathbb{R}} |f(x)| \leq C \sup_{x \in \mathcal{K}} |f(x)| \]

\[ f(x) = \sum_{\lambda_n \in \Lambda} c_n e^{\lambda_n x}, \quad c_n \neq 0, \quad \Lambda \subset \mathbb{R}^d. \]
Meyer’s work

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\[ f(x) = \sum_{\lambda_n \in \Lambda} c_n e^{\lambda_n x}, \quad c_n \neq 0, \quad \Lambda \subset \mathbb{R}^d. \]

Problems:

- How to construct \( \Lambda \)
- The properties of \( \Lambda \)
Meyer’s work

Starting point: the local controls the global

\[
\sup_{x \in \mathbb{R}} |f(x)| \leq C \sup_{x \in \mathcal{K}} |f(x)|
\]

\[
f(x) = \sum_{\lambda_n \in \Lambda} c_n e^{\lambda_n x}, \quad c_n \neq 0, \quad \Lambda \subseteq \mathbb{R}^d.
\]

Problems:

- How to construct \( \Lambda \)
- The properties of \( \Lambda \)

A trivial case: \( \Lambda = \mathbb{Z}, f(x) \) is a periodic function
Delone Set
Delone Set

Discrete
Delone Set

Discrete

Relatively dense
Meyer’s QCs

- A **Meyer’s QC** \( \Lambda \) is a Delone set s.t. \( \Lambda - \Lambda \subset \Lambda + F \) where \( F \) is a finite set.
Meyer’s QCs

- A **Meyer’s QC** $\Lambda$ is a Delone set s.t. $\Lambda - \Lambda \subset \Lambda + F$ where $F$ is a finite set.

- **Meyer’s QCs and Algebraic numbers**

  **Theorem**: If $\Lambda$ is a **Meyer’s QC** and $\theta \Lambda \subset \Lambda \iff \theta$ is either a **Pisot number** or a **Salem number**.
Meyer’s QCs

- A **Meyer’s QC** $\Lambda$ is a Delone set s.t. $\Lambda - \Lambda \subset \Lambda + F$ where $F$ is a finite set.

- **Meyer’s QCs** and **Algebraic numbers**

  **Theorem**: If $\Lambda$ is a **Meyer’s QC** and $\theta \Lambda \subset \Lambda \iff \theta$ is either a **Pisot number** or a **Salem number**.

- **Meyer’s QCs** and **Harmonic analysis**

  **Theorem**: By **duality theory**, $f$ is a **almost periodic function** $f$ when its spectrum lies in a **Meyer’s QC** $\Lambda$. 
Cut-and-Project scheme

A constructive method (Meyer, 1972)

- High-D: Periodic Lattice
- Window: irrational slice
- Low-D: Meyer’s QCs

Cut-and-project scheme can generate tilings.

\[ \tan \alpha = \frac{1 + \sqrt{5}}{2} \]
Dynamical System

Quasi-periodic Schrödinger operator

\[(\mathcal{L}y)(t) = -y''(t) + q(\theta + wt)y(t)\]

\(\theta, w\) is rational independent.
Dynamical System

Quasi-periodic Schrödinger operator

\[(\mathcal{L}y)(t) = -y''(t) + q(\theta + wt)y(t)\]

\(\theta, w\) is rational independent.

The dynamical system

\[(\mathcal{L}y)(t) = Ey(t)\]
Dynamical System

Quasi-periodic Schrödinger operator

$$(\mathcal{L}y)(t) = -y''(t) + q(\theta + wt)y(t)$$

$\theta, w$ is rational independent.

The dynamical system

$$(\mathcal{L}y)(t) = Ey(t)$$

Equivalently

$$\begin{cases} 
\dot{x} = V_{E,q}(\theta)x, \\
\dot{\theta} = w, \\
V_{E,q}(\theta) = \begin{pmatrix} 0 & 1 \\
q(\theta) - E & 0 \end{pmatrix}
\end{cases}$$
Dynamical System

Quasi-periodic Schrödinger operator

\[(Ly)(t) = -y''(t) + q(\theta + wt)y(t)\]

\(\theta, w\) is rational independent.

The dynamical system

\[(Ly)(t) = Ey(t)\]

Equivalently

\[\begin{align*}
\dot{x} &= V_{E,q}(\theta)x, \\
\dot{\theta} &= w,
\end{align*}\]

\[V_{E,q}(\theta) = \begin{pmatrix} 0, & 1 \\ q(\theta) - E, & 0 \end{pmatrix} \]
The First Soft QCs

Dendrimer Liquid QC


$C_{12}H_{25}$
# QCs: Discovery

## Metallic QCs

<table>
<thead>
<tr>
<th>Type of quasicrystal</th>
<th>d-D</th>
<th>n-D</th>
<th>Metric</th>
<th>Symmetry</th>
<th>System</th>
<th>First Report</th>
</tr>
</thead>
<tbody>
<tr>
<td>Icosahedral</td>
<td>3D</td>
<td>6</td>
<td>(\sqrt{5})</td>
<td>m_35</td>
<td>AlMn</td>
<td>Shechtman et al., 1984</td>
</tr>
<tr>
<td>Tetrahedral</td>
<td>3D</td>
<td>6</td>
<td>(\sqrt{3})</td>
<td>m_3</td>
<td>AlLiCu</td>
<td>Donnadieu, 1994</td>
</tr>
<tr>
<td>Decagonal</td>
<td>2D</td>
<td>5</td>
<td>((\sqrt{5}))</td>
<td>10/mmm</td>
<td>AlMn</td>
<td>Chattopadhyay et al., 1985a and Bendersky, 1985</td>
</tr>
<tr>
<td>Dodecagonal</td>
<td>2D</td>
<td>5</td>
<td>(\sqrt{3})</td>
<td>12/mmm</td>
<td>NiCr</td>
<td>Ishimasa et al., 1985</td>
</tr>
<tr>
<td>Octagonal</td>
<td>2D</td>
<td>5</td>
<td>(\sqrt{2})</td>
<td>8/mmm</td>
<td>VNiSi, CrNiSi</td>
<td>Wang et al., 1987</td>
</tr>
<tr>
<td>Pentagonal</td>
<td>2D</td>
<td>5</td>
<td>((\sqrt{5}))</td>
<td>5m</td>
<td>AlCuFe</td>
<td>Bancel, 1993</td>
</tr>
<tr>
<td>Natural Icosahedral</td>
<td>3D</td>
<td>6</td>
<td>((\sqrt{5}))</td>
<td>m_35</td>
<td>khatyrkite</td>
<td>Bindi, 2009</td>
</tr>
</tbody>
</table>

## Soft QCs

<table>
<thead>
<tr>
<th>Soft matter systems</th>
<th>Type of quasicrystal</th>
<th>First Report</th>
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</thead>
<tbody>
<tr>
<td>Dendrimer liquid crystals</td>
<td>Dodecagonal</td>
<td>Zeng et al., 2004</td>
</tr>
<tr>
<td>ABC star copolymers</td>
<td>Dodecagonal</td>
<td>Hayashida et al., 2007</td>
</tr>
<tr>
<td>Colloidal nanoparticle</td>
<td>Dodecagonal</td>
<td>Talapin, 2009</td>
</tr>
<tr>
<td>Colloidal copolymer micelles nanoparticale</td>
<td>Dodecagonal</td>
<td>Talapin, 2009</td>
</tr>
<tr>
<td>ABA'C tetrablock terpolymers</td>
<td>Dodecagonal</td>
<td>Zhang, Bates, 2012</td>
</tr>
<tr>
<td>Mesoporous silica micelles</td>
<td>Dodecagonal</td>
<td>Xiao et al., 2012</td>
</tr>
<tr>
<td>Mesoporous silica nanoparticles</td>
<td>Dodecagonal</td>
<td>Sun et al. 2017</td>
</tr>
</tbody>
</table>

[http://home.iitk.ac.in/~anandh/E-book/Quasicrystals.ppt](http://home.iitk.ac.in/~anandh/E-book/Quasicrystals.ppt)
Experimental QCs

$\text{Mg}_{23}\text{Zn}_{68}\text{Y}_9$ alloy (5-fold)

\[ \tau^2 \Lambda - \tau \Lambda = \Lambda \]
\[ \tau = \frac{1+\sqrt{5}}{2} \text{ Pisot number} \]

Successive spots are at a distance inflated by $\tau$
Successive spots are at a distance inflated by \( \tau \), where

\[
\tau^2 \Lambda - \tau \Lambda = \Lambda
\]

\[
\tau = \frac{1 + \sqrt{5}}{2}
\]

is a Pisot number.

Mg\(_{23}\)Zn\(_{68}\)Y\(_9\) alloy (5-fold)

Experimental QCs \( \cap \) Meyer’s QCs

\( \tau^1, \tau^2, \tau^3, \tau^4 \)
Quasicrystals: Quasiperiodic Crystals

(Levine-Steinhardt, 1986; Mermin, 1999)

\[ f(x) = \sum_{k \in \Lambda} \hat{f}(k)e^{ikx}, \quad x \in \mathbb{R}^d \]

\[ \Lambda: \{k = \sum_{j=1}^{n} h_j b_j, \ b_j \in \mathbb{R}^d, \ h_j \in \mathbb{Z}\} \]

\( b_j \) are reciprocal primitive vectors.

Diffraction of pattern of 10-fold symmetry in experiment
Outline

- Numerical Mathematics
  - Projection method
  - Crystalline approximant method
  - One/multi mode approximation
Difficulties in Computing QCs

- Infinite systems without decay
- Finite domains, suitable boundary conditions
- Evaluate the energy density to high precision
- Put different kinds of ordered structures on an equal footing
Diophantine Approximation

Approximate AP function

\[ f(x) = \cos(2\pi x) + \cos(2\pi \sqrt{2} x) \]

\[ |f(x + n) - f(x)| \leq 2|\sin(\pi \sqrt{2} n)| \leq 2\pi \sqrt{2} n \]
Diophantine Approximation

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Diophantine inequality

\[ \left| \theta - \frac{p}{q} \right| < \frac{1}{q^2} \]
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Continued fraction approximation

\[ \frac{p}{q} : 1, \frac{3}{2}, \frac{7}{5}, \frac{17}{12}, \frac{41}{29}, \frac{99}{70}, \frac{239}{169}, \ldots \rightarrow \sqrt{2} \]
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**Idea:** use a (large) periodic crystal to approximate a QC

- **Frequency domain:** satisfies Diophantine inequality

\[
|Lk - [Lk]| < \varepsilon, \quad k \in \Lambda_{QC}
\]
Error of CAM

- Error: 1. Finity approx. Infinity (Diophantine Approximation error);
  2. Numerical error
Error of CAM

- Error: 1. Finity approx. Infinity (Diophantine Approximation error);
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- 2D 12 fold symmetric QC

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<th>$E_{SDA}$</th>
<th>0.19098</th>
<th>0.17486</th>
<th>0.07042</th>
<th>0.04953</th>
<th>0.03583</th>
<th>0.02961</th>
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<td>$L$</td>
<td>30</td>
<td>208</td>
<td>410</td>
<td>3404</td>
<td>6016</td>
<td>32312</td>
<td>82262</td>
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Computational domain: $[L \times 2\pi)^2$
## Error of CAM

- **Error:**
  1. Infinity approx. Infinity (Diophantine Approximation error);
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- **2D 12 fold symmetric QC**

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- **Computational domain:** $[L \times 2\pi)^2$

- **2D 10 fold symmetric QC**

```
<table>
<thead>
<tr>
<th>$E_{SDA}$</th>
<th>0.1669</th>
<th>0.0918</th>
<th>0.0374</th>
<th>0.0299</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
<td>126</td>
<td>204</td>
<td>3372</td>
<td>53654</td>
<td>...</td>
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</table>
```
CAM

CAM: Fourier spectral method

\[
\phi(x) \approx \sum_{k \in \Lambda_{QC}} \hat{\phi}(Lk) e^{i[Lk] \cdot x}, \quad x \in [0, L \cdot 2\pi)^d
\]
CAM

◆ CAM: Fourier spectral method

\[
\phi(\mathbf{x}) \approx \sum_{\mathbf{k} \in \Lambda_{QC}} \hat{\phi}([L\mathbf{k}]) e^{i[L\mathbf{k}] \cdot \mathbf{x}}, \quad \mathbf{x} \in [0, L \cdot 2\pi)^d
\]

☐ Computational complexity: \( L \) should be small
CAM

CAM: **Fourier spectral method**

\[ \phi(\mathbf{x}) \approx \sum_{\mathbf{k} \in \Lambda_{QC}} \hat{\phi}(\mathbf{Lk}) e^{i[\mathbf{Lk}] \cdot \mathbf{x}}, \quad \mathbf{x} \in [0, L \cdot 2\pi)^d \]

- Computational complexity: \( L \) should be small
- Precision: small SDA error requires that \( L \) is large
CAM

◆ CAM: **Fourier spectral method**

\[
\phi(x) \approx \sum_{k \in \Lambda_{QC}} \hat{\phi}([Lk]) e^{i[Lk] \cdot x}, \quad x \in [0, L \cdot 2\pi)^d
\]

- Computational complexity: \( L \) should be small  **Contradiction**
- Precision: small SDA error requires that \( L \) is large
Projection Method: Motivation

Avoid Diophantine Approximation

\[ f(x) = \cos(2\pi x) + \cos(2\pi \sqrt{2}x) \]
Projection Method: Motivation

Avoid Diophantine Approximation

\[ f(x) = \cos(2\pi x) + \cos(2\pi \sqrt{2}x) \]

\[ f(x) = \cos(2\pi x) + \cos(2\pi y) \]
Projection Method: Motivation
Projection Method: Motivation

12-fold symmetry in Fourier domain

\[ k_1 = (1, 0), \quad k_2 = (0, 1) \]
Projection Method: Motivation

12-fold symmetry in Fourier domain

\[ k_1 = (1, 0) \]  
\[ k_2 = (0, 1) \]  
\[ (\cos(\pi/6), \sin(\pi/6)) \]  
\[ (\cos(\pi/3), \sin(\pi/3)) \]  
\[ (\cos(\pi/3), -\sin(\pi/3)) \]  
\[ (-\cos(\pi/6), \sin(\pi/6)) \]  
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\[ (-\cos(\pi/3), \sin(\pi/3)) \]  
\[ (-\cos(\pi/3), -\sin(\pi/3)) \]
Projection Method: Motivation

12-fold symmetry in Fourier domain

irrational number

\[ k_1 = (1, 0) \]

\[ k_2 = (0, 1) \]

\[ (-\cos(\pi/3), \sin(\pi/3)) \]

\[ (\cos(\pi/3), -\sin(\pi/3)) \]

\[ (-\cos(\pi/6), \sin(\pi/6)) \]

\[ (\cos(\pi/6), -\sin(\pi/6)) \]

\[ (-1, 0) \]

\[ (\cos(\pi/3), \sin(\pi/3)) \]

\[ (\cos(\pi/3), -\sin(\pi/3)) \]
Projection Method: Motivation

12-fold symmetry in Fourier domain
Projection Method: Motivation

12-fold symmetry in Fourier domain
Projection Method: Motivation

12-fold symmetry in Fourier domain

\(-1,0,1,0\)  \((0,0,0,1)\)  \((0,0,1,0)\)
\((0,-1,0,1)\)  \((0,1,0,0)\)
\((-1,0,0,0)\)  \((1,0,0,0)\)
\((0,-1,0,0)\)  \((0,1,0,-1)\)
\((0,0,-1,0)\)  \((1,0,-1,0)\)
\((0,0,0-1)\)
Projection Method: Motivation

12-fold symmetry in Fourier domain

\((-1, 0, 1, 0)\) \(\rightarrow\) \((0, 0, 0, 1)\) \(\rightarrow\) \((0, 0, 1, 0)\)

\((0, -1, 0, 1)\) \(\rightarrow\) \((0, 1, 0, 0)\)

\((-1, 0, 0, 0)\) \(\rightarrow\) \((1, 0, 0, 0)\)

\((0, -1, 0, 0)\) \(\rightarrow\) \((0, 1, 0, -1)\)

\((0, 0, -1, 0)\) \(\rightarrow\) \((1, 0, -1, 0)\)

\((0, 0, 0 - 1)\)

\((-\cos(\pi/3), \sin(\pi/3))\) \(\rightarrow\) \((\cos(\pi/3), \sin(\pi/3))\)

\((-\cos(\pi/6), \sin(\pi/6))\) \(\rightarrow\) \((\cos(\pi/6), \sin(\pi/6))\)

\((-1, 0)\) \(\rightarrow\) \((\cos(\pi/6), -\sin(\pi/6))\)

\((-\cos(\pi/6), -\sin(\pi/6))\) \(\rightarrow\) \((\cos(\pi/6), -\sin(\pi/6))\)

\((-\cos(\pi/3), -\sin(\pi/3))\) \(\rightarrow\) \((\cos(\pi/3), -\sin(\pi/3))\)

\((0, -1)\)
Projection Method: Motivation

12-fold symmetry in Fourier domain

\[(0, 0, 0, 1) \rightarrow (0, 0, 1, 0) \rightarrow (0, 0, 1, 0) \rightarrow (0, 0, 0, 1) \rightarrow \ldots \]

\[
\begin{align*}
(1, 0, 0, 0) \\
(-1, 0, 0, 0) \\
(0, -1, 0, 0) \\
(0, 0, -1, 0) \\
(0, 0, 0, -1)
\end{align*}
\]

\[
\left(\frac{-\pi}{3}, \frac{\pi}{3}\right) \rightarrow \left(\frac{\pi}{3}, \frac{\pi}{3}\right) \rightarrow \left(\frac{\pi}{3}, \frac{\pi}{3}\right) \rightarrow \left(\frac{-\pi}{3}, \frac{-\pi}{3}\right) \rightarrow \ldots
\]

\[
\begin{align*}
(1, 0) \\
(-1, 0) \\
(0, -1) \\
(-1, 0) \\
(0, 0)
\end{align*}
\]
Projection Method: Motivation

12-fold symmetry in Fourier domain

Projection matrix:

\[
\begin{pmatrix}
1 & \cos(\pi/6) & \cos(\pi/3) & 0 \\
0 & \sin(\pi/6) & \sin(\pi/3) & 1
\end{pmatrix}
\]
Projection Method: Motivation

12-fold symmetry in Fourier domain

Projection matrix: \[
\begin{pmatrix}
1 & \cos(\pi/6) & \cos(\pi/3) & 0 \\
0 & \sin(\pi/6) & \sin(\pi/3) & 1
\end{pmatrix}
\]

✓ A d-D QC can be embedded into an n-D periodic structure
✓ Implement in Fourier space
Projection Matrix

**Frequency set**: high-dimension representation

**Projection matrix**: connects high-D and low-D

\[
\Lambda_{12fold} = P \mathbb{Z}^4
\]

\[
P = \begin{pmatrix}
1 & \cos(\pi/6) & \cos(\pi/3) & 0 \\
0 & \sin(\pi/6) & \sin(\pi/3) & 1 
\end{pmatrix}
\]
Projection Matrices

2D 8-fold

\[
\begin{pmatrix}
1 & \cos(\pi/4) & 0 & \cos(3\pi/4) \\
0 & \sin(\pi/4) & 1 & \sin(3\pi/4)
\end{pmatrix}
\]

2D 10-fold

\[
\begin{pmatrix}
1 & \cos(\pi/5) & \cos(2\pi/5) & \cos(3\pi/5) \\
0 & \sin(\pi/5) & \sin(2\pi/5) & \sin(3\pi/5)
\end{pmatrix}
\]

3D Icosahedron

\[
\begin{pmatrix}
1 & \tau/2 & \tau/2 & \tau/2 & 0 & 0 \\
0 & 1/2 & -1/2 & -1/2 & 1 & 0 \\
0 & (1-\tau)/2 & (\tau - 1)/2 & (1-\tau)/2 & 0 & 1
\end{pmatrix}
\]

\[\tau = 2\cos(\pi/5)\]
Projection Method

◆ Projection method

\[ \varphi(x) = \sum_{k \in \Lambda_{QC}} \hat{\varphi}(k)e^{ik \cdot x}, \quad x \in \mathbb{R}^d \]

\[ \Lambda_{QC} : \{ k = PBh, \ h \in \mathbb{Z}^n, \ P \in \mathbb{R}^{d \times n}, \ B \in \mathbb{R}^{n \times n}, \ n \geq d \} \]
Projection Method

- Projection method

\[ \varphi(x) = \sum_{k \in \Lambda_{QC}} \hat{\varphi}(k) e^{ik \cdot x}, \quad x \in \mathbb{R}^d \]

\[ \Lambda_{QC} : \{ k = PBh, \ h \in \mathbb{Z}^n, \ P \in \mathbb{R}^{d \times n}, \ B \in \mathbb{R}^{n \times n}, n \geq d \} \]

- Assume that \( \{ \hat{\varphi}(k) \}_{k \in \Lambda_{QC}} \subset \ell^2(\mathbb{Z}^n) \)
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- Implement in an \( n \)-D unit cell

- Periodic crystals: \( P = I_d \)
In projection method, the **energy density** can be evaluated by

**Theorem:** For a $d$-dimensional quasicrystal $\varphi(\mathbf{x})$, using the projection method expansion, we have

$$
\lim_{R \to \infty} \frac{1}{B(0, R)} \int_{B(0, R)} \varphi(\mathbf{x}) \, d\mathbf{x} = \hat{\varphi}(0)
$$
Optimize Unit Cell

\[ F[\varphi(x)] \quad \rightarrow \quad F[\varphi(x); B] \]

When studying QCs,

\[ \min_{\varphi(x), B} F[\varphi(x); B] \]
One(Multi)-Modes Approximation

- Presuppose some properties of structures

  - 6-fold symmetry and $|k| = 1$

$$\varphi(x) = \sum_{j=1}^{6} \hat{\phi}_1 e^{ik_j \cdot x}$$

$$F[\varphi(x)] \rightarrow F(\hat{\phi}_1)$$
One(Multi)-Modes Approximation

◆ Presuppose some properties of structures

- 6-fold symmetry and $|k| = 1$

\[
\varphi(x) = \sum_{j=1}^{6} \hat{\varphi}_1 e^{ik_j \cdot x}
\]

\[
F[\varphi(x)] \rightarrow F(\hat{\varphi}_1)
\]

✓ Qualitative analysis
✓ Be available to limited cases
Phase Field Crystal Models

Expansion of the free energy with respect to $\varphi(x)$

\[
F[\varphi(x)] = \frac{1}{V} \int_V \left[ -\frac{\varepsilon}{2} \varphi^2(x) - \frac{\alpha}{3} \varphi^3(x) + \frac{1}{4} \varphi^4(x) \right] dx + \frac{1}{V} \int_V \int_V \frac{\gamma}{2} \left[ \varphi(x)G(x, x')\varphi(x') \right] dx dx'
\]

Periodic crystals: one length scale

\[
G(x, x') = (\nabla^2 + 1)^2 \delta(x, x')
\]

QCs: two length scales

\[
G(x, x') = (\nabla^2 + q_1^2)(\nabla^2 + q_2^2)^2 \delta(x, x')
\]

\[
\frac{q_1}{q_2} = 2 \cos\left(\frac{2\pi}{N}\right), \quad N = 8, 10, 12.
\]
Comparison

Projection method can obtain exact energy density.

Take Lifshitz-Petrich model \((PRL, 1997)\) as an example

\[
F[\varphi(\mathbf{x})] = \frac{1}{V} \left\{ \int_{V} \gamma \left[ (1 + \nabla^{2})(q^2 + \nabla^{2})\varphi(\mathbf{x}) \right]^{2} - \frac{\varepsilon}{2} \varphi^{2}(\mathbf{x}) - \frac{\alpha}{3} \varphi^{3}(\mathbf{x}) + \frac{1}{4} \varphi^{4}(\mathbf{x}) \right\} d\mathbf{x}
\]

\[
E_{SDA} = 0.19098
\]
Comparison

Projection method can obtain exact energy density.

Take Lifshitz-Petrich model (PRL, 1997) as an example

\[
F[\varphi(\boldsymbol{x})] = \frac{1}{V} \left\{ \frac{\gamma}{2} \left[ (1 + \nabla^2)(q^2 + \nabla^2)\varphi(\boldsymbol{x}) \right]^2 - \frac{\epsilon}{2}\varphi^2(\boldsymbol{x}) - \frac{\alpha}{3}\varphi^3(\boldsymbol{x}) + \frac{1}{4}\varphi^4(\boldsymbol{x}) \right\} d\boldsymbol{x}
\]

\[E_{SDA} = 0.17486\]
Comparison

Projection method can obtain exact energy density.

Take Lifshitz-Petrich model (PRL, 1997) as an example

\[ F[\varphi(\mathbf{x})] = \frac{1}{V} \left\{ \int_V \frac{\gamma}{2} \left[ (1 + \nabla^2)(q^2 + \nabla^2)\varphi(\mathbf{x}) \right]^2 - \frac{\varepsilon}{2}\varphi^2(\mathbf{x}) - \frac{\alpha}{3}\varphi^3(\mathbf{x}) + \frac{1}{4}\varphi^4(\mathbf{x}) \right\} d\mathbf{x} \]

\[ E_{SDA} = 0.07042 \]
Comparison

Projection method can obtain exact energy density.

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\]
Comparison

Projection method (PM) costs less CPU time.
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The precision is enough.
QCs in LP Model

Projection method can discover more QCs

Figure: Real space densities and their spectra of (a) 12-fold, (b) 10-fold, (c) 8-fold QCs computed by the Projection Method in the 4-D space ($24^4$).
Stability of 2D QCs

Phase diagram

Original phase diagram in Lifshitz-Petrich’s paper (1997, PRL).
3D Icosahedral QCs

$$F[\varphi(\mathbf{x})] = \frac{1}{V} \int_V \int_V \frac{\gamma}{2} \left[ \varphi(\mathbf{x}) G(\mathbf{x}, \mathbf{x}') \varphi(\mathbf{x}') \right] d\mathbf{x} d\mathbf{x}'$$

$$+ \frac{1}{V} \int_V \left[ -\frac{\varepsilon}{2} \varphi^2(\mathbf{x}) - \frac{\alpha}{3} \varphi^3(\mathbf{x}) + \frac{1}{4} \varphi^4(\mathbf{x}) \right] d\mathbf{x}$$

- Gaussian-polynomial potential

$$G'(\mathbf{x}) = e^{\sigma^2 \mathbf{x}^2/2} (c_0 + c_2 \mathbf{x}^2 + c_4 \mathbf{x}^4 + c_6 \mathbf{x}^6 + c_8 \mathbf{x}^8)$$

**Table 1.** Potential parameters used in the present study.

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<th>$d_0$</th>
<th>$d_2$</th>
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<td>0.000087</td>
<td></td>
</tr>
</tbody>
</table>

$$1/(2 \cos(\pi/5))$$
3D Icosahedral QCs

Diffraction pattern of 3d icosahedral QCs obtained by projection method in the 6-D space $^{16^6}$. 
3D Icosahedral QCs

Diffraction pattern of 3d icosahedral QCs obtained by projection method in the 6-D space\(^{(16)}\).

Compare with experiment

Cu-Ga-Mg-Sc alloys, Phil. Mag. Lett. 2002, 82, 483
3D Icosahedral QCs

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Phase Diagrams

Two-modes approximation method
Phase Diagrams

Two-modes approximation method

Projection method
Phase Diagrams

Two-modes approximation method

Projection method

Big Difference!
Phase Diagrams

Big Difference!

Two-modes approximation method

Projection method

Algorithm plays an important role in studying QCs!
Outline

◆ Discussion and Open Problems
QCs and Riemann Conjecture

- Riemann Conjecture
  - \( \zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \)
  - Critical line: \( \frac{1}{2} + ti \)
Problems

- Metallic QCs and Soft QCs
- Phase transition between crystals/QCs and QCs
- ...

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Problems

- What’s a QC in mathematical language?
- Projection method, Cut-and-Projection scheme
- Mathematical, Physical, Experimental QCs
- Which physical model can produce QCs?
- More structures between perfect crystals and disordered
- …
Thank you!

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