Invariance and the structure of matter

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Thanks: Kaushik Dayal, Stefan Müller, Traian Dumitrica
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<th>Name</th>
<th>School</th>
<th>Year</th>
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<td>Millard Beatty</td>
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<td>Samson Adeleke</td>
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<td>Richard James</td>
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<td>Yi-Chao Chen</td>
<td>University of Minnesota-Minneapolis</td>
<td>1985</td>
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<td>Ernest MacMillan</td>
<td>University of Minnesota-Minneapolis</td>
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<td>Giovanni Zanzotto</td>
<td>University of Minnesota-Minneapolis</td>
<td>1990</td>
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According to our current on-line database, Jerald Ericksen has 14 students and 173 descendants.
Jerald L. Ericksen  
Ph.D. Indiana University 1951
Dissertation: Some Geometrical Problems Connected with Ideal Gas Flows

David Gilbarg
Dissertation: On the Structure of the group of p-adic 1-units

Emil Artin  Dr. phil. Universität Leipzig 1921
Dissertation: Quadratische Körper im Gebiete der höheren Kongruenzen
Advisor 1: Gustav Herglotz  
Advisor 2: Otto Ludwig Hölder

Otto Ludwig Hölder
Dissertation: Beiträge zur Potentialtheorie

Gustav Herglotz
Dr. phil. Ludwig-Maximilians-Universität München 1900
Advisor 1: Hugo Hans von Seeliger  
Advisor 2: Ludwig Boltzmann

Paul Du Bois-Reymond
Ph.D. Universität Berlin 1859
Dissertation: De aequilibrio fluidorum

Ludwig Boltzmann
Biography MathSciNet
Dr. phil. Universität Wien 1866
Dissertation: Über die mechanische Bedeutung des zweiten Hauptsatzes mechanischen Wärmetheorie (On the Mechan Law of Thermodyna

Heinrich Ferdinand Scherk
Ph.D. Universität Berlin 1823

Friedrich Wilhelm Bessel
Dr. phil. honoris causa Georg-August-Universität Göttingen 1810

Carl Friedrich Gauß
Dissertation: Demonstratio nova theorematis omnem functionem algebraicam rationalem integram unius variabilis in factores reales primi vel secundi gradus resolvi posse
Three examples

…of invariance under discrete groups, and implications for the structure of matter

- An invariant manifold of molecular dynamics

- Maxwell-Boltzmann equation

- Methods of structure determination for non-crystalline structures (Maxwell’s equations)
Isometry groups

\[ g = (Q|c), \quad Q \in O(3), \quad c \in \mathbb{R}^3 \]

\[ g(x) = Qx + c, \quad x \in \mathbb{R}^3 \]

\[ g_1 = (R_1|c_1), \quad g_2 = (R_2|c_2), \quad g_1 g_2 = (R_1 R_2|c_1 + R_1 c_2) \]

This product rule implies \[ g_1 g_2(x) = g_1(g_2(x)) \]

Identity \[ id = (I|0) \]

The main subject of *The International Tables of Crystallography* are isometry groups containing three linearly independent translations \[ (I|e_1) \quad (I|e_2) \quad (I|e_3) \]
Examples of isometry groups

- Translation group

\[ G_T = \{ t_1^p t_2^q t_3^r : p, q, r \in \mathbb{Z} \} = \{ (I|p)e_1 + qe_2 + re_3 : p, q, r \in \mathbb{Z} \} \]

- Theorem: If a discrete group of isometries does not contain a translation and does not consist entirely of rotations, it is expressible in one of the forms

A \{ h^p : p \in \mathbb{Z} \},
B \{ h^p f^m : p \in \mathbb{Z}, m = 1, 2 \},
C \{ h^p g^q : p \in \mathbb{Z}, q = 1, \ldots, n \},
D \{ h^p g^q f^m : p \in \mathbb{Z}, q = 1, \ldots, n, m = 1, 2 \},

where

1. \( h = (R_\theta \tau e + R_\theta - I)x_0 \), \( R_\theta e = e \), \( |e| = 1 \), \( x_0 \cdot e = 0 \), \( e, x_0 \in \mathbb{R}^3 \), \( \tau \neq 0 \), and \( \theta \) is an irrational multiple of \( 2\pi \).  
2. \( g = (R_\psi |(R_\psi - I)x_0) \), \( R_\psi e = e \), is a proper rotation with angle \( \psi = 2\pi/n \), \( n \in \mathbb{Z} \), \( n \neq 0 \).
3. \( f = (R |(R - I)x_1) \), \( R = -I + 2e_1 \otimes e_1 \), \( |e_1| = 1 \), \( e \cdot e_1 = 0 \) and \( x_1 = x_0 + \xi e \), for some \( \xi \in \mathbb{R} \).
Three examples

...of invariance under discrete groups and implications for the structure of matter

- An invariant manifold of molecular dynamics
- Maxwell-Boltzmann equation
- Methods of structure determination for non-crystalline structures (Maxwell’s equations)
A time-dependent invariant manifold of the equations of molecular dynamics

\[ y_k(t), \ k = 1, \ldots, M \] simulated atoms

\[ G = \{ g_1, g_2, \ldots, g_N \} \] a discrete group of isometries (\( N \) can be infinite)

\[ y_{i,k}(t) = g_i(y_k(t)), \] all of the atoms

\[ i = 1, \ldots, N, \ k = 1, \ldots, M \]

The elements \( g_i \) can depend on \( t > 0 \), but this time dependence must be consistent with

\[ \frac{d^2 y_{j,k}(t)}{dt^2} = \frac{d^2}{dt^2} g_j(y_k(t)) = Q_j \frac{d^2 y_k(t)}{dt^2} \]

\[ g_j = (Q_j|c_j) \in G, \ j = 1, \ldots, N, \ k = 1, \ldots, M \]
Atomic forces

The force on atom $i, k$ is denoted by the suggestive notation $-\partial \varphi / \partial y_{i,k} : \mathbb{R}^{3N} \to \mathbb{R}^3$

The force satisfies

- **Frame-indifference** $\mathbf{Q} \in O(3)$, $\mathbf{c} \in \mathbb{R}^3$

$$\mathbf{Q} \frac{\partial \varphi}{\partial y_{i,k}} (\ldots, y_{i_1,1}, \ldots y_{i_1,M}, \ldots, y_{i_2,1}, \ldots y_{i_2,M}, \ldots)$$

$$= \frac{\partial \varphi}{\partial y_{i,k}} (\ldots, Qy_{i_1,1} + \mathbf{c}, \ldots Qy_{i_1,M} + \mathbf{c}, \ldots, Qy_{i_2,1} + \mathbf{c}, \ldots Qy_{i_2,M} + \mathbf{c}, \ldots)$$

- **Permutation invariance**

$$\frac{\partial \varphi}{\partial y_{\Pi(i,k)}} (\ldots, y_{i_1,1}, \ldots y_{i_1,M}, \ldots, y_{i_2,1}, \ldots y_{i_2,M}, \ldots)$$

$$= \frac{\partial \varphi}{\partial y_{i,k}} (\ldots, y_{\Pi(i_1,1)}, \ldots y_{\Pi(i_1,M)}, \ldots, y_{\Pi(i_2,1)}, \ldots y_{\Pi(i_2,M)}, \ldots)$$

where $\Pi$ is a permutation that preserves species.

Preservation of species means that if $(i, k) = \Pi(j, \ell)$ then the species (i.e., atomic mass and number) of atom $i, k$ is the same as the species of atom $j, \ell$. 

(These conditions satisfied, e.g., by the Hellmann-Feynman force based on Born-Oppenheimer quantum mechanics)
Potential energy

These conditions can be found by formally differentiating the frame-indifference and permutation invariance of the potential energy,

\[ \varphi(\ldots, Y_{i_1,1}, \ldots, Y_{i_1,M}, \ldots, Y_{i_2,1}, \ldots Y_{i_2,M}, \ldots) \]

\[ = \varphi(\ldots, Y_{\Pi(i_1,1)}, \ldots Y_{\Pi(i_1,M)}, \ldots, Y_{\Pi(i_2,1)}, \ldots, Y_{\Pi(i_2,M)}, \ldots) \]

\[ = \varphi(\ldots, Qy_{i_1,1} + c, \ldots Qy_{i_1,M} + c, \ldots, Qy_{i_2,1} + c, \ldots, Qy_{i_2,M} + c, \ldots) \]

( but of course this calculation would not make sense when \( N = \infty \) )
Theorem

Assume the restrictions on the potential energy above and let \( G = \{g_1, g_2, \ldots, g_N\} \) be a time-dependent discrete group of isometries satisfying the restriction on the time-dependence given above. If \( y_k(t), k = 1, \ldots, M \) satisfy the equations of molecular dynamics, i.e.,

\[
m_k \ddot{y}_k = -\frac{\partial \varphi}{\partial y_{1,k}}(\ldots, y_{i,1}, \ldots, y_{i,M}, y_{i+1,1}, \ldots y_{i+1,M}, \ldots)
\]

\[
= -\frac{\partial \varphi}{\partial y_{1,k}}(\ldots, g_i(y_1), \ldots, g_i(y_M), g_{i+1}(y_1), \ldots g_{i+1}(y_M), \ldots)
\]

\[
y_k(0) = y_k^0, \quad \dot{y}_k(0) = v_k^0, \quad k = 1, \ldots, M
\]

then \( y_{j,k}(t) \) also satisfy the equations of molecular dynamics:

\[
m_k \ddot{y}_{j,k}(t) = -\frac{\partial \varphi}{\partial y_{j,k}}(\ldots, y_{i,1}(t), \ldots, y_{i,M}(t), y_{i+1,1}(t), \ldots, y_{i+1,M}(t), \ldots)
\]
Proof

There is a permutation $\Pi$, depending on the choice of $g$, such that

$$y_{\Pi(i,k)}(t) = g(y_{i,k}(t)), \; i = 1, \ldots, N, \; k = 1, \ldots, M$$

Fix $j \in \{1, \ldots, N\}$ and choose $g = g_j^{-1} = (Q_j^T | - Q_j^T c_j)$

The corresponding permutation $\Pi$ satisfies $\Pi(j,k) = (1,k)$

$$m_k \ddot{y}_{j,k}(t) = m_k Q_j \ddot{y}_k(t) = -Q_j \frac{\partial \varphi}{\partial y_{1,k}} (\ldots, y_{i,1}(t), \ldots, y_{i,M}(t), y_{i+1,1}(t), \ldots, y_{i+1,M}(t), \ldots)$$

$$= -Q_j \frac{\partial \varphi}{\partial y_{\Pi(i,k)}} (\ldots, y_{i,1}(t), \ldots, y_{i,M}(t), y_{i+1,1}(t), \ldots, y_{i+1,M}(t), \ldots)$$

$$= -Q_j \frac{\partial \varphi}{\partial y_{\Pi(i,1)}} (\ldots, y_{\Pi(i,1)}(t), \ldots, y_{\Pi(i,M)}(t), \ldots, y_{\Pi(i+1,1)}(t), \ldots, y_{\Pi(i+1,M)}(t), \ldots)$$

$$= -Q_j \frac{\partial \varphi}{\partial y_{j,k}} (\ldots, g_j^{-1}(y_{i,1}(t)), \ldots, g_j^{-1}(y_{i,M}(t)), g_j^{-1}(y_{i+1,1}(t)), \ldots, g_j^{-1}(y_{i+1,M}(t)), \ldots)$$

$$= -Q_j \frac{\partial \varphi}{\partial y_{j,k}} (\ldots, Q_j^T y_{i,1}(t) - Q_j^T c_j, \ldots, Q_j^T y_{i,M}(t) - Q_j^T c_j, \ldots)$$

$$= -Q_j^T y_{i+1,1}(t) - Q_j^T c_j, \ldots, Q_j^T y_{i+1,M}(t) - Q_j^T c_j, \ldots)$$

$$= -\frac{\partial \varphi}{\partial y_{j,k}} (\ldots, y_{i,1}(t), \ldots, y_{i,M}(t), y_{i+1,1}(t), \ldots, y_{i+1,M}(t), \ldots)$$
Allowed time dependence of the group elements

\[ g_j = (Q_j | c_j), \quad Q_j \in O(3), \quad c_j \in \mathbb{R}^3 \]

\[ \frac{d}{dt}Q_j = Q_j W_j \] (no sum), where \( W_j = -W_j^T \)

The permitted time-dependence,

\[ \frac{d^2}{dt^2} (Q_j y_k + c_j) = Q_j \frac{d^2 y_k(t)}{dt^2} \]

that is,

\[ \ddot{c}_j = -Q_j (W_j^2 y_k + \dot{W}_j y_k + 2W_j \dot{y}_k) \]

\[ k = 1, \ldots, M, \quad t > 0 \]

This is satisfied (in the absence of excessive assumptions on the solution)
if and only if

\[ \ddot{c}_j = 0 \quad \text{and} \quad W_j = 0 \]

That is, \( Q_j \in O(3) \) must be constant and \( c_j = a_j t + b_j \) must be an affine function of \( t \)
This is an invariant manifold of the equations of molecular dynamics

\[ p = \{p_1, \ldots, p_N\} \]

\[ q = \{q_1, \ldots, q_N\} \]

\[ (p_0, q_0) \]

In the case of the translation group...

\[ p = \{m_k \dot{y}_{i,k}\} = m_k \frac{d}{dt} g_i(y_{1,k}, t) = m_k Q_i y_{1,k} + m_k a_i \]

\[ q = \{y_{i,k}\} = g_i(y_{1,k}, t) = Q_i y_{1,k} + a_i t + b_i \]

The form of the manifold is independent of the material
Simplest case - translation group

\[ G_T = \{(I|\nu^1e_1 + \nu^2e_2 + \nu^3e_3) : \nu^1, \nu^2, \nu^3 \in \mathbb{Z}\} \]

discrete translation group

all of the atoms

\[ y_{\nu,k}(t), \quad \nu \in \mathbb{Z}^3, \quad k = 1, \ldots, M, \quad t > 0 \]

simulated atoms

\[ y_k(t) = y_{(0,0,0),k}(t), \quad k = 1, \ldots, M \]

\[ y_{\mu,k}(t) = g_\mu(y_k(t)) = y_k(t) + \mu^i e_i + \mu^i tAe_i = y_k(t) + (I + tA)(\mu^i e_i) \]

permitted time-dependence

October 24, 2015
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All of continuum mechanics inherits this (these) invariant manifold(s)

\[
\begin{align*}
\mathbf{y}(\mathbf{x}, t) &= (\mathbf{I} + t\mathbf{A})\mathbf{x} & \mathbf{v}(\mathbf{y}, t) &= A(\mathbf{I} + t\mathbf{A})^{-1}\mathbf{y}
\end{align*}
\]

because

\[
\rho(\mathbf{v}_t + \nabla \mathbf{v} \mathbf{v}) = \nabla \cdot \sigma = 0
\]

If thermodynamics is included, the energy equation becomes an ODE for the temperature

\[
\theta(\mathbf{x}, t) = \tilde{\theta}(t)
\]

The solution for the temperature is not universal.
Other groups besides the translation group


B. de St. Venant, Memoire sur la torsion des prisms, Mem. Des Savants Etrangers 14 (1855), 233-560
Three examples

...of invariance under discrete groups and implications for the structure of matter

- An invariant manifold of molecular dynamics

- Maxwell-Boltzmann equation

- Methods of structure determination for non-crystalline structures (Maxwell’s equations)
Maxwell-Boltzmann equation

\[ f : \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}^\geq \quad f(t, y, \mathbf{v}) \]

Maxwell-Boltzmann equation

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{y}} = \mathcal{C} f(\mathbf{v}) = \int_{\mathbb{R}^3} \int_{\mathcal{S}} (f' f' - f_\ast f) B(\mathbf{v}_\ast - \mathbf{v}, \omega) \, d\omega d\mathbf{v}_\ast \]

\[ f_\ast = f(t, y, \mathbf{v}_\ast) = f(t, y, \mathbf{v}_\ast - ((\mathbf{v}_\ast - \mathbf{v}) \cdot \mathbf{e}) \mathbf{e}) \]

\[ f' = f(t, y, \mathbf{v}') = f(t, y, \mathbf{v} + ((\mathbf{v}_\ast - \mathbf{v}) \cdot \mathbf{e}) \mathbf{e}) \]

\[ f_\ast = f(t, y, \mathbf{v}_\ast) \]

\[ f = f(t, y, \mathbf{v}) \]

\[ H(t) = \frac{1}{n} \int_{\mathbb{R}^3} f \log f \, d\mathbf{v} = \frac{1}{n} \int_{\mathbb{R}^3} g \log g \, d\mathbf{w} \]
Solutions on the invariant manifold have their own “statistics”

- Use translation group (i.e., gases fill volumes)

- The velocities at $0$ are $\dot{y}_i, \ i = 1, \ldots, M$

- The velocities at $y = (I + tA)x$ are $\dot{y}_i + Ax, \ i = 1, \ldots, M$

- Or, in the Eulerian form used in the kinetic theory, the velocities at $y$ are $\dot{y}_i + A(I + tA)^{-1}y, \ i = 1, \ldots, M$

$$f(t, y, \mathbf{v} + A(I + tA)^{-1}y) = f(t, 0, \mathbf{v})$$
This yields an exact reduction of the Maxwell-Boltzmann equation

\[
\begin{align*}
f(t, y, v) &= f(t, 0, v - A(I + tA)^{-1}y) \\
&= g(t, v - A(I + tA)^{-1}y), \quad v \in \mathbb{R}^3, \ y \in \mathbb{R}^3, \ t > 0
\end{align*}
\]

\(g(t, w)\) satisfies

\[
\frac{\partial g}{\partial t} + \frac{\partial g}{\partial w} \cdot A(I + tA)^{-1}w = \int_{\mathbb{R}^3} \int_{S} (g'_{\ast}g' - g_{\ast}g)B \, d\omega \, dv_{\ast}
\]

- Includes many (all?) known exact solutions of the equations of the moments for special force laws
- Does not include the Bobylev-Krook-Wu solution
Further simplification for inverse 5th power molecules

Return to the reduced Maxwell-Boltzmann equation:

\[
\frac{\partial g}{\partial t} + \frac{\partial g}{\partial \mathbf{w}} \cdot \mathbf{A}(\mathbf{I} + t\mathbf{A})^{-1}\mathbf{w} = \int_{\mathbb{R}^3} \int_S (g'_*g' - g_*g)B \, d\omega dv_*
\]

Assume \( g(t, \mathbf{w}) = \xi(t)G(\eta(t)\mathbf{w}) \)

Choose \( \xi(t) \) and \( \eta(t) \) to remove the time dependence. Get

\[
\text{div} \left[ G \left( t(\text{cof}\mathbf{A}^T)^D + \beta \mathbf{I} - \mathbf{A}^D \right) \mathbf{w} \right] = \mathcal{C}G
\]

\((\text{cof}\mathbf{A}^T)^D = 0\) removes the time dependence

(In each case get explicit formulas for \( \xi(t) \) and \( \eta(t) \))
Example 1

1. $A = a \otimes n$, $a \cdot n = 0$

$$u(y, t) = A(I + tA)^{-1}y = (n \cdot y)a$$

$$\rho(t) = \rho_0, \quad u(t, y) = \kappa y_2 e_1, \quad T(t) = T_0 e^{-2\beta t}, \quad e(t) = -(\text{tr} T_0 / 2\rho_0) e^{-2\beta t} = \frac{3\rho_0}{2\rho_0} e^{-2\beta t}$$

$$H(t) = 3\beta t + H_0$$

$$= -\log \frac{e^{3/2}(t)}{\rho} + \text{const.}!$$
2. \( A = a \otimes n, \quad a \cdot n \neq 0 \) \( u(t, y) = \frac{1}{1 + (a \cdot n)t}(n \cdot y) \)

\[
\rho(t) = \frac{\rho_0}{1 + (a \cdot n)t}, \quad T(t) = (1 + (a \cdot n)t)^{-\left(\frac{2\beta}{a \cdot n} + \frac{5}{3}\right)}T_0, \quad c(t) = \frac{3\rho_0}{2\rho_0}(1 + (a \cdot n)t)^{-\left(\frac{2\beta}{a \cdot n} + \frac{5}{3}\right)}
\]

\[
H(t) = \frac{3\beta}{a \cdot n} \log (1 + (a \cdot n)t) + H_0
\]

\[
= -\log \frac{e^{3/2}(t)}{\rho(t)} + \text{const. !}
\]
Remarks

- Caveat: we have not (yet) given an existence theorem for the initial datum \( G(w) \), i.e., for

\[
\text{div} \left[ G (\beta I - A^D) w \right] = CG
\]

- Consistency of the behavior of \( H \) and its definition?

\[
H(t) = \frac{1}{n} \int_{\mathbb{R}^3} f \log f \, dv = \frac{1}{n} \int_{\mathbb{R}^3} g \log g \, dw
\]

- Both the solutions of Boltzmann and the numerical results on pulling carbon nanotubes at constant strain rate suggest that there is a statistical mechanics for the invariant manifold. If so, it cannot be based on the invariant measure of ordinary statistical mechanics (Gibbs measure) because

\[
\text{Hamiltonian} \neq \text{constant}
\]
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- An invariant manifold of molecular dynamics
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X-ray diffraction

**X-Ray Crystallography (XRC, Max von Laue, 1912)**

- Polychromatic x-ray source
- Single crystal
- Screen/detector
- Electron density of a unit cell

+ Structural information
+ High resolution
- For crystals only

**Coherent Diffraction Imaging (CDI, John Miao, 1999)**

- Highly brilliant x-ray source
- General structure
- Screen/detector
- Projection of the electron density

- No structural information
- Low resolution
+ For general structures

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Coherent diffractive imaging requires a coherent source of hard x-rays, \( \ldots \), i.e., one of these:

LINAC at SLAC:
2 mile long linear accelerator, longest in the world

$ 400,000,000.00$
Some of the most interesting structures today are not crystals

Buckyball (Smalley, Kurl, Kroto, Nobel Prize 1996)

Graphene (Geim and Novoselov, Nobel Prize 2010)

Myovirus bacteriophage

Amyloid protein (causes Alzheimer's, Parkinson's and Creutzfeldt-Jakob disease)

H1N1 bird flu virus

“Objective structures”

Ebola virus

Forthcoming work on the crystallization problem for these kinds of structures: B. Schmidt and P. Dondl
Our method

- Focus on structures generated by isometry groups (objective structures)
- Exploit the mathematical analog

\[ e^{i \mathbf{k} \cdot \mathbf{x}} \]

\{ 
  \text{eigenfunction of the Laplacian (i.e., solves the time-harmonic wave equation)} 
  
  \text{eigenfunction of the translation group:} 
  \[ e^{i \mathbf{k} \cdot (\mathbf{x}+\mathbf{c})} = e^{i \mathbf{k} \cdot \mathbf{c}} e^{i \mathbf{k} \cdot \mathbf{x}} \] 

\[ ?(\mathbf{x}) \]

\{ 
  \text{eigenfunction of the Laplacian (i.e., solves the time-harmonic wave equation)} 
  
  \text{eigenfunction of the isometry group* that generates the objective structure} 
\}

- Design radiation for the inverse problem

Key point:
isometries are in invariance group of the Helmholtz equation. Hence, structural invariance coincides with invariance of the PDE
Remarks

- The solution is vector-valued, and the required action is

\[ g \mathbf{E}_0(\mathbf{x}) = \mathbf{Q} \mathbf{E}_0(\mathbf{Q}^T(\mathbf{x} - \mathbf{c})) \quad g = (\mathbf{Q}|\mathbf{c}) \]

- The design criterion is

\[ g \mathbf{E}_0 = \chi(g)\mathbf{E}_0 \quad \text{for some } \chi : G \to \mathbb{C} \]

- \( \chi : G \to \mathbb{C} \) is a character of \( G \). We do not know the structure ahead of time, so, which group \( G \)?
Explicit form of the design criterion for the simplest helical group

- We design in a super group $G'$
  $$G' = \{(R_\theta|\tau e) : \theta \in [0, 2\pi), \tau \in \mathbb{R}\} \quad R_\theta e = e$$

  $G$ that generates the structure is a discrete subgroup of $G'$

- $G'$ is isomorphic to
  $$(\mathbb{T} \times \mathbb{R}, +) \quad \text{i.e., } (R_\theta, \tau e) \rightarrow (\theta, \tau)$$

- This implies the character
  $$\chi(\theta, \tau) = e^{i(\alpha \theta + \beta \tau)} \quad \alpha \in \mathbb{Z}, \beta \in \mathbb{R}$$

- The explicit form of the design criterion is
  $$R_\theta E_0(R_{-\theta}(x - \tau e)) = e^{i(\alpha \theta + \beta \tau)} E_0(x) \quad x \in \mathbb{R}^3, (\alpha, \beta) \in \mathbb{Z} \times \mathbb{R}$$

- Problem: find functions of this form satisfying Helmholtz, i.e., of the form
  $$E_0(x) = \int_{\frac{\omega}{c} S^2} n(k) e^{i(k \cdot x - \omega t)} dH^2(k) \quad n(k) \cdot k = 0$$
GP is a transmembrane fusion protein. It forms trimers on the virion surface and mediates virus attachment and entry to the host cell. [1]*

The viral membrane may contain human proteins, such as components of the histocompatibility complex or other surface receptors [2], which — in some cases — can increase the infectivity of the enveloped viruses. [3, 4]

VP40 and VP24 are Ebola major and minor matrix proteins. They form a layer beneath the membrane and are crucial for virus budding. [5, 6]

Ebola RNA is packed with the NP protein. Together, they make a nucleocapsid — a spiral structure in the very center of the virion. [7]

L stands for the large Ebola protein — the polymerase. It is responsible for the synthesis of positive sense virus RNA. [8]

VP35 and VP30 are minor Ebola proteins. They act as interferon antagonists and transcription activation factors. [9, 10]

The budding viral particle is wrapped in the lipid membrane taken from the human cell. [11]

*For more information and references visit www.visualsciencecompany.com/ebola

Konstantinov et al., Visual Science nsf.gov
Solution: twisted waves

\[ E(r, \varphi, z, t) = \]

\[ e^{i(\alpha \varphi + \beta z - \omega t)} \begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1 \\
\end{pmatrix} \begin{pmatrix}
\frac{n_1 + in_2}{2} & \frac{n_1 - in_2}{2} & 0 \\
\frac{n_2 + in_1}{2} & \frac{n_2 - in_1}{2} & 0 \\
0 & 0 & n_3 \\
\end{pmatrix} \begin{pmatrix}
J_{\alpha + 1}(\gamma r) \\
J_{\alpha - 1}(\gamma r) \\
J_\alpha(\gamma r) \\
\end{pmatrix} \]

and the magnetic field is given by

\[ B = -\frac{i}{\omega} \text{curl} E \]

Important parameters:

\[ \alpha, \beta \]
Twisted waves interact with helical structures in the same way as plane waves do for crystals

Slightly off resonance: **destructive** interference (A. Weil’s theorem)

On resonance: **constructive** interference
How do you build the machine?

(...for under $ 400,000,000.)

Theoretical concept:
Example: reconstruction of Pf1

- Formula for far-field scattered radiation
- Reconstruction algorithm (JFJ + Elser)
- Unbiased: random initial phases, no structural information used

Jüstel, Friesecke, James