

周期的極小曲面に拘束された 電子の量子力学

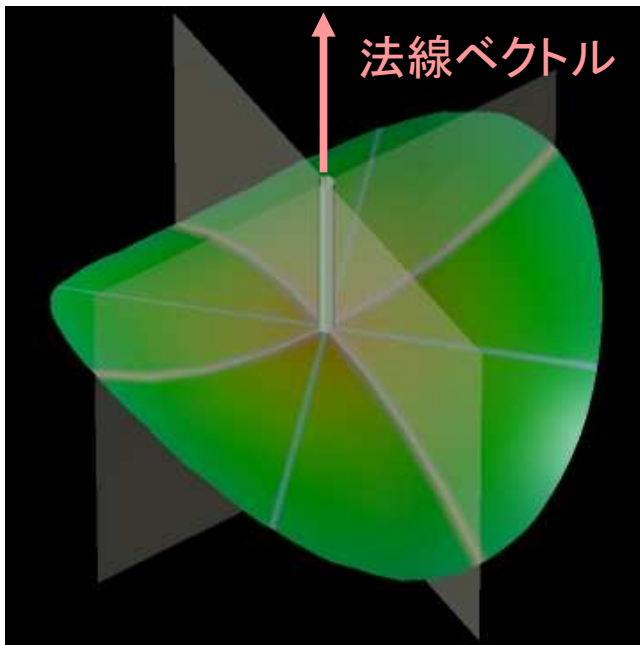
東北大多元研 藤田伸尚

骨子

1. 曲面の幾何学
2. 周期的極小曲面
3. 曲面に拘束された電子
4. P, D, G表面のバンド構造
5. 波動関数の対称性とノード線
6. まとめ

1 . 曲面の幾何学

曲率の定義



主曲率

$$\kappa_1 = 1/R_1$$

$$\kappa_2 = 1/R_2$$

平均曲率

$$H = \frac{1}{2}(\kappa_1 + \kappa_2)$$

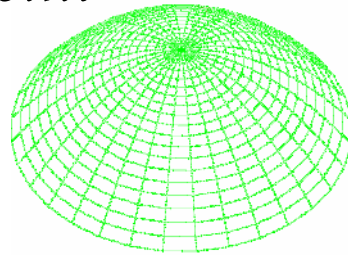
ガウス曲率

$$K = \kappa_1 \kappa_2$$

曲面上の様々な点

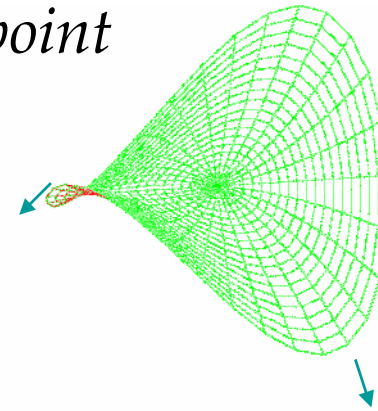
Elliptic point

$$K > 0$$



Saddle point

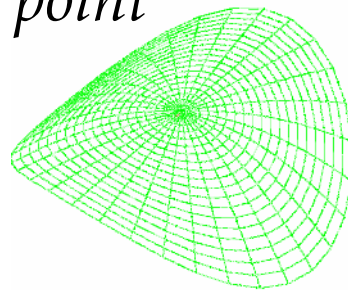
$$K < 0$$



Parabolic point

$$K = 0$$

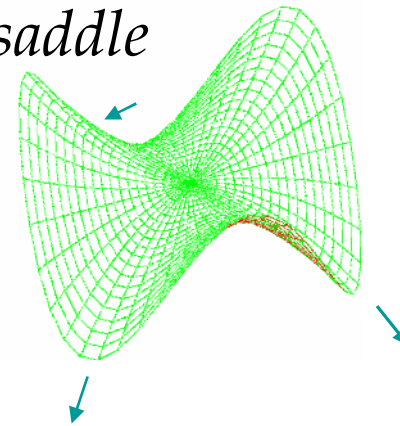
$$(\kappa_1 = 0, \kappa_2 \neq 0)$$



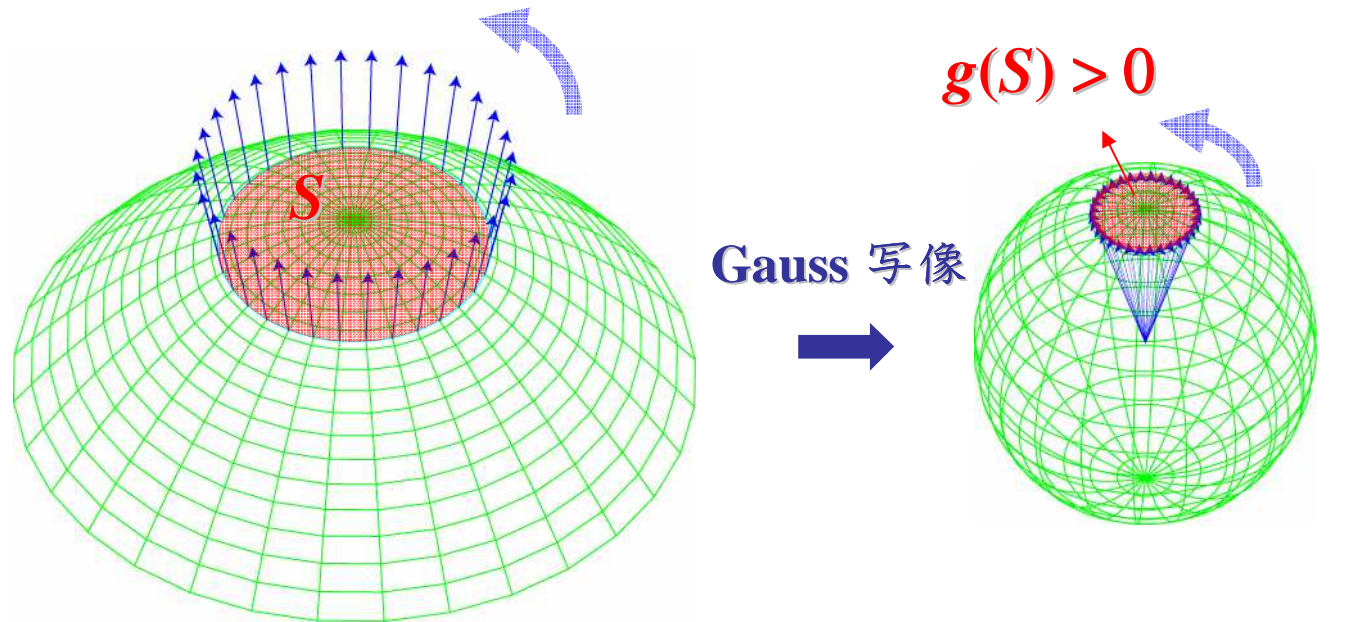
Monkey saddle

$$K = 0$$

$$(\kappa_1 = \kappa_2 = 0)$$



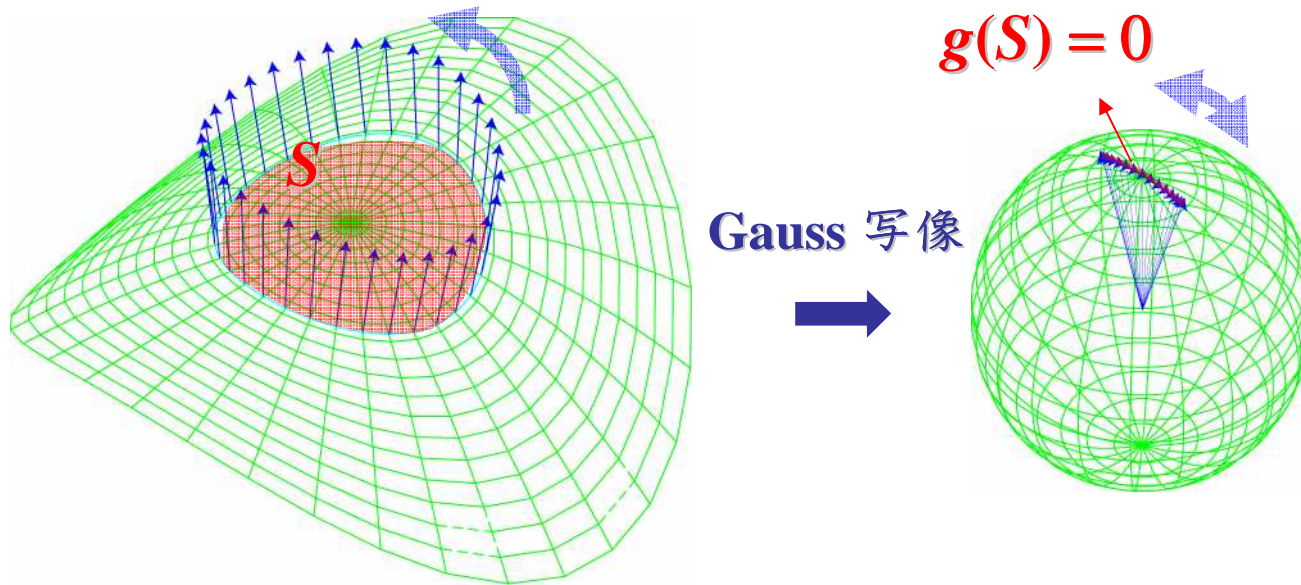
ガウス曲率



$$K = \lim_{S \rightarrow 0} \frac{g(S)}{S} > 0$$

Elliptic point (楕円点)

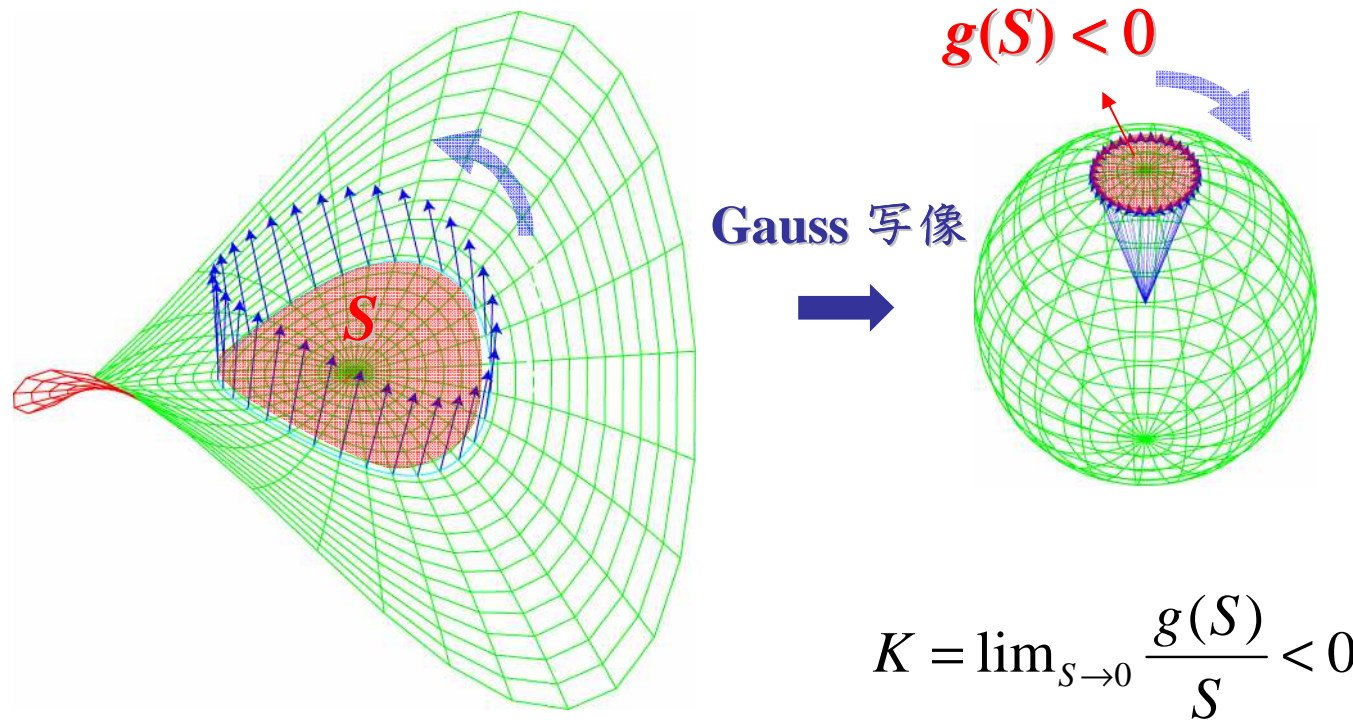
ガウス曲率



$$K = \lim_{S \rightarrow 0} \frac{g(S)}{S} = 0$$

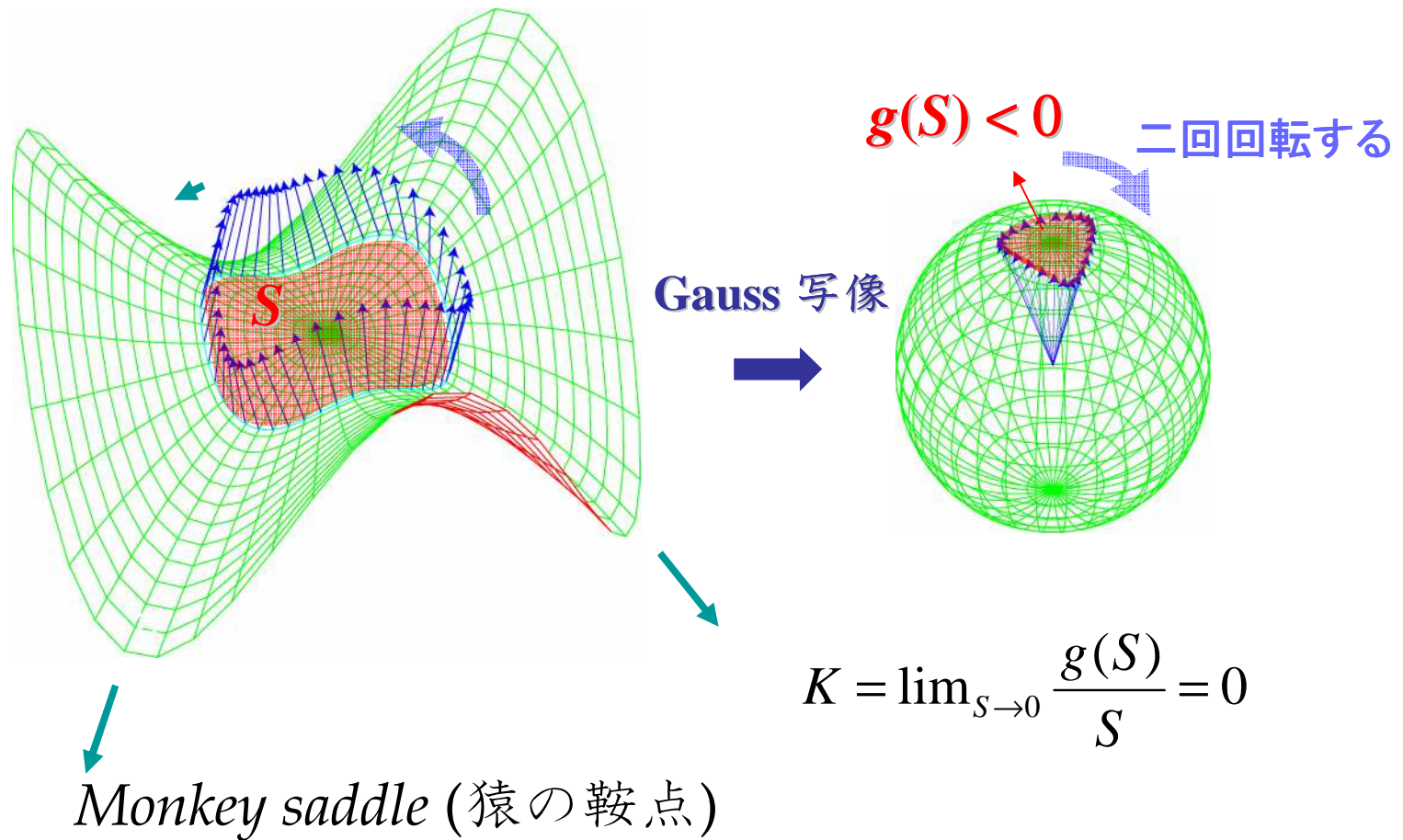
Parabolic point (放物点)

ガウス曲率



Saddle point (鞍点)
= *Hyperbolic point* (双曲点)

ガウス曲率



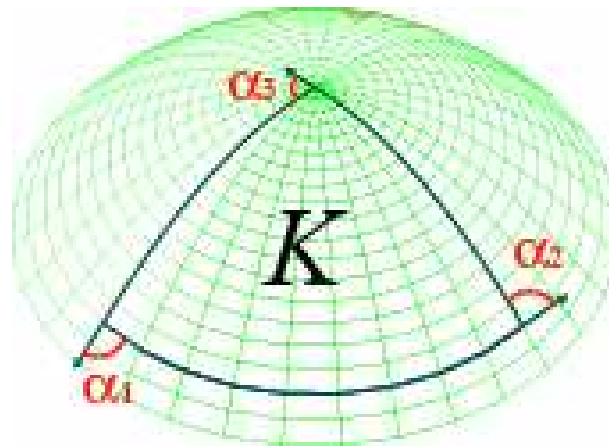
ガウス-ボンネの定理

(Gauss-Bonnet Theorem)

$$\iint_T K dS = 2\pi - \sum_{j=1}^3 \alpha_j$$

測地線三角形 T の内角の和
はガウス曲率の面積積分
(対応するガウス球面上の
面積) だけ増加する。

$$\iint_T K dS = \iint_{g(T)} dS_g$$



2. 周期的極小曲面

プラトー問題 (19世紀)

針金の枠に張られた石鹼膜 →
表面張力エネルギーを最小化



$$E = \gamma \iint_{\partial} dS$$

(\approx 表面積を最小化)



c.f. Laplace law for soap films

$$p_2 - p_1 = 2\gamma H$$

極小曲面

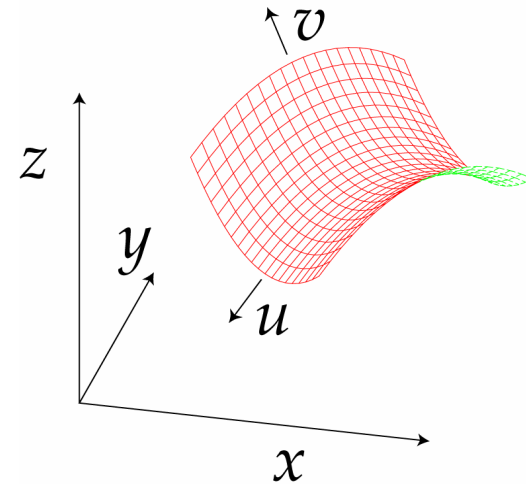
極小曲面：平均曲率 H が至る所で
ゼロである曲面



与えられた境界線を持つ極小曲面は
ユニークに決まる → 面積最小曲面

Weierstrass-Enneper表現

あらゆる極小曲面は、
有理型関数 $F(\zeta)$ を用い
て解析的に表現できる



$$\vec{x}(u, v) = \vec{x}(\zeta = u + iv) = \ell \operatorname{Re} \left(e^{i\alpha} \vec{\xi}(\zeta) \right) \quad (\in \mathbf{R}^3)$$

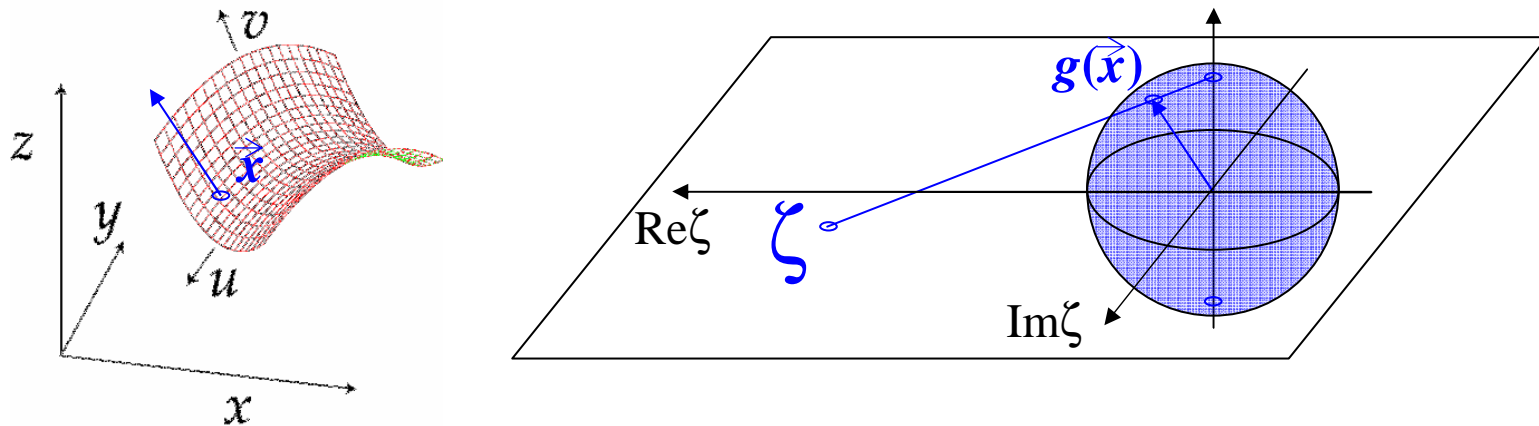
$$\vec{\xi}(\zeta) \quad (\in \mathbf{C}^3)$$

$\alpha = \text{Bonnet angle}$

$$= \left(\int^{\zeta} F(\zeta_1)(1 - \zeta_1^2) d\zeta_1, \int^{\zeta} iF(\zeta_1)(1 + \zeta_1^2) d\zeta_1, \int^{\zeta} 2F(\zeta_1)\zeta_1 d\zeta_1 \right)$$

Weierstrass-Enneper表現

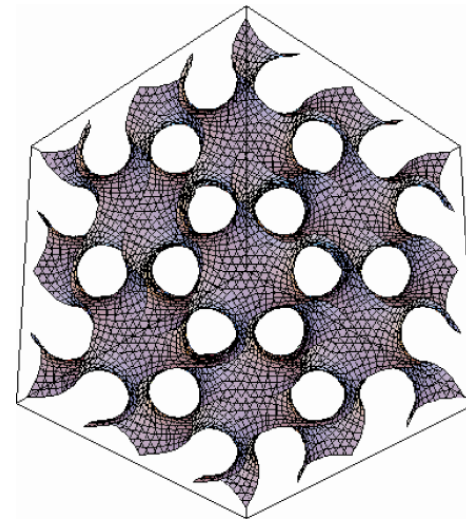
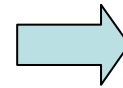
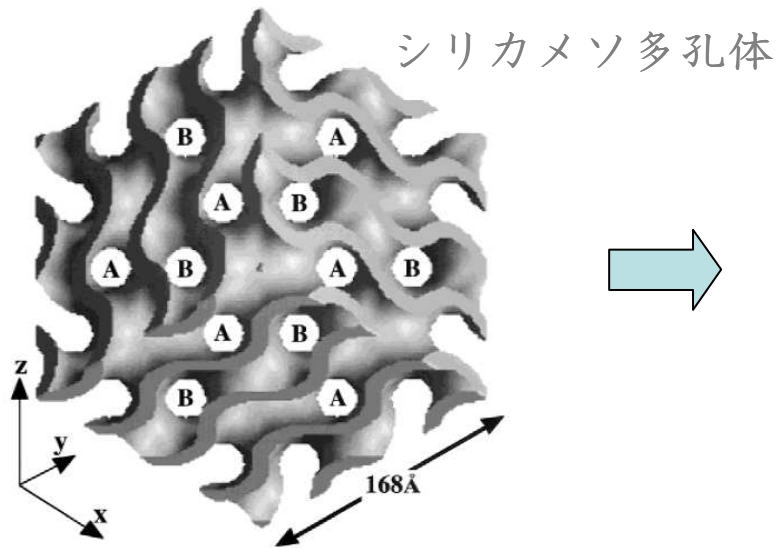
変数 $\zeta (= u+iv)$ ~ 曲面上の各点の Gauss 写像に
対するステレオ投影 (複素数による表現)



$$g(\vec{x}) = \frac{\partial_u \vec{x} \times \partial_v \vec{x}}{|\partial_u \vec{x} \times \partial_v \vec{x}|} = \left(\frac{2 \operatorname{Re} \zeta}{|\zeta|^2 + 1}, \frac{2 \operatorname{Im} \zeta}{|\zeta|^2 + 1}, \frac{|\zeta|^2 - 1}{|\zeta|^2 + 1} \right)$$

周期的極小曲面

液晶・高分子などの系において自己組織化により生成する周期的な界面構造を良く記述できる（代表例：P, D, G表面）



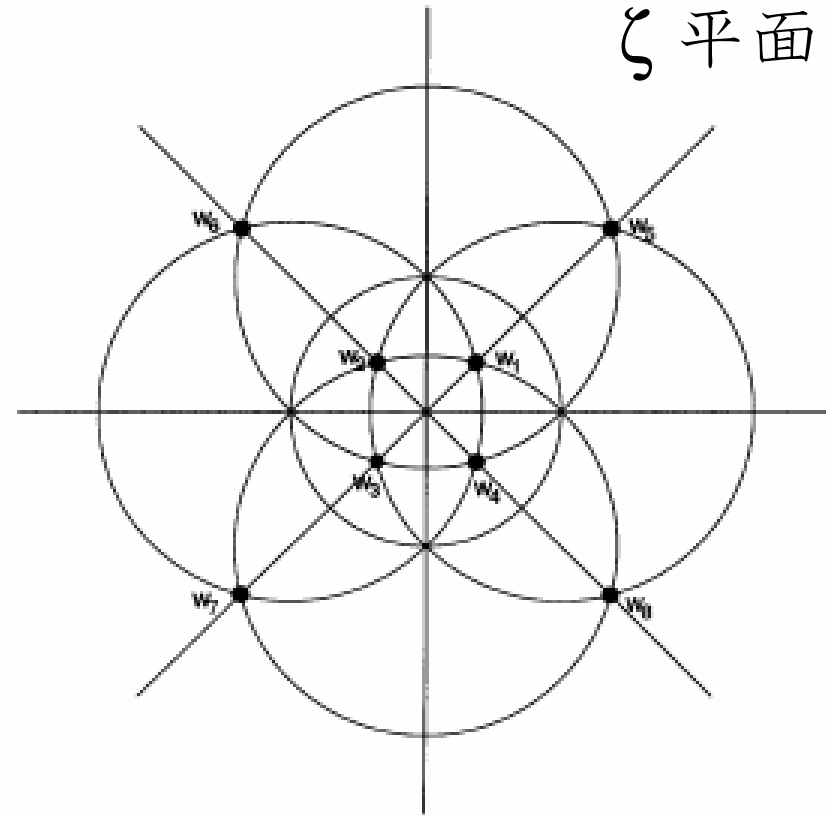
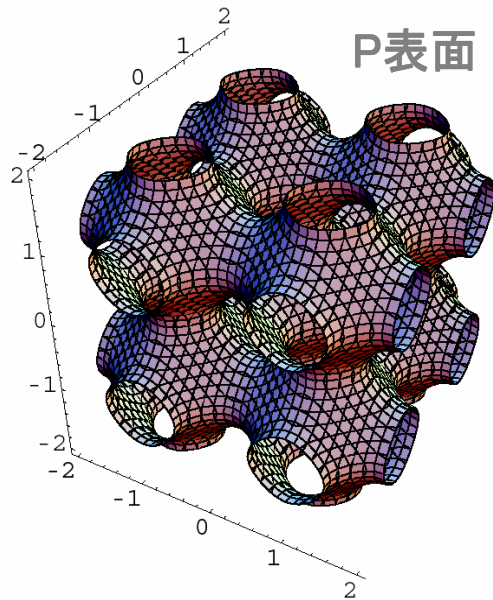
Gyroid (G表面)

視線方向 - 3 回軸

O. Terasaki et al.
Microsc. Microanal. 8, 35 (2002).

P表面 (Schwarz,1890)

$$F(\zeta) = \frac{1}{\sqrt{1+14\zeta^4 + \zeta^8}}$$

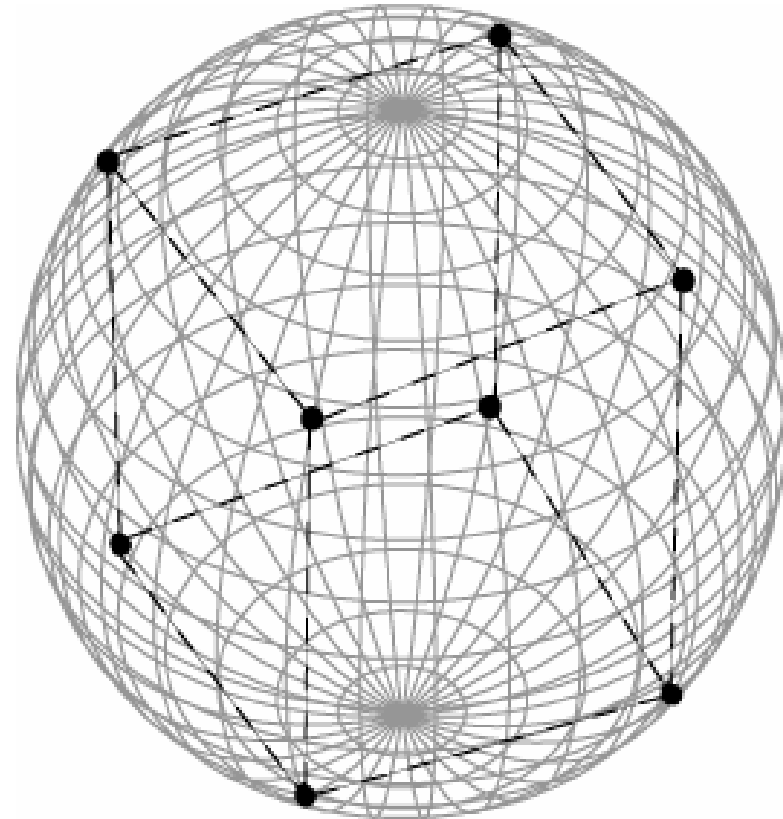
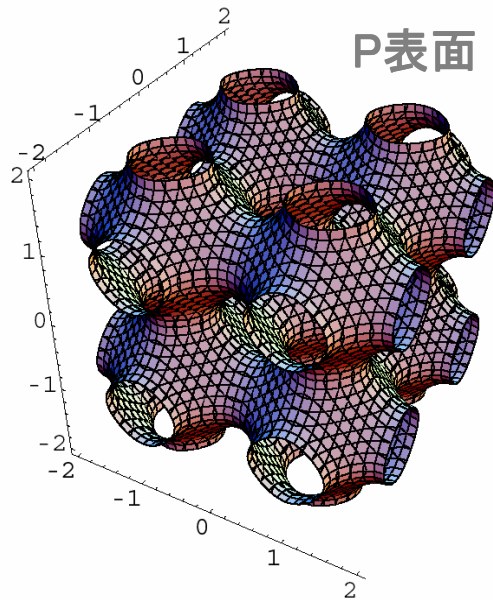


$F(\zeta)$: 二価関数、
8個の特異点(branch point)を持つ

$$\frac{\sqrt{3} \pm 1}{\sqrt{2}} e^{i \frac{(2n+1)\pi}{4}} \quad (n = 0, 1, 2, 3)$$

P表面 (Schwarz,1890)

$$F(\zeta) = \frac{1}{\sqrt{1+14\zeta^4 + \zeta^8}}$$

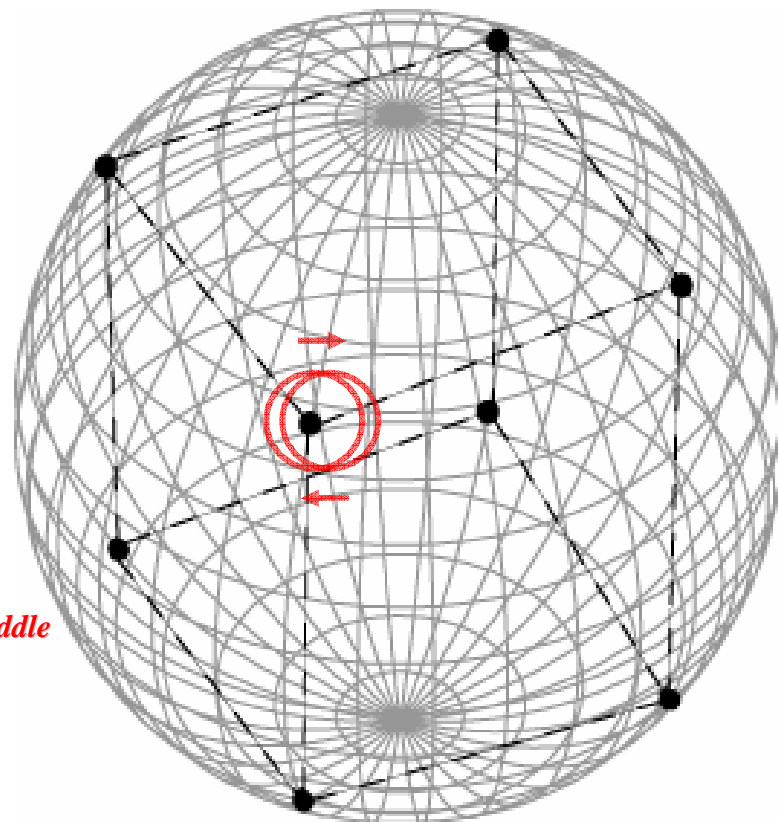
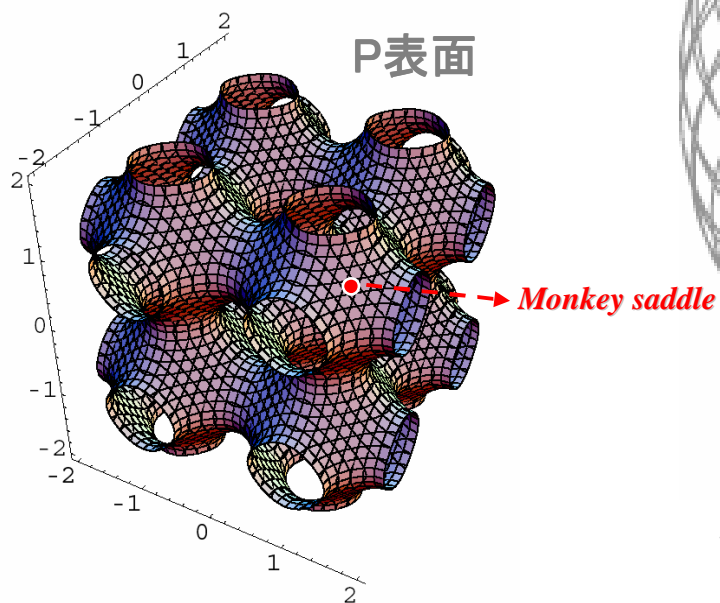


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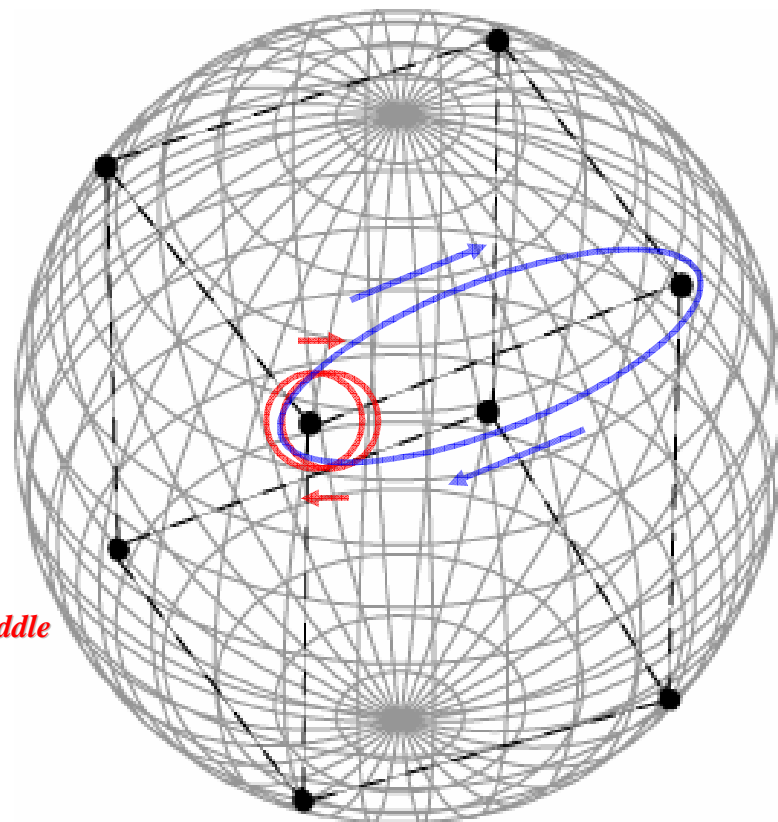
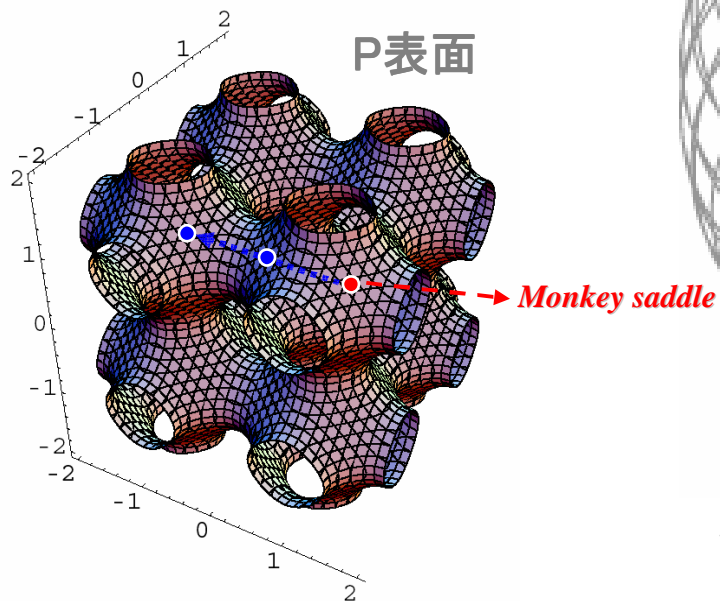


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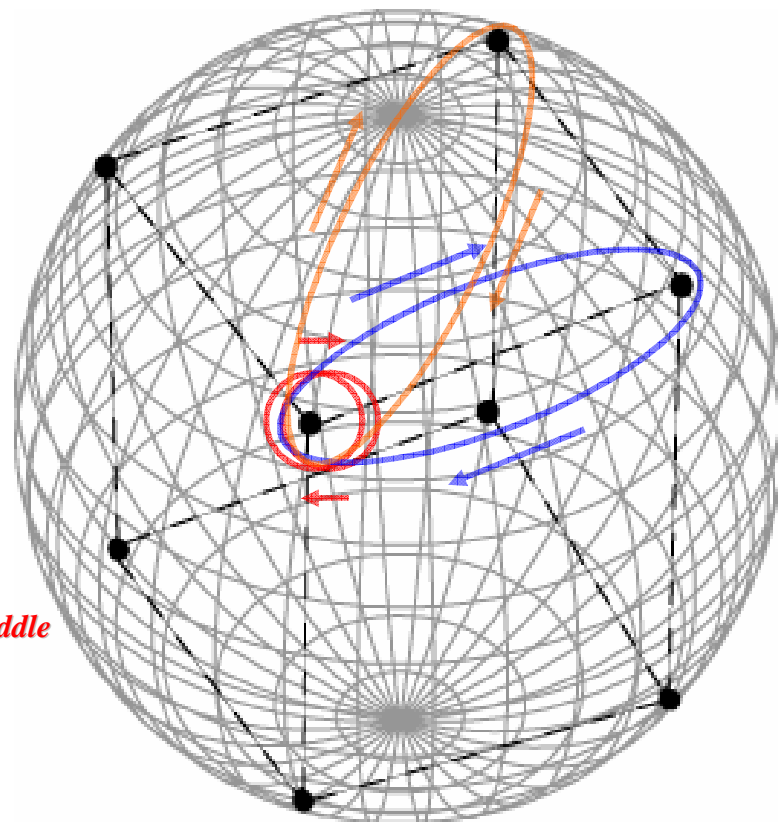
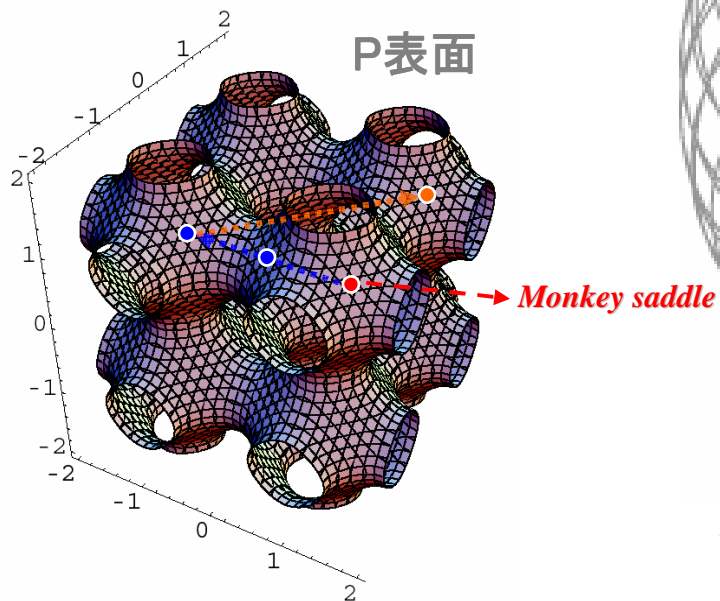


$F(\zeta)$: 二価関数、
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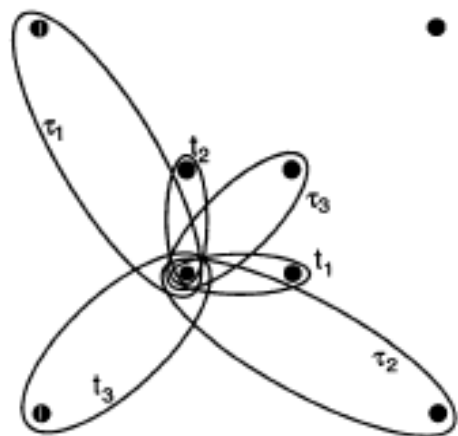
\mathbb{C}^3 空間における基本周期

$$\vec{x}(u, v) = \vec{x}(\zeta = u + iv) = \ell \operatorname{Re}(e^{i\alpha} \vec{\xi}(\zeta)) \quad (\in \mathbb{R}^3) \quad \text{Weierstrass-Enneper rep.}$$

$$\vec{\xi}(\zeta) \quad (\in \mathbb{C}^3)$$

$\alpha = \text{Bonnet angle}$

$$= \left(\int^\zeta F(\zeta_1)(1 - \zeta_1^2) d\zeta_1, \int^\zeta iF(\zeta_1)(1 + \zeta_1^2) d\zeta_1, \int^\zeta 2F(\zeta_1)\zeta_1 d\zeta_1 \right)$$



ζ 平面

$$\begin{pmatrix} \vec{T}_1 & \vec{T}_2 & \vec{T}_3 & \vec{T}_4 & \vec{T}_5 & \vec{T}_6 \end{pmatrix} = \begin{pmatrix} r & -is & is & 0 & r-is & -r-is \\ is & r & -is & -r-is & 0 & r-is \\ -is & is & r & r-is & -r-is & 0 \end{pmatrix}$$

$$r - is = 2e^{-\pi i/6} K(e^{-2\pi i/3})$$

$$r \approx 2.156, s = 1.686$$

Oguey & Sadoc, J. Phys. I France **3**, 839 (1993)

\mathbb{R}^6 空間における基本周期

$$\begin{aligned}
 & (\vec{T}_1 \quad \vec{T}_2 \quad \vec{T}_3 \quad \vec{T}_4 \quad \vec{T}_5 \quad \vec{T}_6) \quad \text{in } \mathbb{C}^3 \\
 & = \begin{pmatrix} r & -is & is & 0 & r-is & -r-is \\ is & r & -is & -r-is & 0 & r-is \\ -is & is & r & r-is & -r-is & 0 \end{pmatrix} \quad \begin{aligned} r-is &= 2e^{-\pi i/6} K(e^{-2\pi i/3}) \\ r &\approx 2.156, s=1.686 \end{aligned}
 \end{aligned}$$



$$\begin{aligned}
 & (\tilde{T}_1 \quad \tilde{T}_2 \quad \tilde{T}_3 \quad \tilde{T}_4 \quad \tilde{T}_5 \quad \tilde{T}_6) = \begin{pmatrix} r & 0 & 0 & 0 & r & -r \\ 0 & r & 0 & -r & 0 & r \\ 0 & 0 & r & r & -r & 0 \\ 0 & -s & s & 0 & -s & -s \\ s & 0 & -s & -s & 0 & -s \\ -s & s & 0 & -s & -s & 0 \end{pmatrix} \left. \begin{array}{l} \text{real parts} \\ \text{imaginary parts} \end{array} \right\} \\
 & \mathbb{C}^3 \simeq \mathbb{R}^6
 \end{aligned}$$

\mathbb{R}^3 空間への投影と Bonnet 角 α

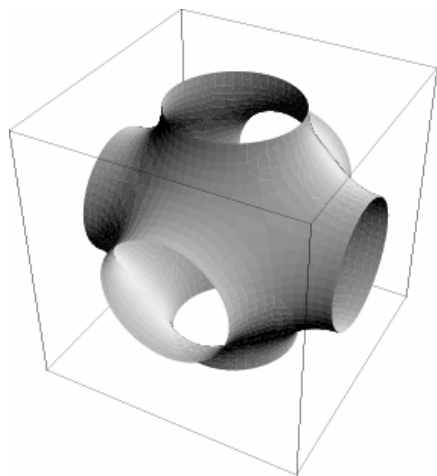
$$\text{Re}(e^{i\alpha}(\vec{T}_1 \ \vec{T}_2 \ \vec{T}_3 \ \vec{T}_4 \ \vec{T}_5 \ \vec{T}_6)) = \downarrow_{\alpha}(\tilde{T}_1 \ \tilde{T}_2 \ \tilde{T}_3 \ \tilde{T}_4 \ \tilde{T}_5 \ \tilde{T}_6)$$

$$\downarrow_{\alpha} := (\mathbf{I}\cos\alpha \quad -\mathbf{I}\sin\alpha)$$

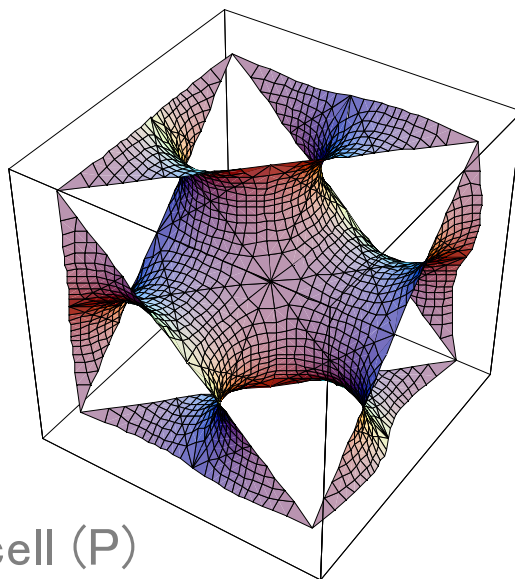
$$\downarrow_0(\tilde{T}_1 \ \tilde{T}_2 \ \tilde{T}_3 \ \tilde{T}_4 \ \tilde{T}_5 \ \tilde{T}_6) = r \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 1 & -1 & 0 \end{pmatrix} \quad \text{P(SC)}$$

$$\downarrow_{\pi/2}(\tilde{T}_1 \ \tilde{T}_2 \ \tilde{T}_3 \ \tilde{T}_4 \ \tilde{T}_5 \ \tilde{T}_6) = s \begin{pmatrix} 0 & 1 & -1 & 0 & 1 & 1 \\ -1 & 0 & 1 & 1 & 0 & 1 \\ 1 & -1 & 0 & 1 & 1 & 0 \end{pmatrix} \quad \text{D(FCC)}$$

$$\downarrow_{\arctan(r/s)}(\tilde{T}_1 \ \tilde{T}_2 \ \tilde{T}_3 \ \tilde{T}_4 \ \tilde{T}_5 \ \tilde{T}_6) = \frac{rs}{\sqrt{r^2+s^2}} \begin{pmatrix} 1 & 1 & -1 & 0 & 2 & 0 \\ -1 & 1 & 1 & 0 & 0 & 2 \\ 1 & -1 & 1 & 2 & 0 & 0 \end{pmatrix} \quad \text{G(BCC)}$$



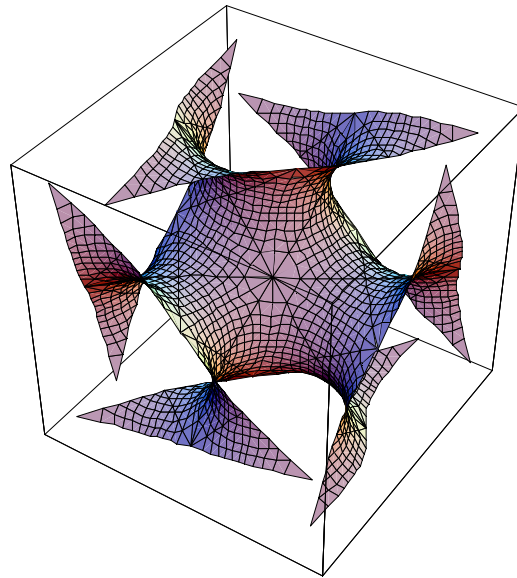
P表面



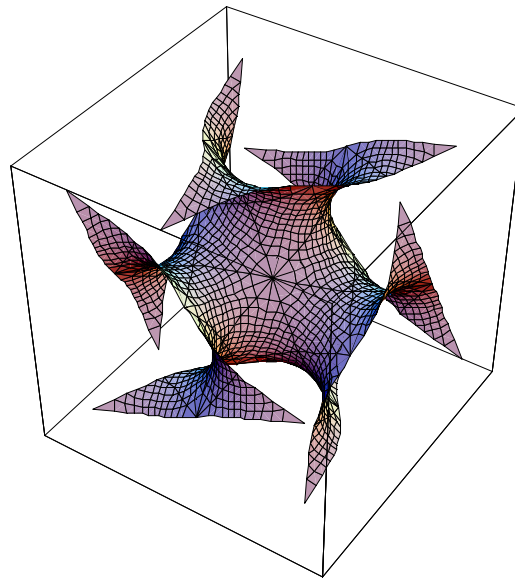
primitive cell (P)

$\alpha=0^\circ$

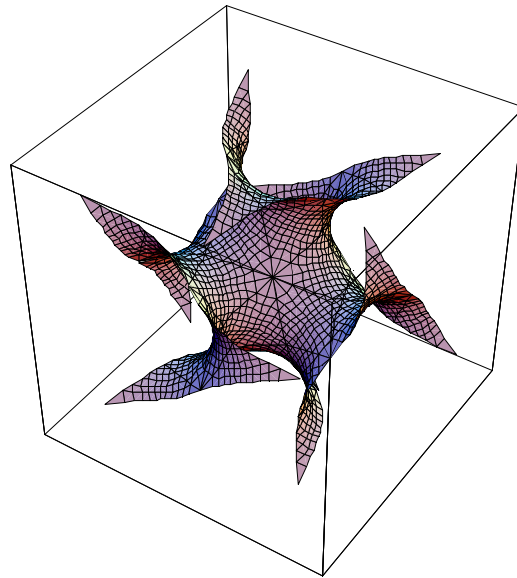
$\alpha=9^\circ$



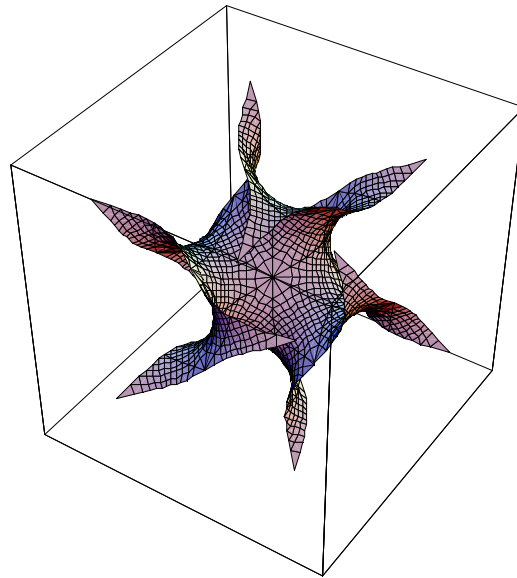
$\alpha=18^\circ$



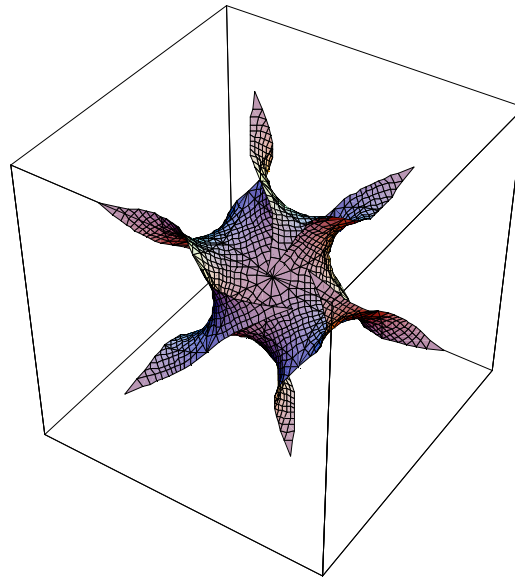
$\alpha=27^\circ$

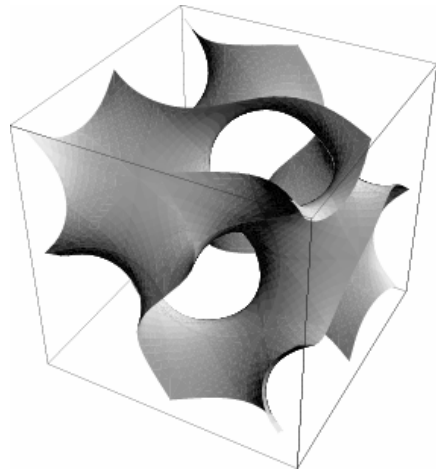


$$\alpha=36^\circ$$

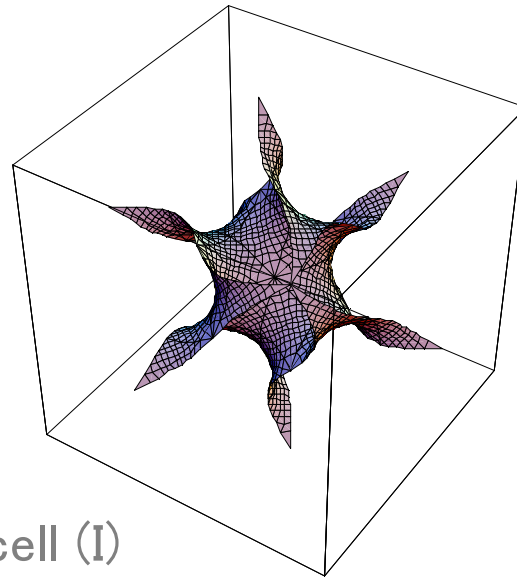


$\alpha=45^\circ$





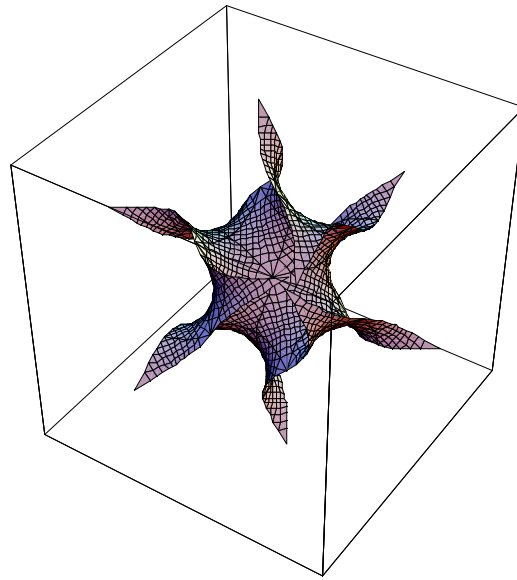
G表面



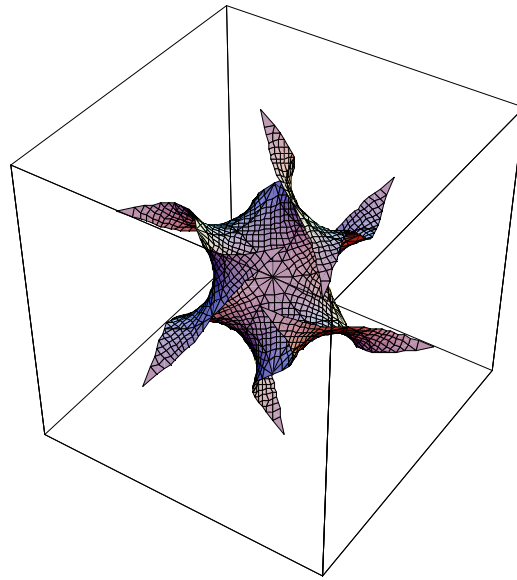
primitive cell (I)

$$\alpha = 51.985^\circ$$
$$= \arctan \frac{r}{s}$$

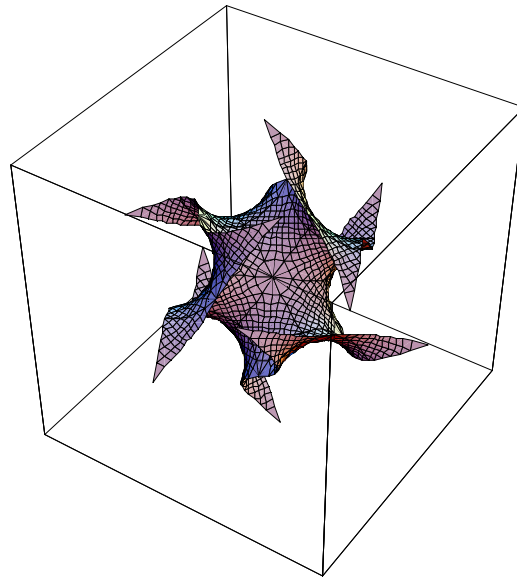
$\alpha=54^\circ$



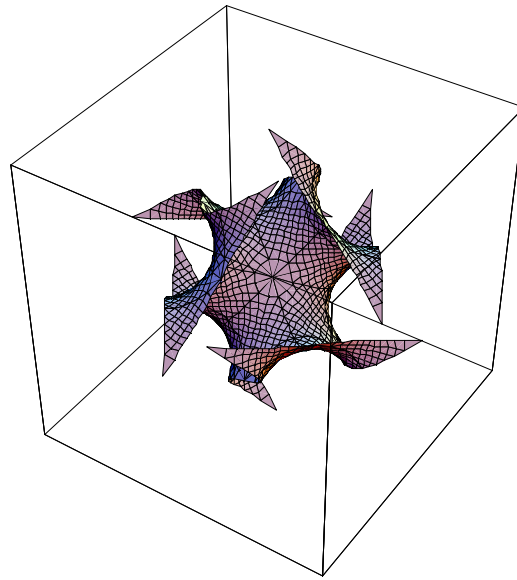
$\alpha=63^\circ$

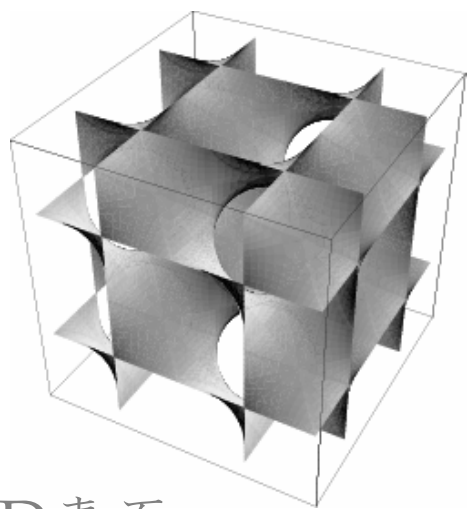


$$\alpha=72^\circ$$

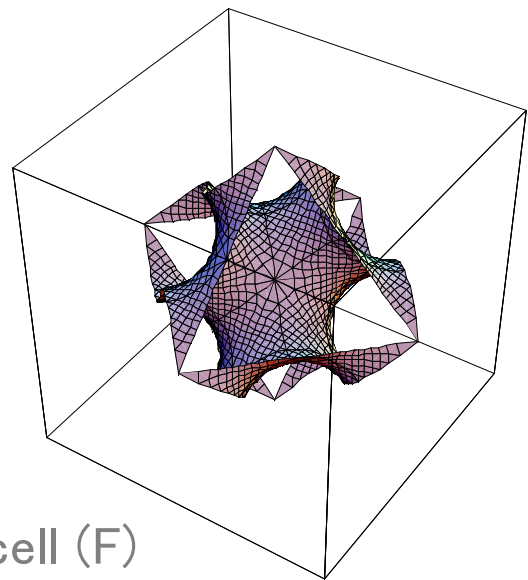


$\alpha=81^\circ$





D表面



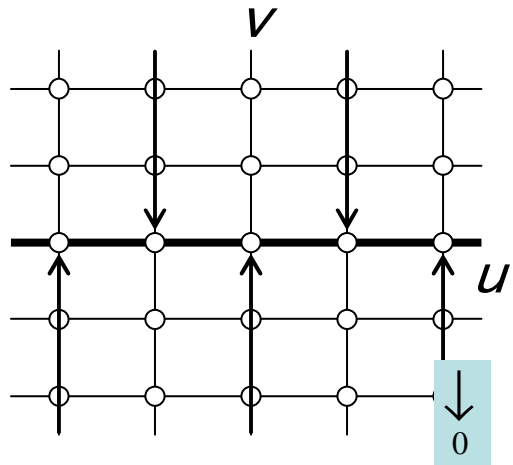
primitive cell (F)

$$\alpha=90^\circ$$

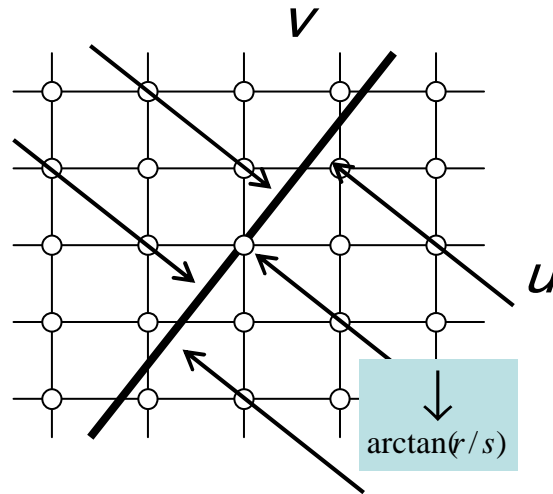
Bonnet変換

同一の $F(\zeta)$ に対して、一般に異なる
Bonnet角 α を持つ幾つかの極小曲面が
存在する。（極小曲面のBonnet族）

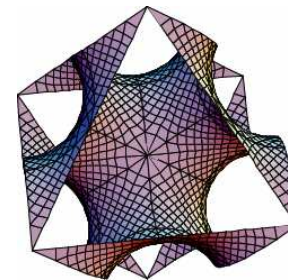
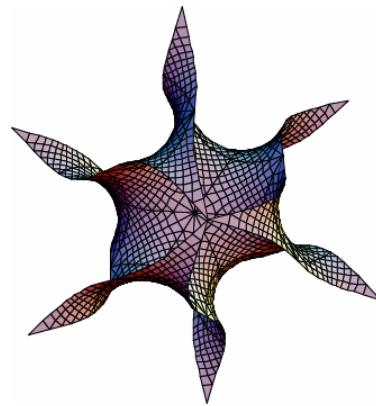
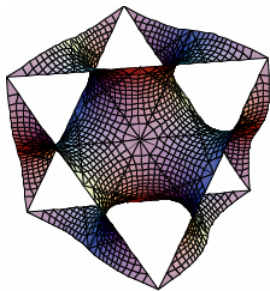
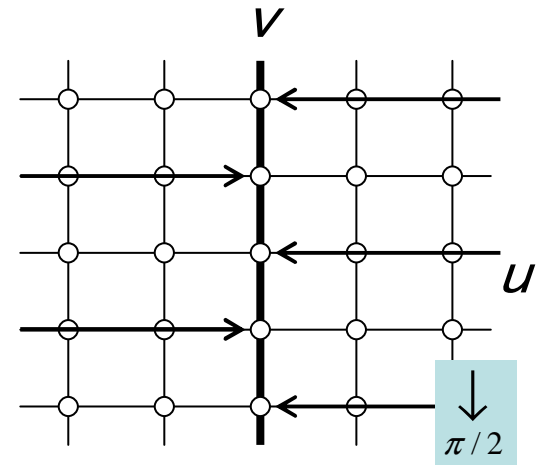
P(SC)



G(BCC)

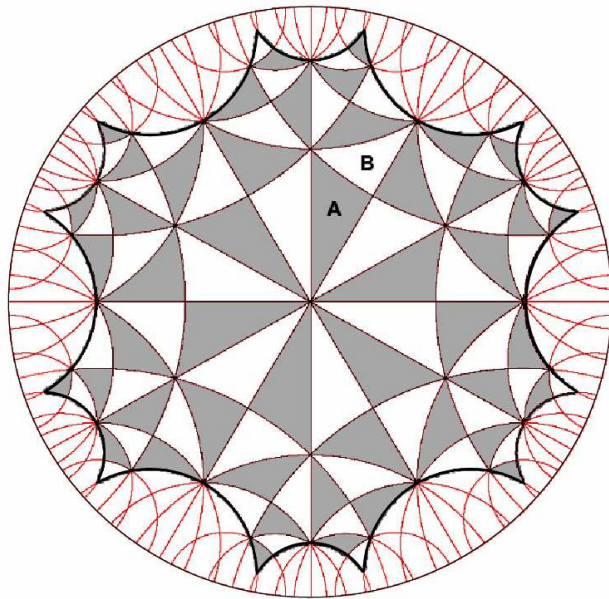


D(FCC)



補足

\mathbb{C}^3 空間の周期曲面 $\vec{\xi}(\zeta)$ は、負の定曲率平面（双曲平面）内の測地線12角形による周期タイリングと位相同型



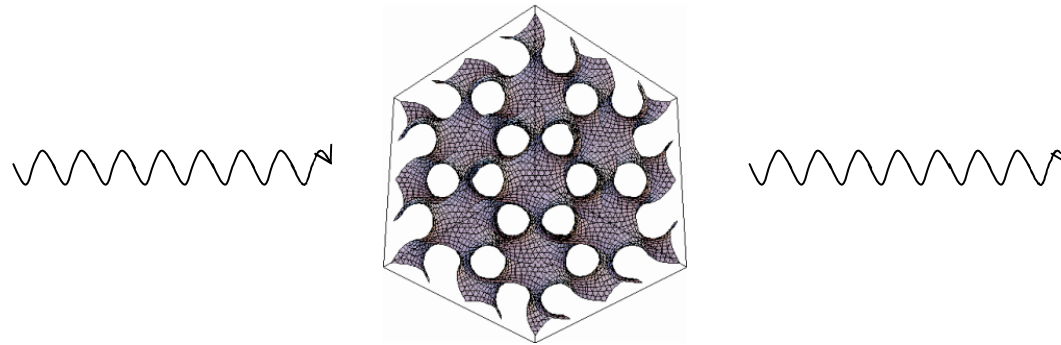
6方向の基本周期を持つ

双曲平面(Poincaréモデル)中の12角形タイル～96個の合同な(2,4,6)三角形に分割できる

3. 曲面に拘束された電子

曲面上に拘束された電子

曲率・対称性・トポロジーが電子波の干渉を規定し、定常波（共鳴状態）を決定する



幾何学的に制御された電子構造(スペクトル)

“Can one hear the shape of a drum?”

Marc Kac, Am. Math. Mon. **73**, 1-23 (1966).

曲面上のSchrödinger 方程式

Jensen & Koppe, *Quantum Mechanics with Constraints*,
Ann. Phys. 63, 586 (1971).

da Costa, *Quantum mechanics of a constrained particle*
Phys. Rev. A 23, 1982 (1981)

Ikegami & Nagaoka, *Quantum Mechanics of an Electron on a Curved Interface*
Prog. Theor. Phys. 106, 235 (1991)

Ikegami, Nagaoka, Takagi & Tanzawa, *Quantum Mechanics of a Particle on a Curved Surface – Comparison of Three Different Approaches*
Prog. Theor. Phys. Suppl. 88, 229 (1992)

一般的な曲面の場合

デカルト座標 曲線座標

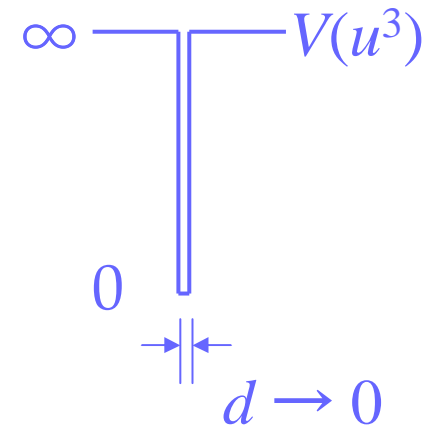
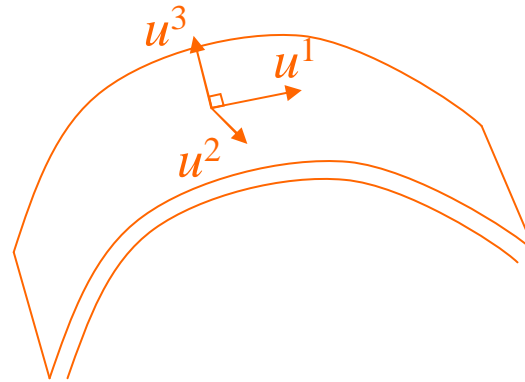
$$(x, y, z) \rightarrow (u^1, u^2, u^3)$$

計量テンソル g

$$ds^2 = dx^2 + dy^2 + dz^2 = g_{\mu\nu} du^\mu du^\nu$$

ラプラシアン

$$\nabla^2 = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^\mu} \sqrt{g} g^{\mu\nu} \frac{\partial}{\partial u^\nu}$$



シュレーディンガー方程式

$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^\mu} \sqrt{g} g^{\mu\nu} \frac{\partial}{\partial u^\nu} + V(u^3) \right\} \Psi(\{u^\mu\}) = E \Psi(\{u^\mu\})$$

一般的な曲面の場合

デカルト座標 曲線座標

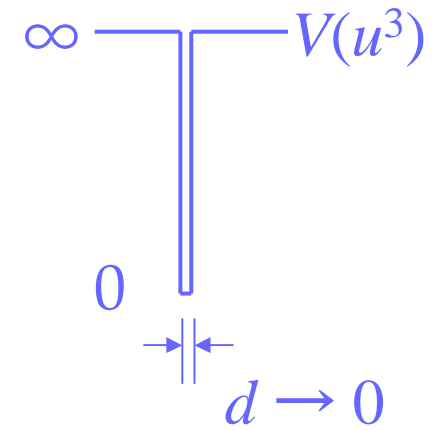
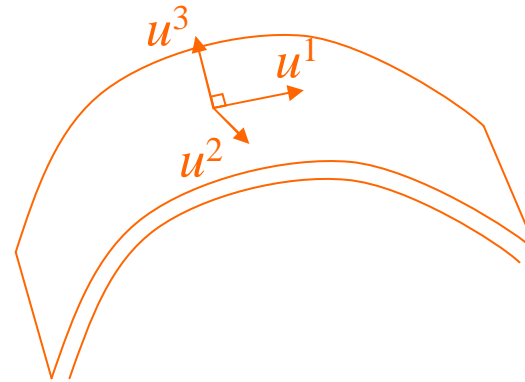
$$(x, y, z) \rightarrow (u^1, u^2, u^3)$$

計量テンソル g

$$ds^2 = dx^2 + dy^2 + dz^2 = g_{\mu\nu} du^\mu du^\nu$$

ラプラシアン

$$\nabla^2 = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^\mu} \sqrt{g} g^{\mu\nu} \frac{\partial}{\partial u^\nu}$$



シュレーディンガー方程式

$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^\mu} \sqrt{g} g^{\mu\nu} \frac{\partial}{\partial u^\nu} + V(u^3) \right\} \Psi(\{u^\mu\}) = E \Psi(\{u^\mu\})$$



$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^j} \sqrt{g} g^{jk} \frac{\partial}{\partial u^k} - \frac{\hbar^2}{8m} (\kappa_1 - \kappa_2)^2 \right\} \psi(u^1, u^2) = E \psi(u^1, u^2)$$

極小曲面の場合

曲面座標

曲面の計量

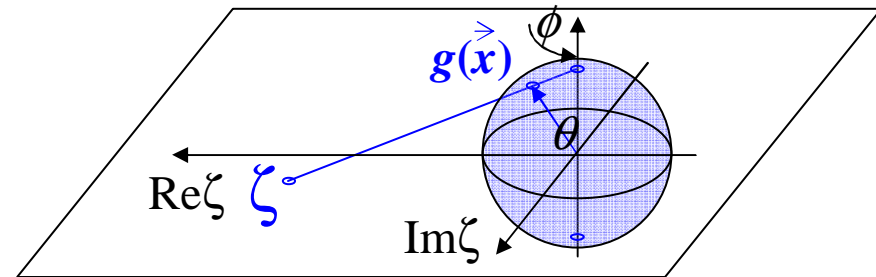
$$\zeta = u + iv \quad ds^2 = \mu(\zeta)(du^2 + dv^2), \quad \mu(\zeta) = \frac{\ell^2}{4} |F(\zeta)|^2 (1 + |\zeta|^2)^2$$

シュレーディンガー方程式

$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{\mu} \left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) - \frac{\hbar^2}{8m} (\kappa_1 - \kappa_2)^2 \right\} \psi(u, v) = E \psi(u, v)$$

$$|\kappa_1 - \kappa_2| = \frac{8}{|F(\zeta)| (1 + |\zeta|^2)^2}$$

$$\zeta = u + iv = \cot \frac{\theta}{2} e^{i\phi}$$



Aoki, Koshino, Takeda, Morise & Kuroki, *Electronic structure of periodic curved surfaces: Topological band structure*, Phys. Rev. B 65, 035102 (2001).

極小曲面の場合

曲面座標

曲面の計量

$$\zeta = u + iv \quad ds^2 = \mu(\zeta)(du^2 + dv^2), \quad \mu(\zeta) = \frac{\ell^2}{4} |F(\zeta)|^2 (1 + |\zeta|^2)^2$$

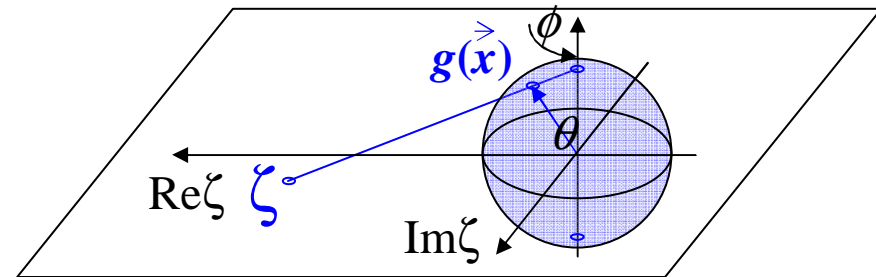
シュレーディンガー方程式

$$-\frac{(1 - \cos \theta)^4}{|F(\zeta)|^2} \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + 1 \right) \psi(\theta, \phi) = \varepsilon \psi(\theta, \phi)$$

$$\varepsilon = \frac{8m\ell^2 E}{\hbar^2}$$

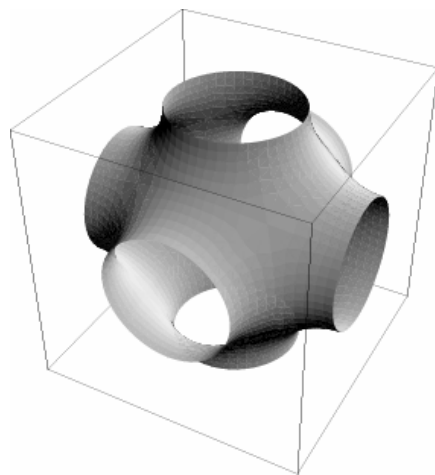


$$\zeta = u + iv = \cot \frac{\theta}{2} e^{i\phi}$$

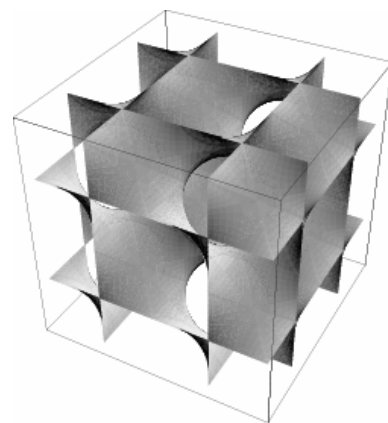


Aoki, Koshino, Takeda, Morise & Kuroki, *Electronic structure of periodic curved surfaces: Topological band structure*, Phys. Rev. B 65, 035102 (2001).

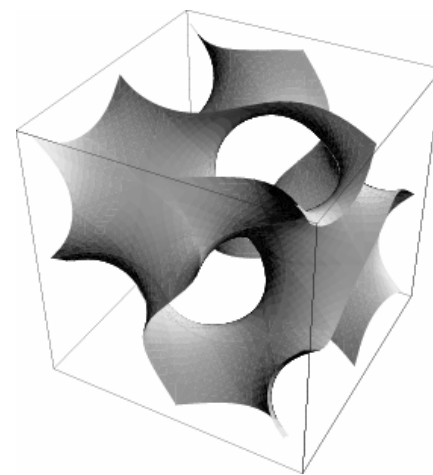
4. P, D, G表面のバンド構造



P



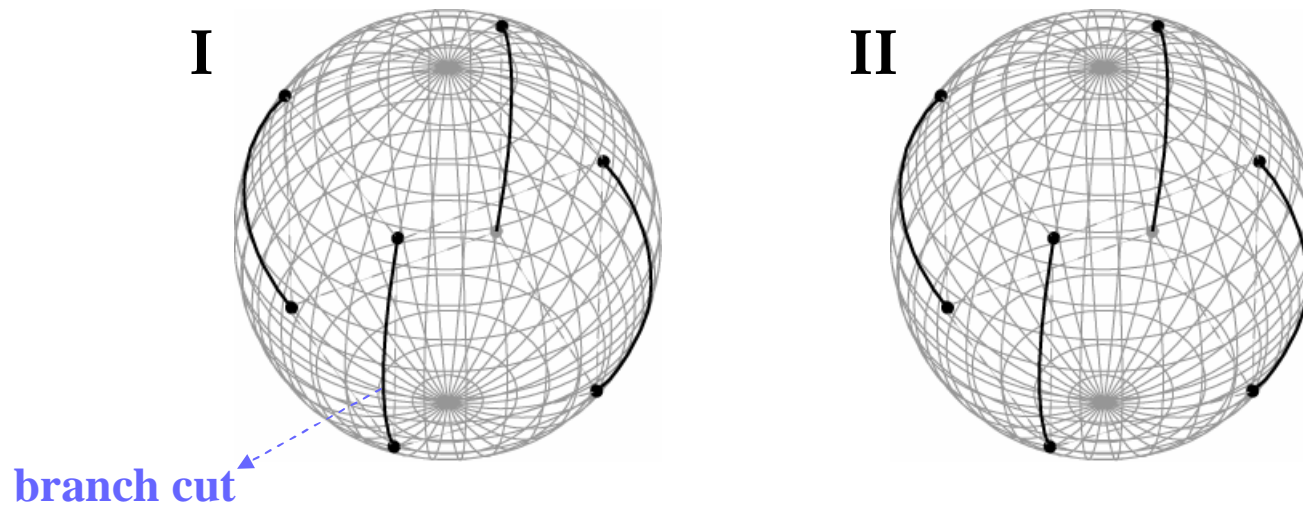
D



G

P, D, G表面の単位胞

基本単位胞 \mathcal{U} (12角形パッチ)のGauss写像は
branch cutで互いに接続した二つの球面

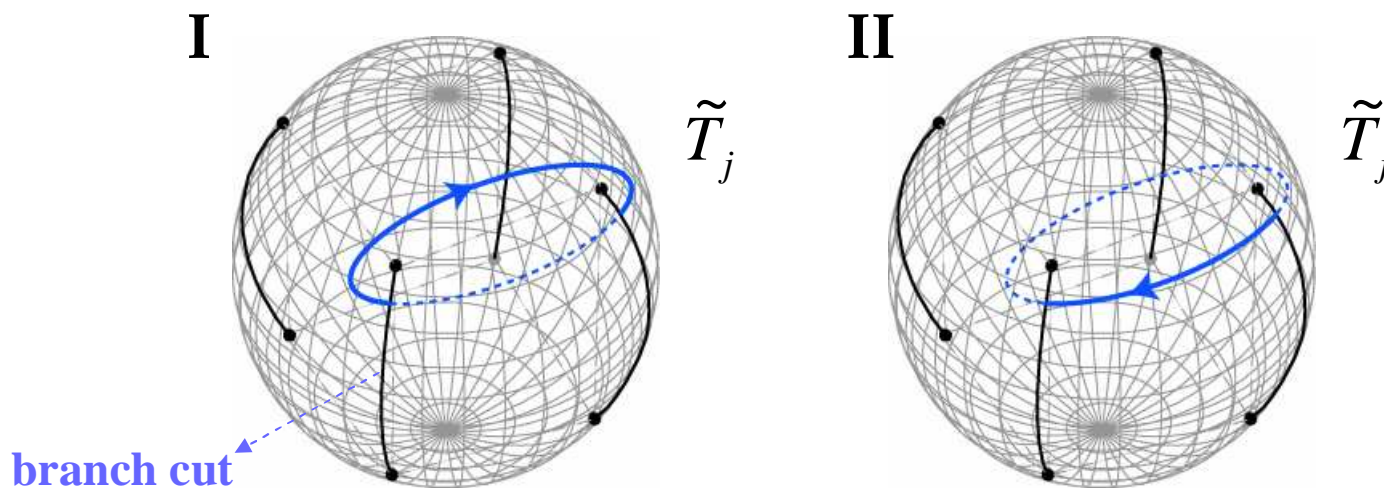


$$-\frac{(1-\cos\theta)^4}{|F(\zeta)|^2} \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + 1 \right) \psi(\theta, \phi) = \varepsilon\psi(\theta, \phi)$$

注： Gauss球面上で表したSchrödinger方程式はBonnet角に依存しない

Bloch条件

基本並進ベクトルに対応する閉曲線の周りの位相の回転を指定する



$$\Psi_{\vec{k}}(\zeta) \rightarrow e^{2\pi i \vec{k} \cdot \vec{T}_j^\alpha} \Psi_{\vec{k}}(\zeta) \quad (\text{位相の回転: } \alpha \text{ 依存})$$

$$\vec{T}_j^\alpha = \downarrow_{\alpha} \tilde{T}_j$$

六次元のバンド構造

六次元の波数空間 \tilde{k} の導入

$$\Psi_{\tilde{k}}(\zeta) \rightarrow e^{2\pi i \tilde{k} \cdot \tilde{T}_j} \Psi_{\tilde{k}}(\zeta) \quad (\text{位相の回転: } \alpha \text{ 非依存})$$

$$\varepsilon(\tilde{k} + \tilde{K}) = \varepsilon(\tilde{k}), \quad \forall \tilde{K} \in \left\{ \sum_j m_j \tilde{Q}_j \right\} \quad \text{六次元のバンド構造}$$

$$\left(\tilde{Q}_1 \quad \tilde{Q}_2 \quad \tilde{Q}_3 \quad \tilde{Q}_4 \quad \tilde{Q}_5 \quad \tilde{Q}_6 \right) = \left(\left(\tilde{T}_1 \quad \tilde{T}_2 \quad \tilde{T}_3 \quad \tilde{T}_4 \quad \tilde{T}_5 \quad \tilde{T}_6 \right)^{-1} \right)^{\mathbf{T}}$$

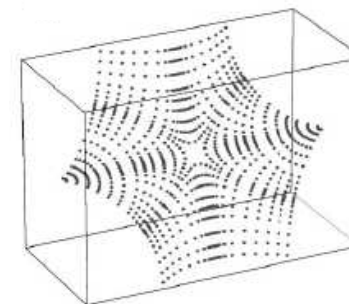
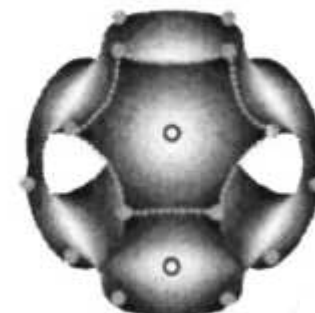
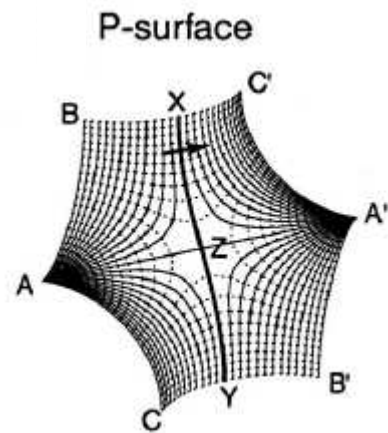
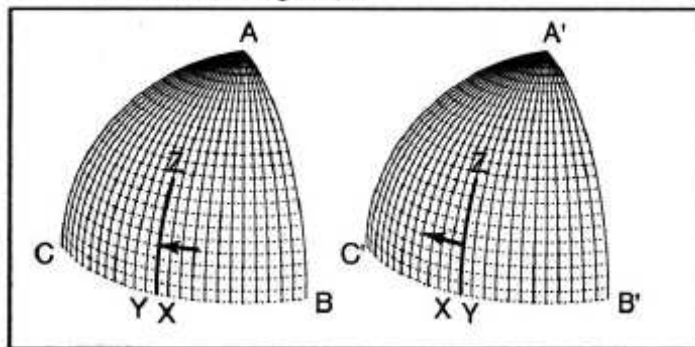
六次元の基本逆格子ベクトル

各極小表面のバンド構造は、対応する部分空間上の三次元断面 $\varepsilon(\tilde{k}_\alpha(\vec{k}))$ で与えられる

変数の離散化による数値計算

(Stereographic map)

$$w = \cot(\theta/2) \exp(i\phi)$$



Schrödinger eq.

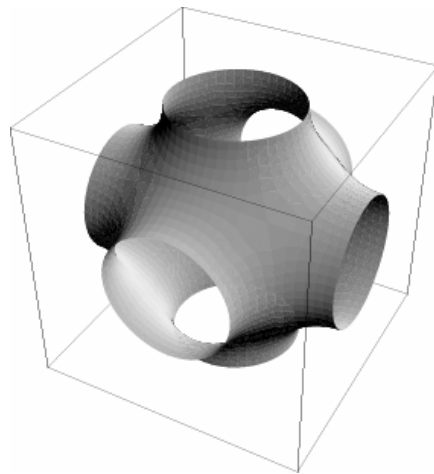
$$-\frac{(1 - \cos \theta)^4}{|F(w)|^2} \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + 1 \right) \psi(\theta, \phi) = \epsilon \psi(\theta, \phi)$$

$$\epsilon = 8m\ell^2 E / \hbar^2$$

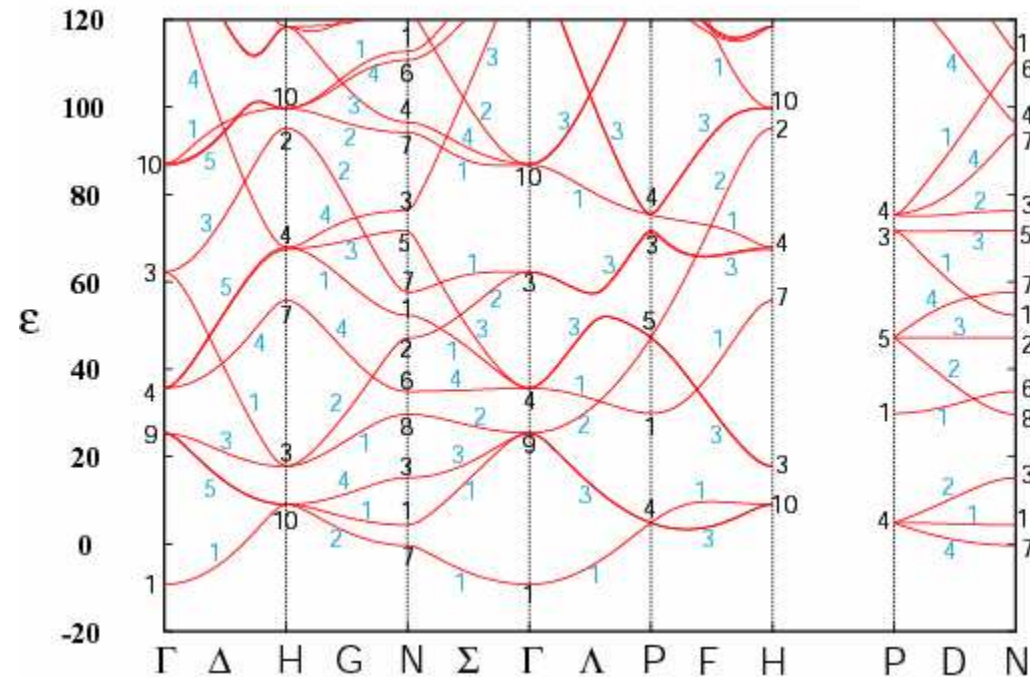
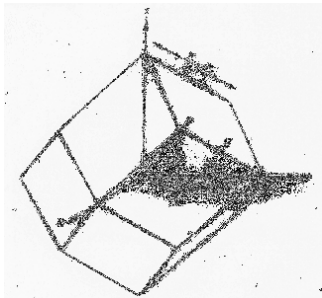
H.Aoki et al, Phys. Rev. B **65**, 035102 (2001).

P表面のバンド構造

4096 mesh pnts per \mathcal{U}



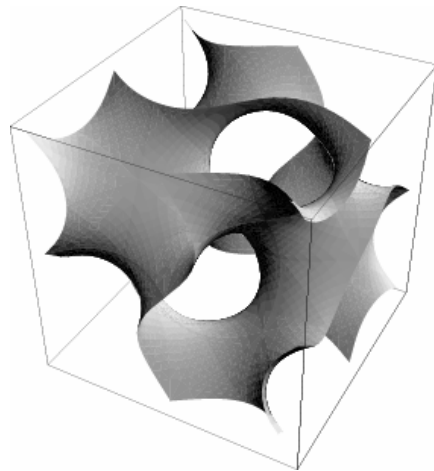
$Im\bar{3}m / Pm\bar{3}m$



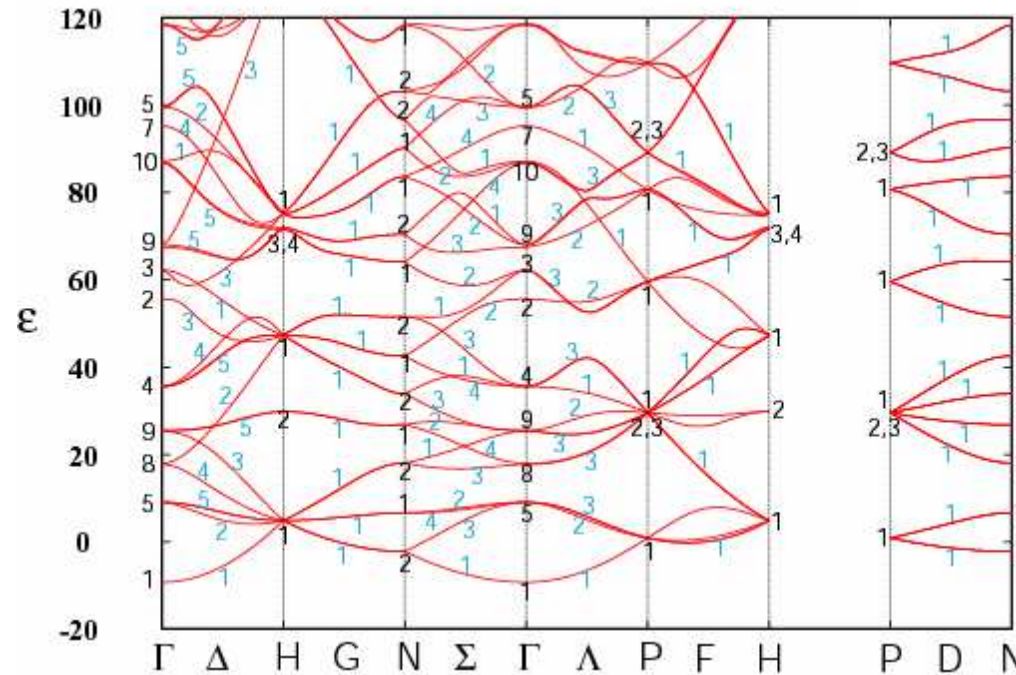
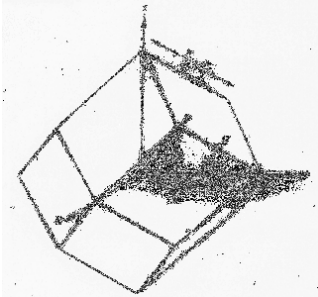
The numbers correspond to the specific irreducible representations for the space groups given by J. Zak et al, “*The Irreducible Representations of Space Groups*” (Benjamin, New York, 1969)

G表面のバンド構造

4096 mesh pnts per \mathcal{U}



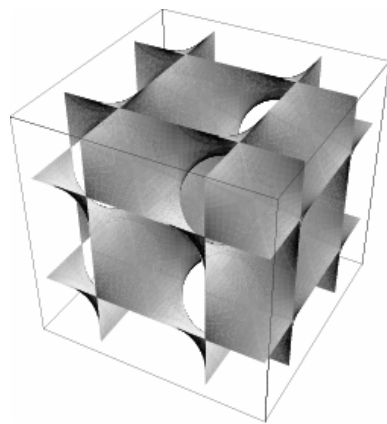
$Ia\bar{3}d / I4_132$



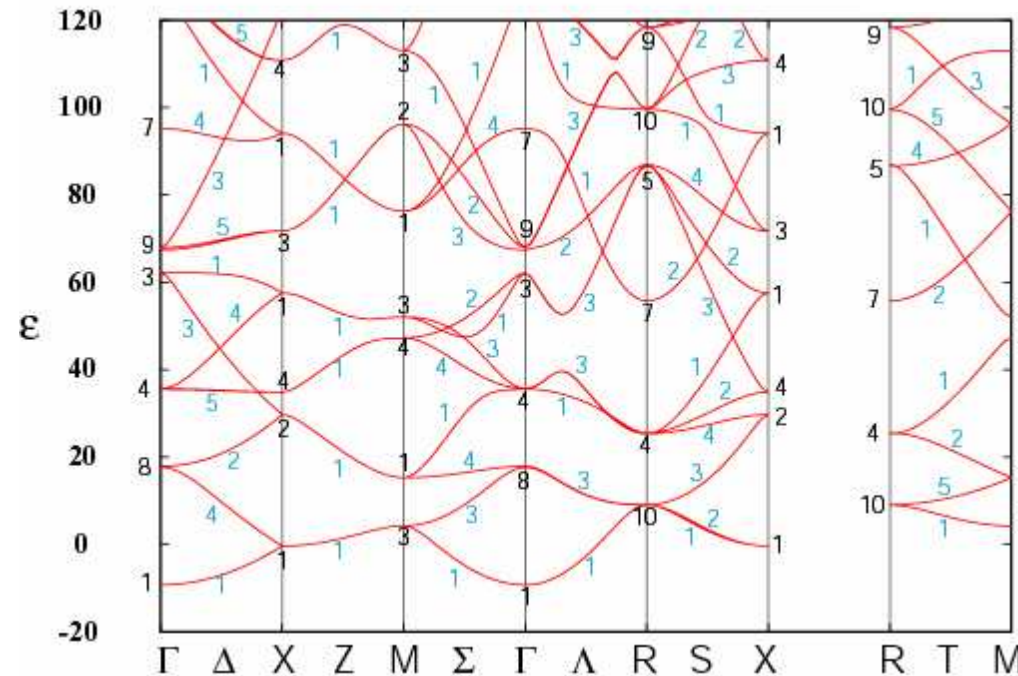
The numbers correspond to the specific irreducible representations for the space groups given by J. Zak et al, “*The Irreducible Representations of Space Groups*” (Benjamin, New York, 1969)

D表面のバンド構造

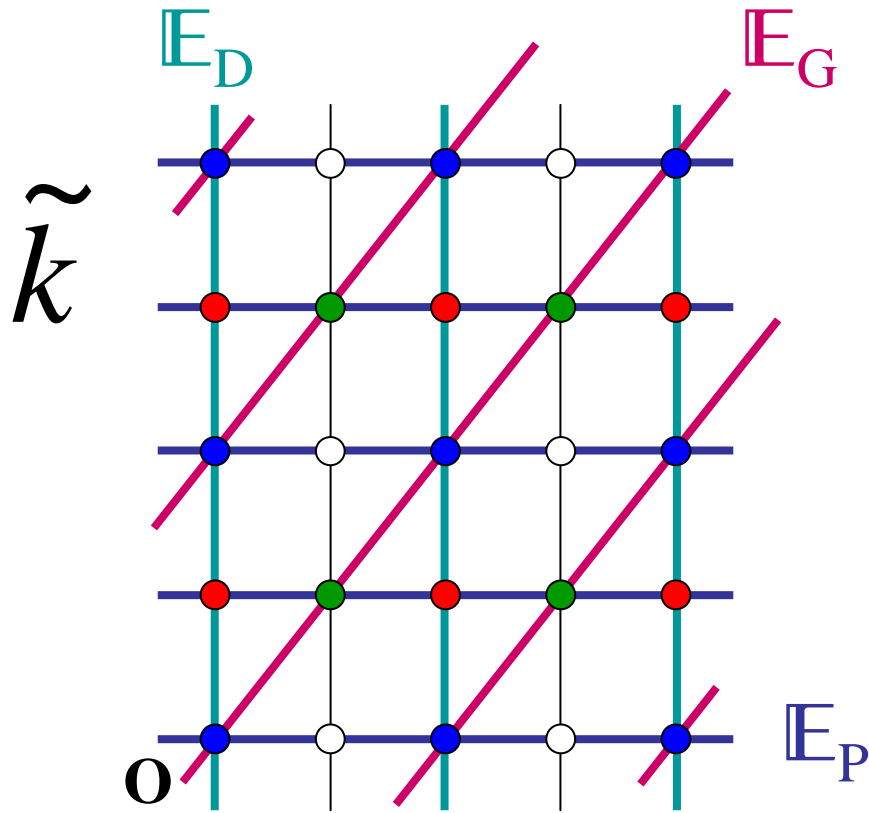
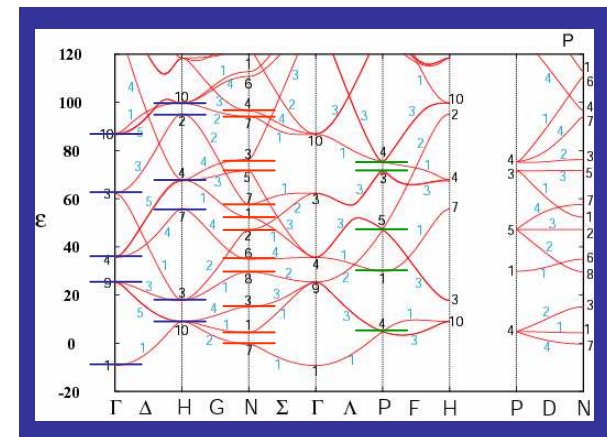
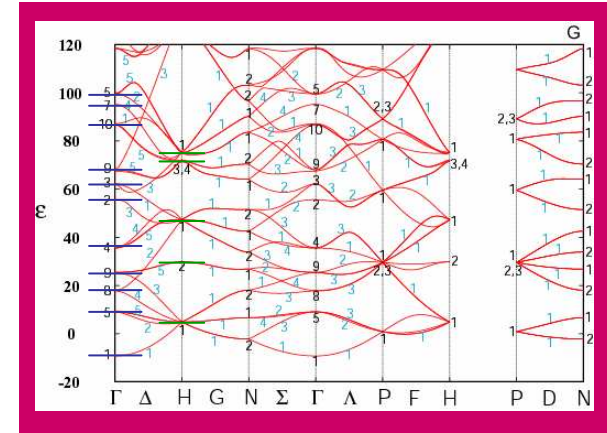
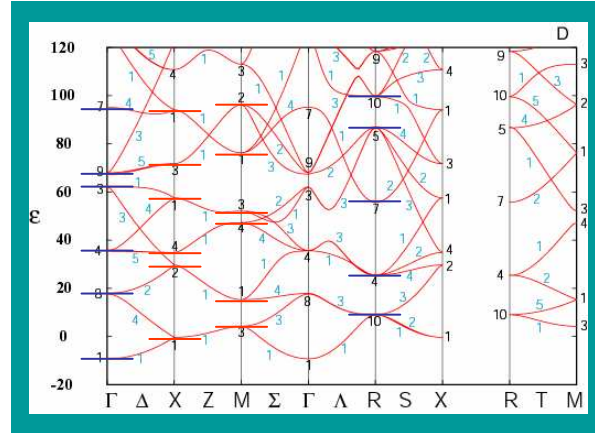
4096 mesh pnts per \mathcal{U}

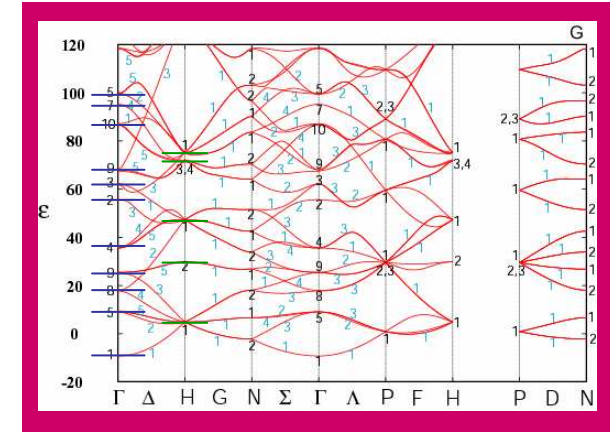
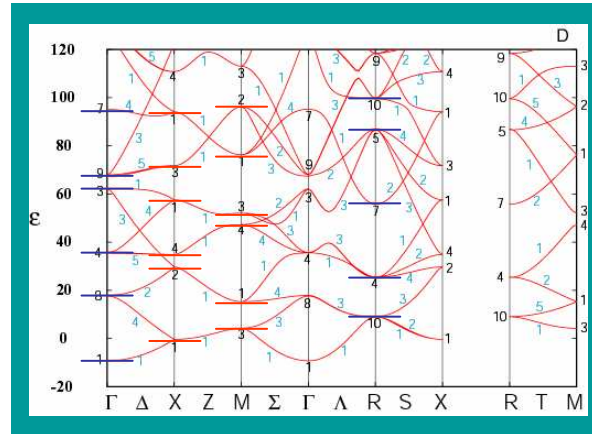


$Pn\bar{3}m / Fd\bar{3}m$



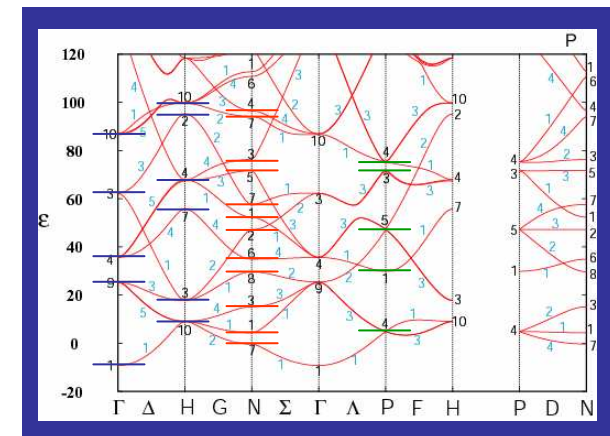
The numbers correspond to the specific irreducible representations for the space groups given by J. Zak et al, “*The Irreducible Representations of Space Groups*” (Benjamin, New York, 1969)





バンド交差による
エネルギー固有値の一致

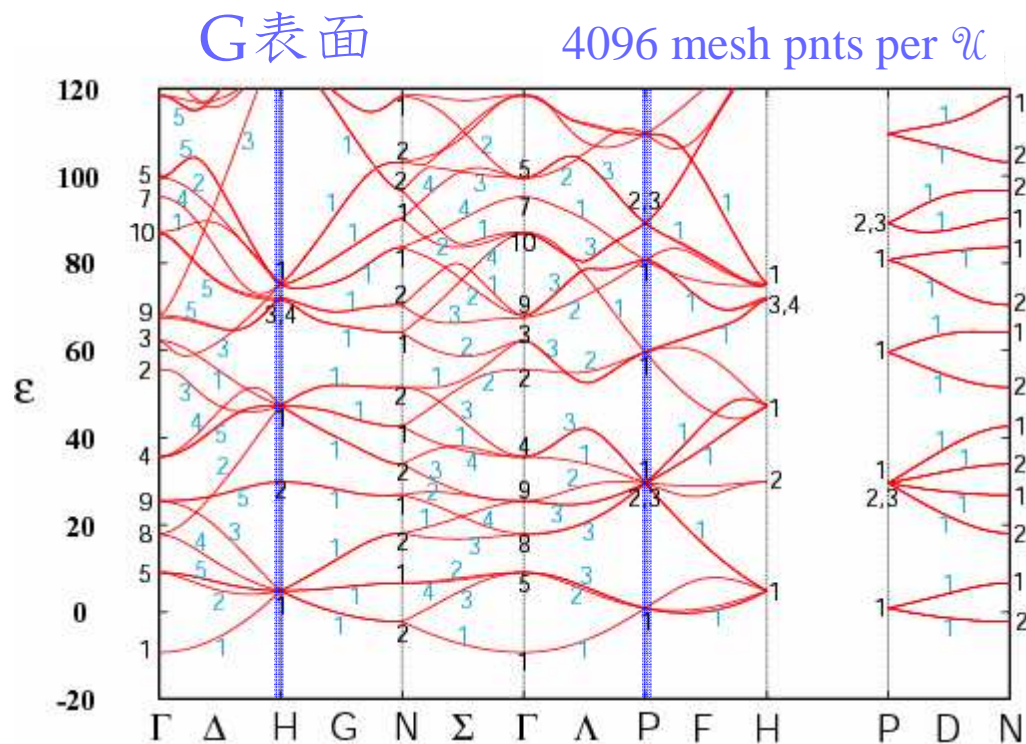
P-surface	D-surface	G-surface
Γ (Γ, H)	Γ (Γ, R)	Γ
M (N^2)	X (M, X)	—
R (P^2)	—	H



5. 波動関数の対称性と ノード線

空間群の既約表現による分類

Brillouin ゾーン内の特殊点における準位の縮退度は対応する既約表現の次元数に等しい



$Ia\bar{3}d$

非共型空間群
(non-symmorphic)
→ 螺旋軸、映進面

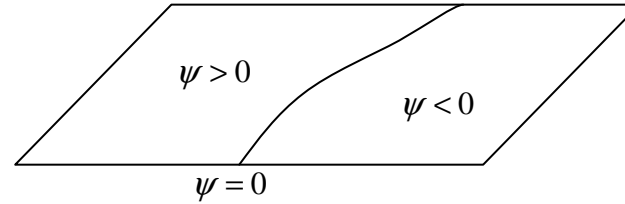
H_1 — 6-fold

P_1 — 4-fold

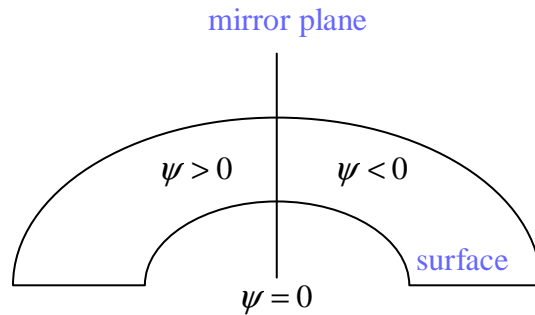
H_2, H_3, H_4, P_2, P_3 — 2-fold

時間反転対称性による縮退

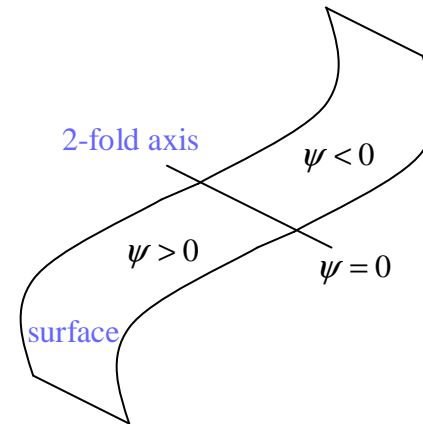
ノード線



曲面上の曲線を不変に保つ対称操作に対して既約表現が奇ならば、ノード線が存在する

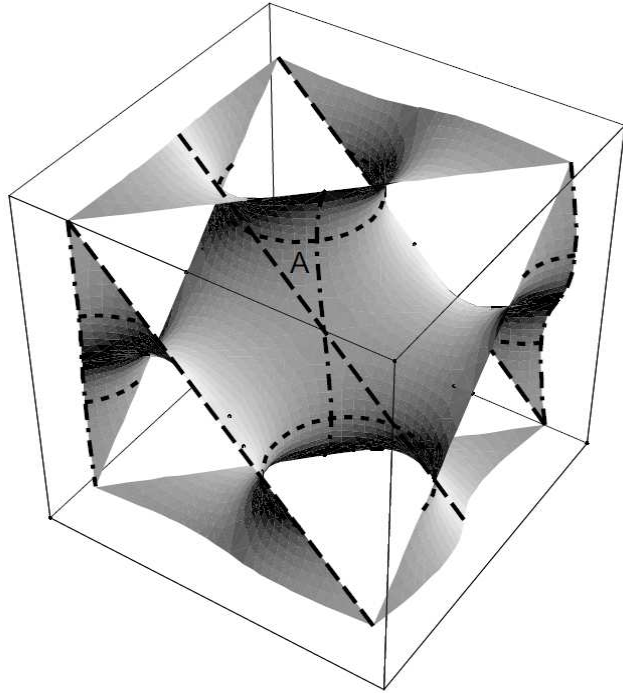


曲面と垂直交差する鏡映面



曲面上の二回軸

P 表面



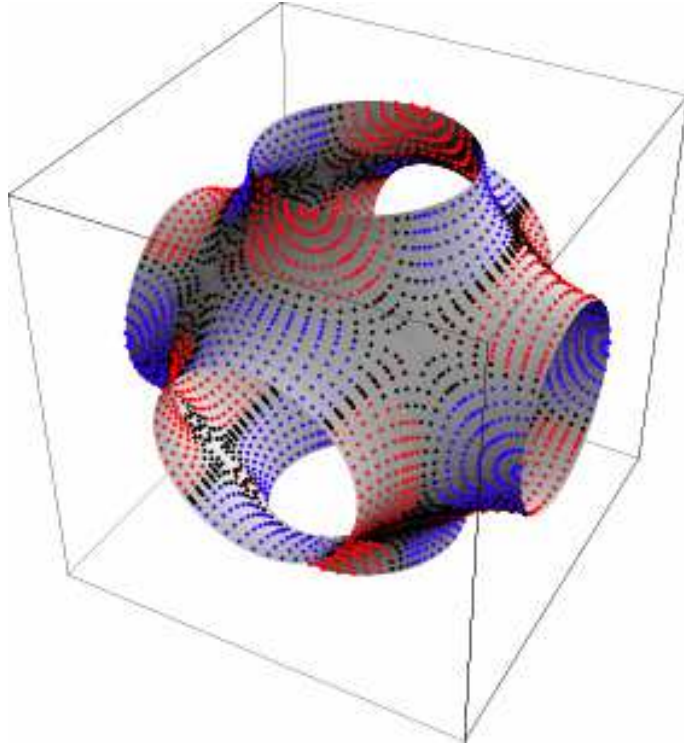
(two-fold axes U_d) $U^{xy}, U^{\bar{x}y}, U^{yz}, U^{\bar{y}z}, U^{zx}, U^{\bar{z}x}$,

(mirrors σ_d) $\sigma^{xy}, \sigma^{\bar{x}y}, \sigma^{yz}, \sigma^{\bar{y}z}, \sigma^{zx}, \sigma^{\bar{z}x}$,

(mirrors σ) $\sigma^x, \sigma^y, \sigma^z$.

k-point	G_k/T	IR (nodal lines)
$\Gamma (0, 0, 0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(3\sigma, 6\sigma_d), \Gamma_7(6U_d, 3\sigma), \Gamma_8(3\sigma)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma, 2\sigma_d), \Delta_3(2\sigma_d), \Delta_4(2\sigma)$
$H (1, 0, 0)$	O_h	$H_1(6U_d), H_2(6\sigma_d), H_6(6U_d, 3\sigma, 6\sigma_d), H_7(3\sigma), H_8(3\sigma)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(U_d, \sigma_d), \Sigma_3(\sigma, \sigma_d), \Sigma_4(U_d, \sigma)$
$G (k_x, 1 - k_x, 0)$	C_{2v}	$G_1(U_d), G_2(\sigma_d), G_3(U_d, \sigma, \sigma_d), G_4(\sigma)$
$N (\frac{1}{2}, \frac{1}{2}, 0)$	D_{2h}	$N_1(U^{\bar{x}y}), N_2(\sigma^{\bar{x}y}, \sigma^z), N_3(U^{xy}, U^{\bar{x}y}, \sigma^z, \sigma^{xy}), N_4(U^{xy}, \sigma^{xy}, \sigma^{\bar{x}y}),$ $N_5(U^{\bar{x}y}, \sigma^z, \sigma^{xy}, \sigma^{\bar{x}y}), N_6(\sigma^{xy}), N_7(U^{xy}, U^{\bar{x}y}, \sigma^{\bar{x}y}), N_8(U^{xy}, \sigma^z)$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$F (k_x, 1 - k_x, 1 - k_x)$	C_{3v}	$F_2(3\sigma_d)$
$D (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{2v}	$D_2(\sigma^{xy}), D_3(\sigma^{xy}, \sigma^{\bar{x}y}), D_4(\sigma^{\bar{x}y})$
$P (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	T_d	$P_2(6\sigma_d)$
$\Xi (k_x, k_y, 0)$	C_s	$\Xi_2(\sigma)$
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$B (k_x, 1 - k_x, k_z)$	C_s	$B_2(\sigma_d)$

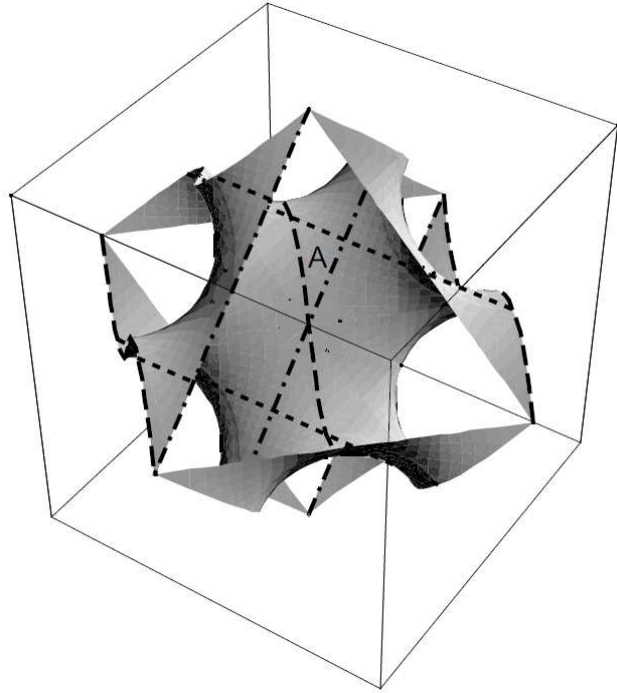
P 表面



(two-fold axes U_d) $U^{xy}, U^{\bar{x}y}, U^{yz}, U^{\bar{y}z}, U^{zx}, U^{\bar{z}x}$,
 (mirrors σ_d) $\sigma^{xy}, \sigma^{\bar{x}y}, \sigma^{yz}, \sigma^{\bar{y}z}, \sigma^{zx}, \sigma^{\bar{z}x}$,
 (mirrors σ) $\sigma^x, \sigma^y, \sigma^z$.

k-point	G_k/T	IR (nodal lines)
$\Gamma (0,0,0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(3\sigma, 6\sigma_d), \Gamma_7(6U_d, 3\sigma), \Gamma_8(3\sigma)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma, 2\sigma_d), \Delta_3(2\sigma_d), \Delta_4(2\sigma)$
$H (1, 0, 0)$	O_h	$H_1(6U_d), H_2(6\sigma_d), H_6(6U_d, 3\sigma, 6\sigma_d), H_7(3\sigma), H_8(3\sigma)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(U_d, \sigma_d), \Sigma_3(\sigma, \sigma_d), \Sigma_4(U_d, \sigma)$
$G (k_x, 1 - k_x, 0)$	C_{2v}	$G_1(U_d), G_2(\sigma_d), G_3(U_d, \sigma, \sigma_d), G_4(\sigma)$
$N (\frac{1}{2}, \frac{1}{2}, 0)$	D_{2h}	$N_1(U^{\bar{x}y}), N_2(\sigma^{\bar{x}y}, \sigma^z), N_3(U^{xy}, U^{\bar{x}y}, \sigma^z, \sigma^{xy}), N_4(U^{xy}, \sigma^{xy}, \sigma^{\bar{x}y}),$ $N_5(U^{\bar{x}y}, \sigma^z, \sigma^{xy}, \sigma^{\bar{x}y}), N_6(\sigma^{xy}), N_7(U^{xy}, U^{\bar{x}y}, \sigma^{\bar{x}y}), N_8(U^{xy}, \sigma^z)$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$F (k_x, 1 - k_x, 1 - k_x)$	C_{3v}	$F_2(3\sigma_d)$
$D (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{2v}	$D_2(\sigma^{xy}), D_3(\sigma^{xy}, \sigma^{\bar{x}y}), D_4(\sigma^{\bar{x}y})$
$P (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	T_d	$P_2(6\sigma_d)$
$\Xi (k_x, k_y, 0)$	C_s	$\Xi_2(\sigma)$
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$B (k_x, 1 - k_x, k_z)$	C_s	$B_2(\sigma_d)$

D表面



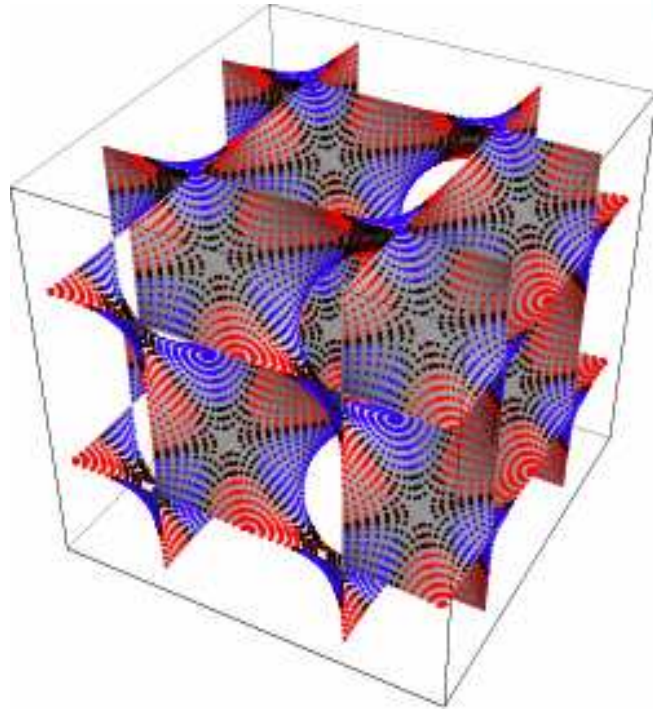
(mirrors σ_d) $\sigma^{xy}, \sigma^{\bar{x}y}, \sigma^{yz}, \sigma^{\bar{y}z}, \sigma^{zx}, \sigma^{\bar{z}x},$

(two-fold axes U_d) $U^{xy}, U^{\bar{x}y}, U^{yz}, U^{\bar{y}z}, U^{zx}, U^{\bar{z}x},$

(two-fold axes U) $U^x, U^y, U^z.$

k-point	G_k/T	IR (nodal lines)
$\Gamma (0, 0, 0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(6\sigma_d), \Gamma_7(6U_d)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma_d), \Delta_3(2\sigma_d), \Delta_5(U)$
$X (\frac{1}{2}, 0, 0)$	D_{4h}	$X_2(2\sigma_d), X_3(U^x, U^{yz}, U^{\bar{y}z}), X_4(U^x)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(\sigma_d, U_d), \Sigma_3(\sigma_d), \Sigma_4(U_d)$
$Z (k_x, \frac{1}{2}, 0)$	C_{2v}	—
$M (\frac{1}{2}, \frac{1}{2}, 0)$	D_{4h}	$M_1(U^z), M_2(U^z, 2\sigma_d), M_4(U^{xy}, U^{\bar{x}y})$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$S (\frac{1}{2}, k_y, k_y)$	C_{2v}	$S_3(\sigma^{\bar{y}z}), S_4(\sigma^{\bar{y}z})$
$T (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{4v}	$T_2(U^z), T_3(U^z), T_4(U^z), T_5(U^z)$
$R (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	O_h	$R_1(3U, 6U_d), R_2(3U, 6\sigma_d), R_3(3U), R_6(3U, 6U_d, 6\sigma_d), R_7(3U), R_8(3U)$
$\Xi (k_x, k_y, 0)$	C_s	—
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$A (\frac{1}{2}, k_y, k_z)$	C_s	—

D表面



(mirrors σ_d) $\sigma^{xy}, \sigma^{\bar{x}y}, \sigma^{yz}, \sigma^{\bar{y}z}, \sigma^{zx}, \sigma^{\bar{z}x}$,

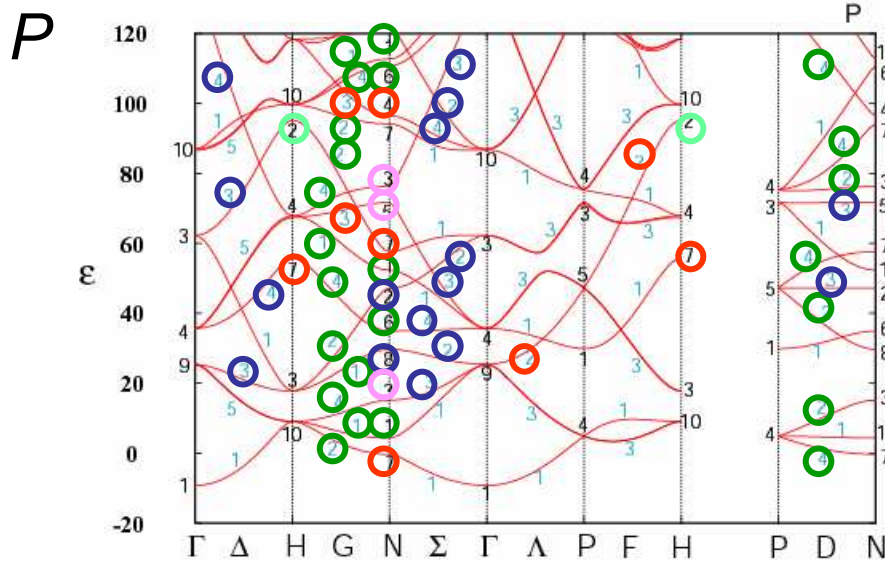
(two-fold axes U_d) $U^{xy}, U^{\bar{x}y}, U^{yz}, U^{\bar{y}z}, U^{zx}, U^{\bar{z}x}$,

(two-fold axes U) U^x, U^y, U^z .

k-point	G_k/T	IR (nodal lines)
$\Gamma (0, 0, 0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(6\sigma_d), \Gamma_7(6U_d)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma_d), \Delta_3(2\sigma_d), \Delta_5(U)$
$X (\frac{1}{2}, 0, 0)$	D_{4h}	$X_2(2\sigma_d), X_3(U^x, U^{yz}, U^{\bar{y}z}), X_4(U^x)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(\sigma_d, U_d), \Sigma_3(\sigma_d), \Sigma_4(U_d)$
$Z (k_x, \frac{1}{2}, 0)$	C_{2v}	—
$M (\frac{1}{2}, \frac{1}{2}, 0)$	D_{4h}	$M_1(U^z), M_2(U^z, 2\sigma_d), M_4(U^{xy}, U^{\bar{x}y})$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$S (\frac{1}{2}, k_y, k_y)$	C_{2v}	$S_3(\sigma^{\bar{y}z}), S_4(\sigma^{\bar{y}z})$
$T (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{4v}	$T_2(U^z), T_3(U^z), T_4(U^z), T_5(U^z)$
$R (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	O_h	$R_1(3U, 6U_d), R_2(3U, 6\sigma_d), R_3(3U), R_6(3U, 6U_d, 6\sigma_d), R_7(3U), R_8(3U)$
$\Xi (k_x, k_y, 0)$	C_s	—
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$A (\frac{1}{2}, k_y, k_z)$	C_s	—

The existence of nodal lines in an eigenstate necessitate a sufficient amount of kinetic energy, so that IR's with a large number of nodal lines cannot appear in a lowest part of the energy spectrum. It is also seen that IR's with nodal lines appear roughly in the increasing order in the number of nodal lines as one goes up the energy axis.

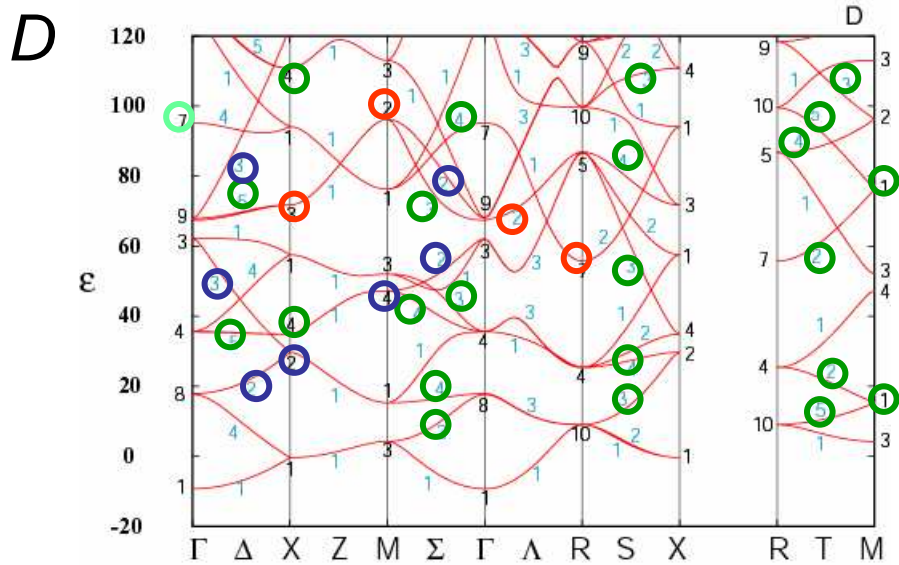
Therefore, nodal lines can be regarded as an important feature of eigenstates present in real-space in order to understand the overall characteristics of the systems.



k-point	G_k/T	IR (nodal lines)
$\Gamma (0, 0, 0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(3\sigma, 6\sigma_d), \Gamma_7(6U_d, 3\sigma), \Gamma_8(3\sigma)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma, 2\sigma_d), \Delta_3(2\sigma_d), \Delta_4(2\sigma)$
$H (1, 0, 0)$	O_h	$H_1(6U_d), H_2(6\sigma_d), H_6(6U_d, 3\sigma, 6\sigma_d), H_7(3\sigma), H_8(3\sigma)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(U_d, \sigma_d), \Sigma_3(\sigma, \sigma_d), \Sigma_4(U_d, \sigma)$
$G (k_x, 1 - k_x, 0)$	C_{2v}	$G_1(U_d), G_2(\sigma_d), G_3(U_d, \sigma, \sigma_d), G_4(\sigma)$
$N (\frac{1}{2}, \frac{1}{2}, 0)$	D_{2h}	$N_1(U^{xy}), N_2(\sigma^{xy}, \sigma^z), N_3(U^{xy}, U^{xy}, \sigma^z, \sigma^{xy}), N_4(U^{xy}, \sigma^{xy}, \sigma^{xy}), N_5(U^{xy}, \sigma^z, \sigma^{xy}, \sigma^{xy}), N_6(\sigma^{xy}), N_7(U^{xy}, U^{xy}, \sigma^{xy}), N_8(U^{xy}, \sigma^z)$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$F (k_x, 1 - k_x, 1 - k_x)$	C_{3v}	$F_2(3\sigma_d)$
$D (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{2v}	$D_2(\sigma^{xy}), D_3(\sigma^{xy}, \sigma^{xy}), D_4(\sigma^{xy})$
$P (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	T_d	$P_2(6\sigma_d)$
$\Xi (k_x, k_y, 0)$	C_s	$\Xi_2(\sigma)$
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$B (k_x, 1 - k_x, k_z)$	C_s	$B_2(\sigma_d)$

The existence of nodal lines in an eigenstate necessitate a sufficient amount of kinetic energy, so that IR's with a large number of nodal lines cannot appear in a lowest part of the energy spectrum. It is also seen that IR's with nodal lines appear roughly in the increasing order in the number of nodal lines as one goes up the energy axis.

Therefore, nodal lines can be regarded as an important feature of eigenstates present in real-space in order to understand the overall characteristics of the systems.



k-point	G_k/T	IR (nodal lines)
$\Gamma (0, 0, 0)$	O_h	$\Gamma_2(6U_d, 6\sigma_d), \Gamma_6(6\sigma_d), \Gamma_7(6U_d)$
$\Delta (k_x, 0, 0)$	C_{4v}	$\Delta_2(2\sigma_d), \Delta_3(2\sigma_d), \Delta_5(U)$
$X (\frac{1}{2}, 0, 0)$	D_{4h}	$X_2(2\sigma_d), X_3(U^x, U^{yz}, U^{yz}), X_4(U^x)$
$\Sigma (k_x, k_x, 0)$	C_{2v}	$\Sigma_2(\sigma_d, U_d), \Sigma_3(\sigma_d), \Sigma_4(U_d)$
$Z (k_x, \frac{1}{2}, 0)$	C_{2v}	—
$M (\frac{1}{2}, \frac{1}{2}, 0)$	D_{4h}	$M_1(U^z), M_2(U^z, 2\sigma_d), M_4(U^{xy}, U^{xy})$
$\Lambda (k_x, k_x, k_x)$	C_{3v}	$\Lambda_2(3\sigma_d)$
$S (\frac{1}{2}, k_y, k_y)$	C_{2v}	$S_3(\sigma^{yz}), S_4(\sigma^{yz})$
$T (\frac{1}{2}, \frac{1}{2}, k_z)$	C_{4v}	$T_2(U^z), T_3(U^z), T_4(U^z), T_5(U^z)$
$R (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	O_h	$R_1(3U, 6U_d), R_2(3U, 6\sigma_d), R_3(3U), R_6(3U, 6U_d, 6\sigma_d), R_7(3U), R_8(3U)$
$\Xi (k_x, k_y, 0)$	C_s	—
$\Theta (k_x, k_x, k_z)$	C_s	$\Theta_2(\sigma_d)$
$A (\frac{1}{2}, k_y, k_z)$	C_s	—

6. まとめ

- 同一のBonnet族に属する周期的極小曲面に拘束された電子は、リーマン面上等価なSchrödinger方程式に従う
- 所与の波数ベクトルに対し、リーマン面上の特異点を囲む任意の閉曲線における位相の回転が曲面のトポロジーによって指定される (Bloch条件)
- 曲面のトポロジーは六次元におけるトポロジーの投影として与えられ、そのバンド構造は六次元の仮想的バンド構造の三次元断面として記述できる (各バンド構造の接続)
- ノード線の発生は空間群の既約表現を用いて理解できる

7. 課題？

準古典論に基づく位相不変量（winding数）の導入によるバンド構造の連結性の説明、など

