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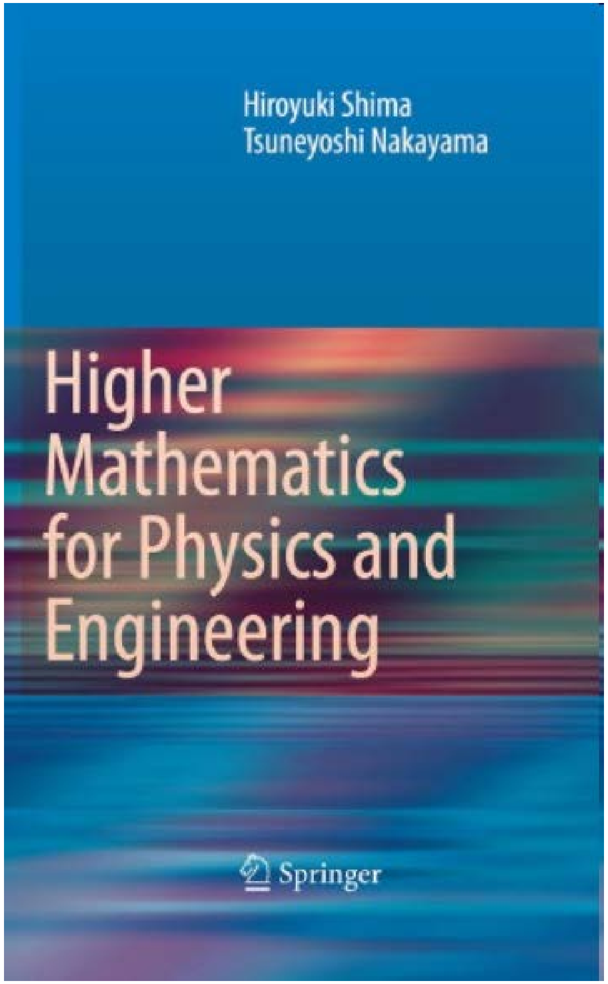

Higher Mathematics for Physics and Engineering

H. Shima & T. Nakayama

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(EQualS 2013) at University Putra Malaysia
22-24, November 2013

Geometry-Property Relationship in Condensed Matter Physics

Hiroyuki Shima

Dept. of Environmental Sciences
University of Yamanashi, Japan

Fuji-Minori
("Minori" = "Berry")

Fuji-Yama
("Yama"="Mountain")

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Department of Local Produce and Food Sciences

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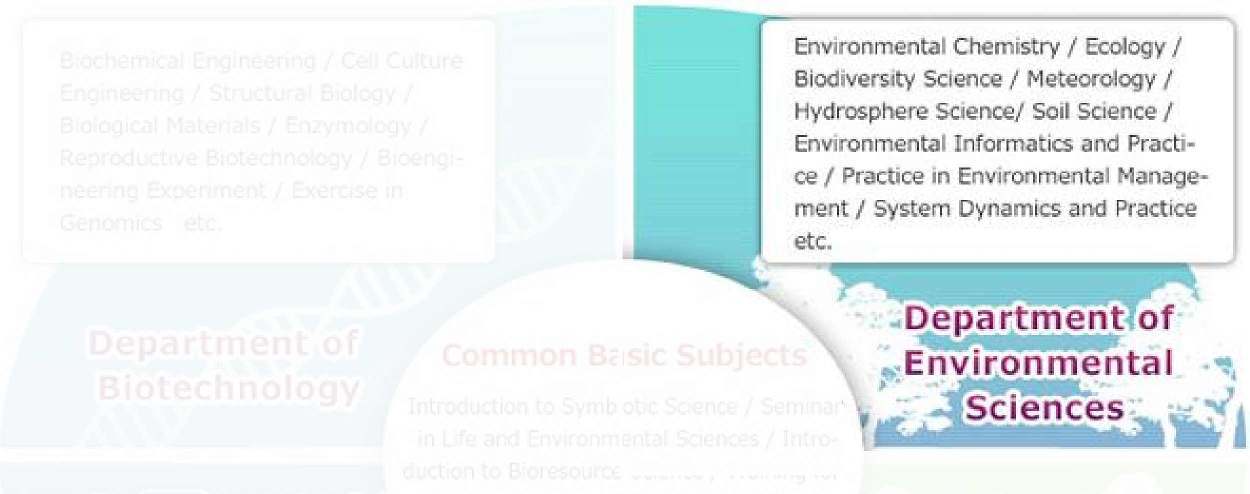
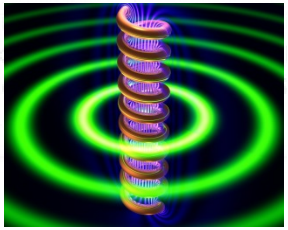


Environmental Sciences =
Physics + Chemistry + Biology + Geoscience




- Complex dynamics of environment
- Fundamental origin of natural phenomena
- Mathematical methods for environment analyses

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Geometry-Property Relationship in Condensed Matter Physics

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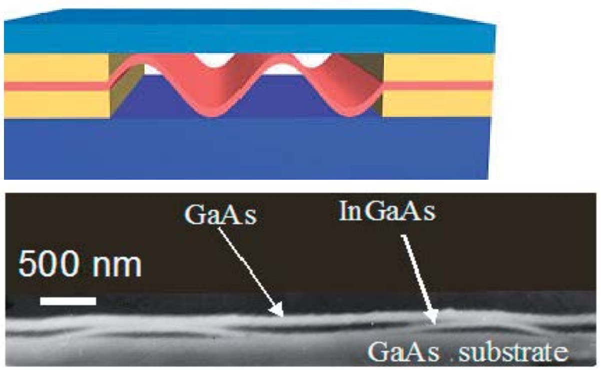
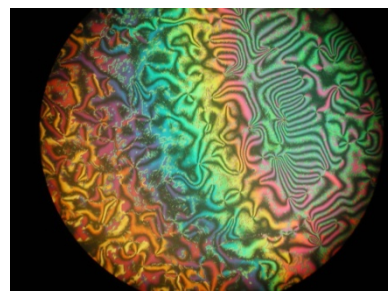
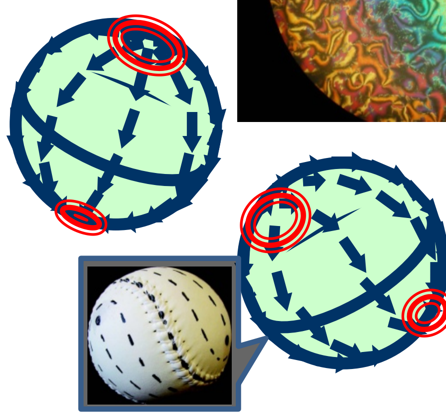
Quantum mechanics on Curved surfaces



Phys. Rev. B **86**, 035415 (2012)
EPL **96** 27011 (2011)
Phys. Rev. B **79,** 201401 (2009)

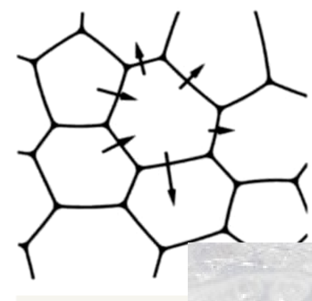
Liquid crystal on Curved substrates





J. Phys. Soc. Jpn. **79**, 074607 (2010).

Foam Dynamics



J. Phys. Soc. Jpn. **79**, 074601 (2010).

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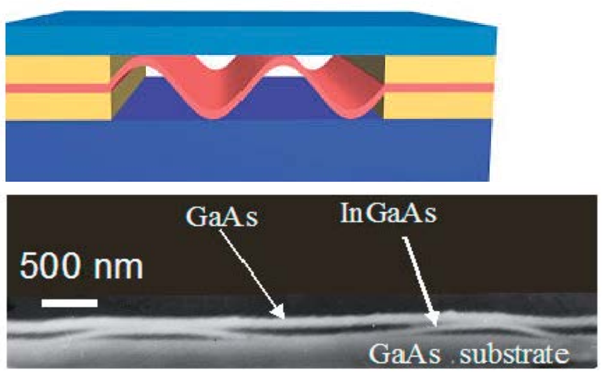

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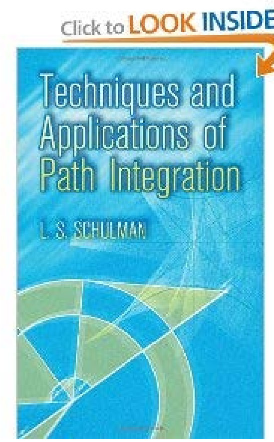
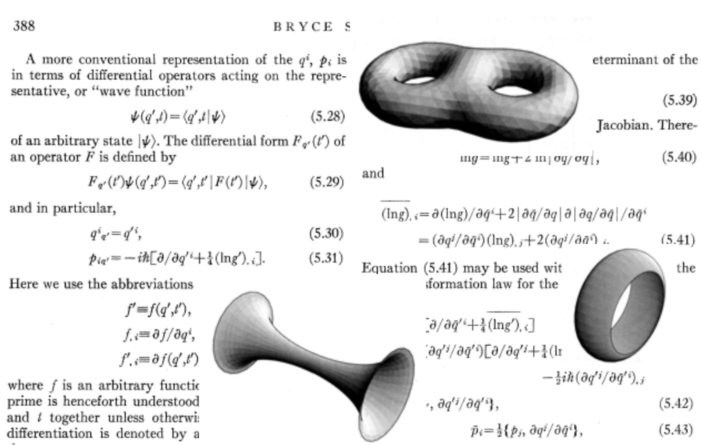
1. History of QM on curved surfaces



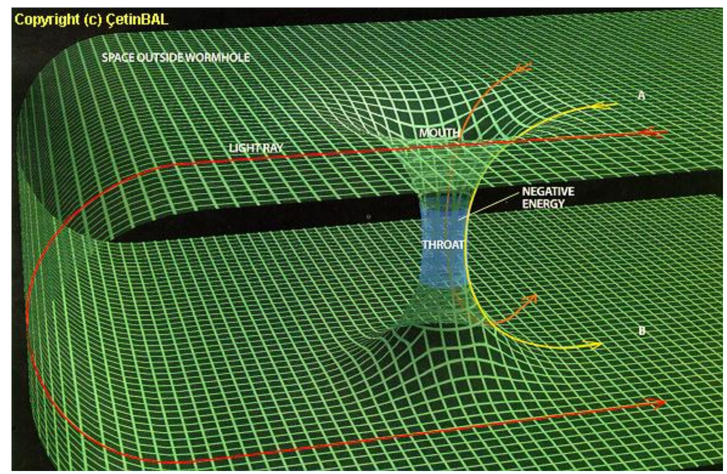
> *"If you like excitement, conflict, and controversy, especially when nothing very serious is at stake, then you will love the history of quantization on curved spaces."*

L.S. Schulman, "*Techniques and Applications of Path Integration*", (Wiley, 1981)

[1] Mathematical foundations of quantum mechanics



[2] Quantum gravity, Early universe

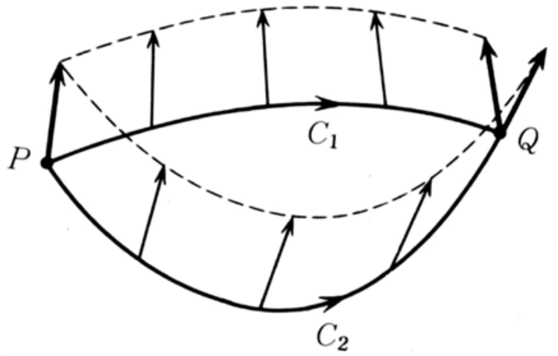


[3] Quantum physics of curved nano-materials

2. Gaussian curvature

… Geometry-induced scalar potential stems from non-zero Gaussian curvature.

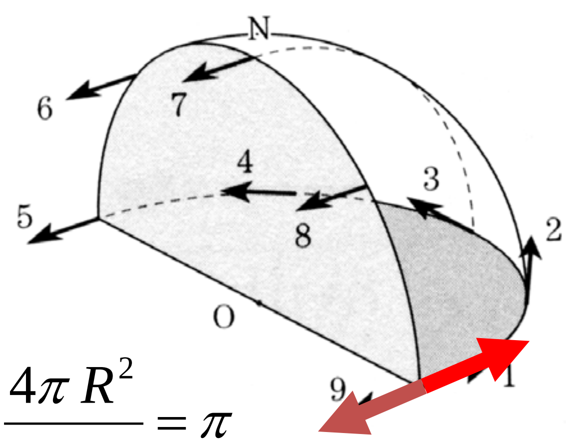
Defintion of Gaussian curvature:



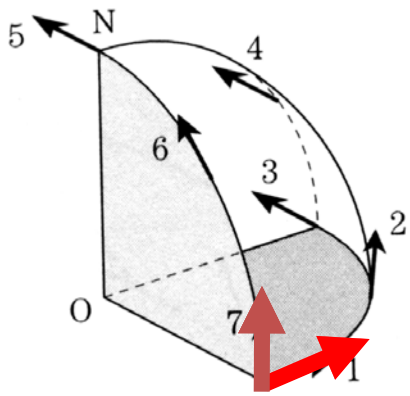
On a curved surface, parallel displacement of a vector along a closed loop causes its rotation by the angle $\Delta\theta$:

$$\Delta\theta = \iint_S K d\sigma$$: Gauss-Bonnet's theorem

K: Gaussian curvature $\left(= \frac{1}{R^2}\right)$



$$\Delta\theta = \frac{1}{R^2} \times \frac{4\pi R^2}{4} = \pi$$



$$\Delta\theta = \frac{1}{R^2} \times \frac{4\pi R^2}{8} = \frac{\pi}{2}$$

2. Gaussian curvature

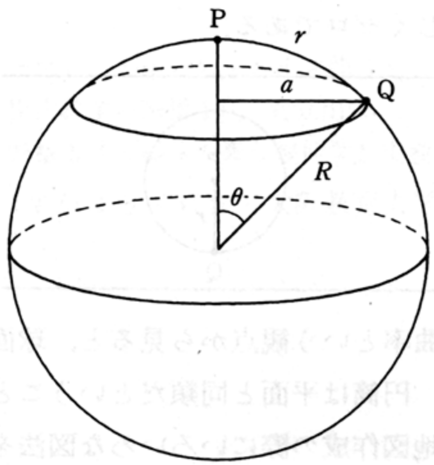
Practical formula

GC at point P: $$K = \lim_{r \to 0} \frac{3[2\pi r - \ell(r)]}{\pi r^3}$$

r : geodesic distance from P

$\ell(r)$: length of an enclosing curve around P

ex.) Spherical surface



The length of a closed contour:

$$\ell(r) = 2\pi a \ = 2\pi R \sin(r/R)$$

$$= 2\pi r - 2\pi \frac{r^3}{3! R^2} + \cdots$$

The Gaussian curvature of the sphere:

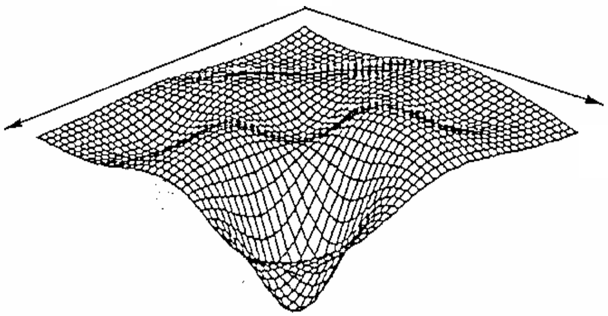
$$K = 1/R^2 > 0$$

Classes of curved surfaces:

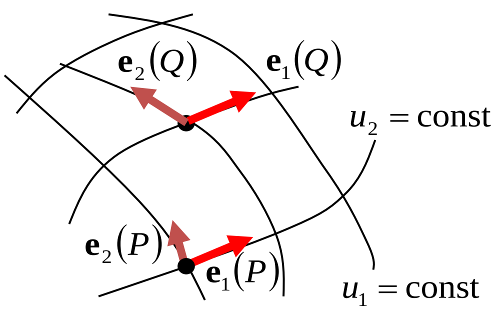
- Positively curved surface: $K > 0$
- Flat plane : $K = 0$
- Negatively curved surface: $K < 0$

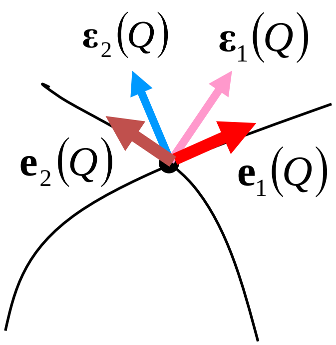
2'. Gaussian curvature .vs Metric tensor

Suppose a curved surface associated with the curvilinear coordinate system u_1, u_2 .
Then, …



$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ $\quad g^{ij} = \boldsymbol{\varepsilon}^i \cdot \boldsymbol{\varepsilon}^j$: Metric tensor





$$\Gamma^m_{ij} = \frac{g^{mp}}{2}\left(\partial_j g_{pi} + \partial_i g_{pj} - \partial_p g_{ij}\right) \text{ : Connection}$$

$$R^m{}_{ilj} = \partial_l \Gamma^m_{ij} - \partial_j \Gamma^m_{il} + \Gamma^m_{pl}\Gamma^p_{ij} - \Gamma^m_{pj}\Gamma^p_{il}$$

$$R_{kilj} = g_{km} R^m{}_{ilj} \text{ : Riemann tensor}$$

$$R_{ij} = g^{kl} R_{kilj} \text{ : Ricci tensor}$$

$$R = g^{ij} R_{ij} \text{ : Scalar curvature}$$

Exact definition: $K = -\dfrac{R}{2}$

For general 2D systems, we obtain

$$K = -\frac{R_{1212}}{\det g_{ij}}$$

Landau & Lifshitz,
"The Classical Theory of Fields"

3. Constraint motion of a particle

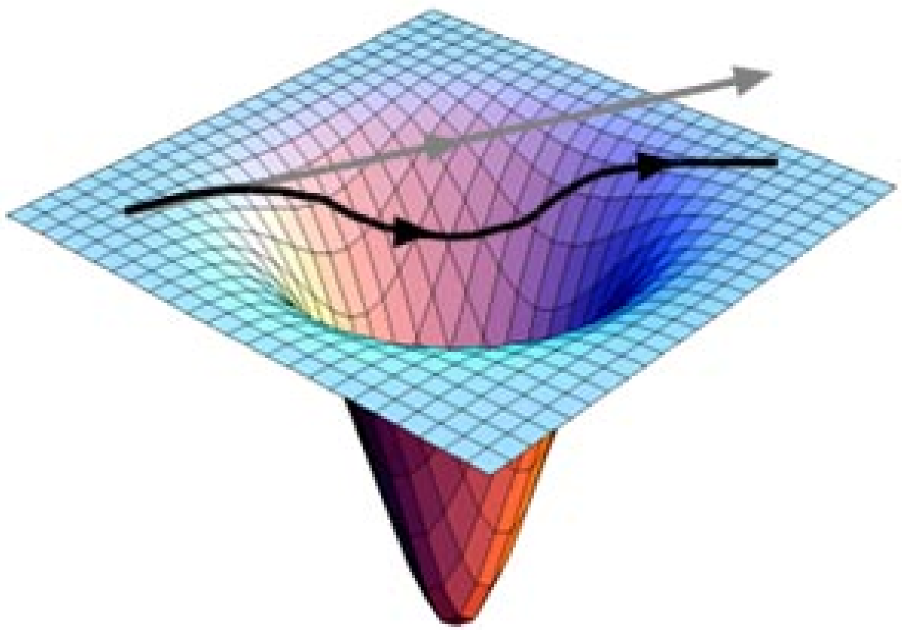
Lagrangian method:

Using a 2D curved coordinate system

$$H(\mathbf{r},\mathbf{p}) = g_{ij}\ p^i\ p^j$$

$$(i, j = 1 \text{ or } 2)$$

➡ Ambiguity of the operator ordering



Newtonian method:

3D free motion + constraint force

= 2D motion along a curved surface

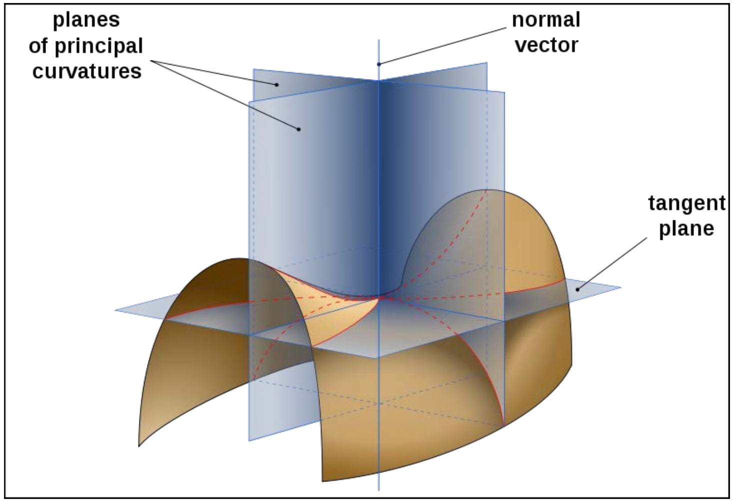
$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial x_i}\left(\sqrt{g}\,g^{ij}\frac{\partial}{\partial x_j}\psi\right)-\frac{\hbar^2}{8m}(\kappa_1-\kappa_2)^2\psi = E\psi$$

g_{ij} : Metric tensor κ_1, κ_2 : Principal curvatures

4. Curvature effect on QM

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial x_i}\left(\sqrt{g}\,g^{ij}\frac{\partial}{\partial x_j}\psi\right)-\frac{\hbar^2}{8m}(\kappa_1-\kappa_2)^2\psi=E\psi$$

g_{ij} : Metric tensor κ_1, κ_2 : Principal curvatures



Modulation in the effective mass

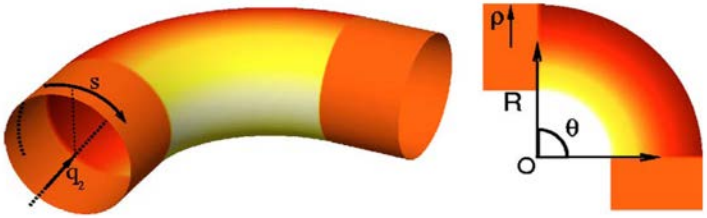
… affects **quantum transport** through the curved surface

Curvature-induced potential

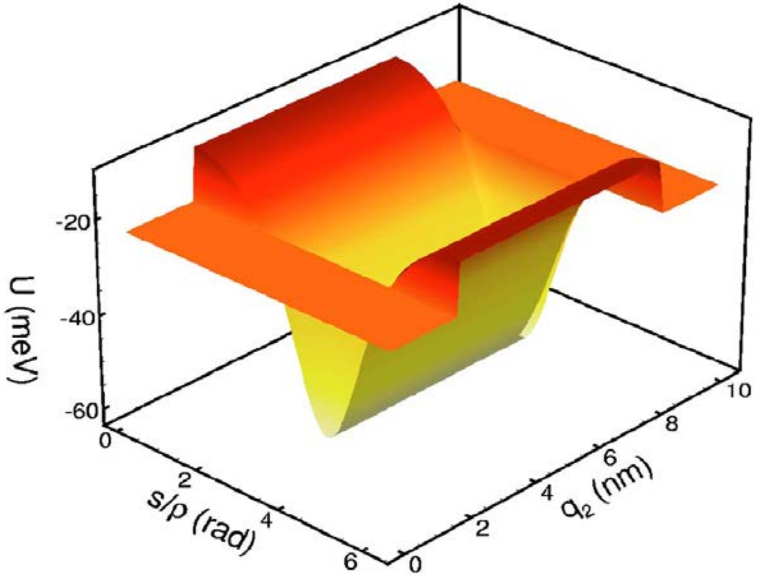
… yields **spatial localization** of conducting electrons around deformed regions

Locally-deformed hollow cylinder

Marchi *et al.*, PRB **72** (2005) 035403.



$R = 4\text{ nm}\quad \rho = 1.55\text{ nm}$



5. Geometry-induced effective potential

Quantum systems with curved geometry:

$$H = -\frac{1}{2\sqrt{g}}\left(\partial_\mu - iA_\mu\right)g^{\mu\nu}\sqrt{g}\left(\partial_\nu - iA_\nu\right) + P$$

Scalar potential (curvature-induced)

$$P = \frac{1}{8}g^{\mu\nu}g^{\rho\sigma}\left(\alpha^i_{\mu\nu}\alpha^i_{\rho\sigma} - 2\alpha^i_{\mu\rho}\alpha^i_{\nu\sigma}\right)I$$

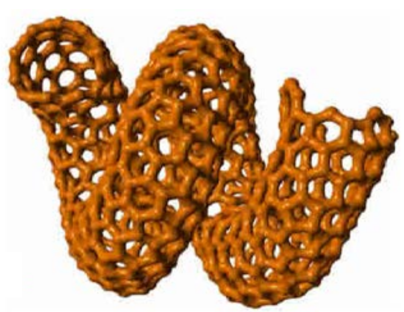
R.C.A. da Costa, Phys. Rev. A **23** (1981) 1980.

Vector potential (torsion-induced)

$$A_\mu = \frac{1}{2}S_\mu^{rs}L_{sr}$$

Schuster & and Jaffe, Ann.Phys. **307** (2003) 132.

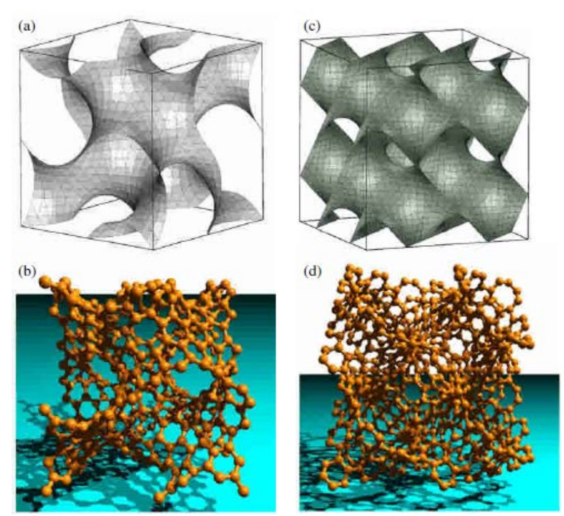
Nano-spring



Twisted carbon nanotube

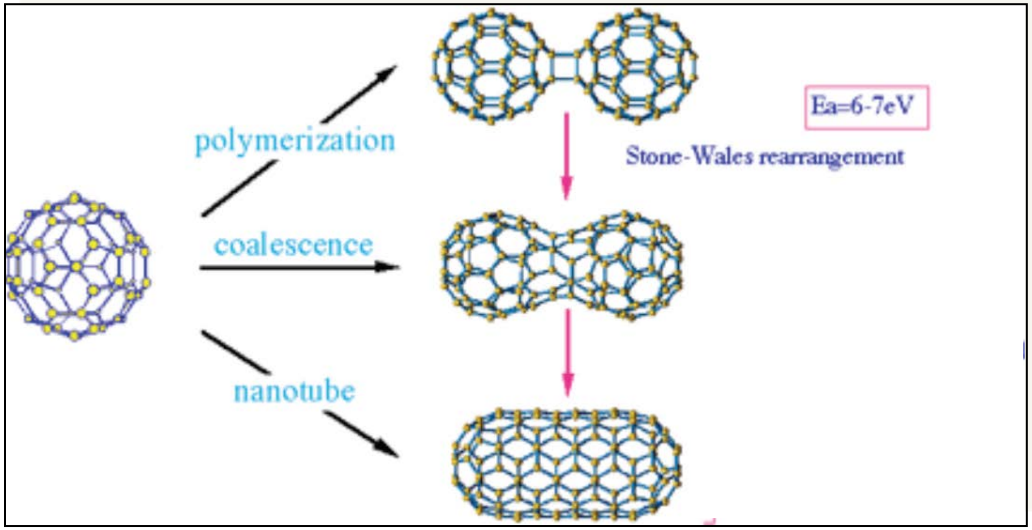
Arias & Arroyo, PRL **100** (2008) 085503.

Minimal nano-surface

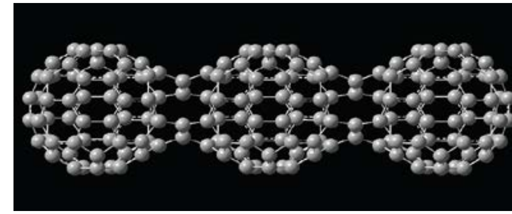


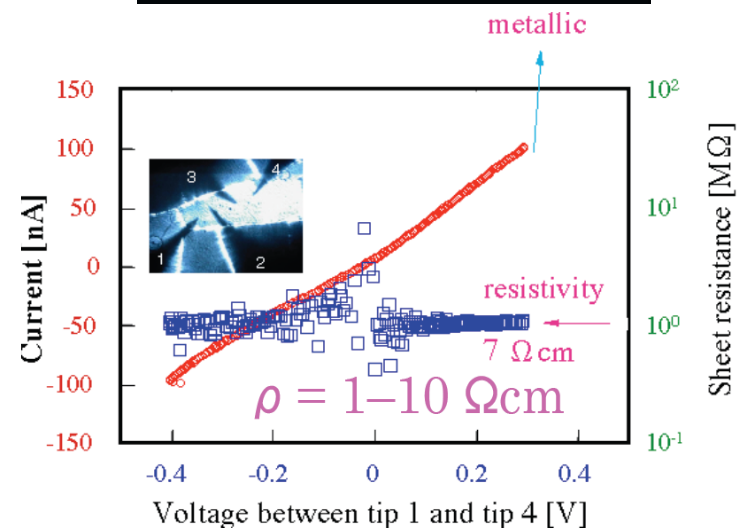
6. Peanut-shaped C_{60} polymer

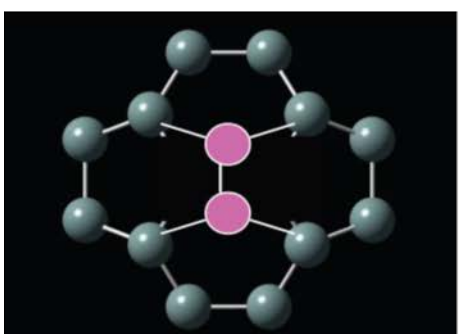
… is an exemplary nano-carbon materials. = Quasi-one dimensional metal !



J. Onoe *et al.,* Appl. Phys. Lett. **82**, 595 (2003)







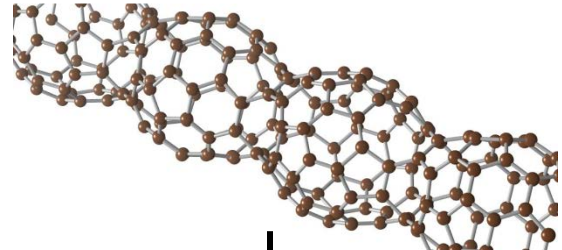
Stone-Wales transformation

= rotation of atom pairs about their bond centre.

The activation energy for this process in C_{60} ~6.2 eV.

A.J. Stone & D.J. Wales, Chem. Phys. Lett. **128**, 501 (1986).

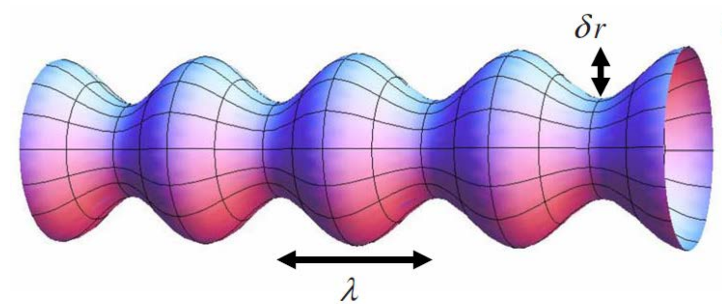
7. Continuum approximation



Peanut-shaped C60 polymers

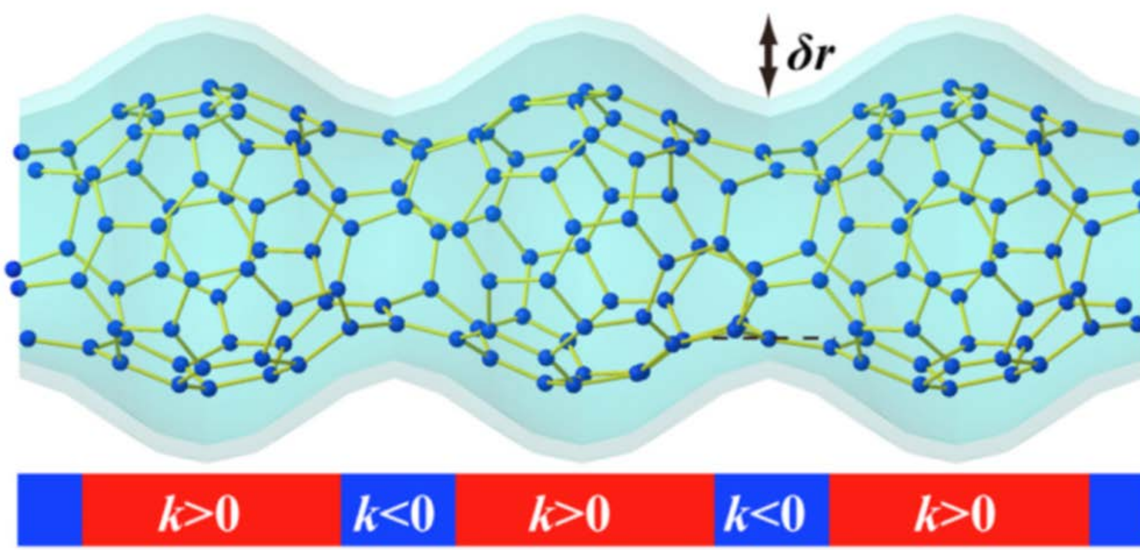
↓ is mapped onto

Periodically modulated hollow cylinders



$$-\frac{\hbar^2}{2m}\left[\frac{1}{r\sqrt{1+r'^2}}\frac{d}{dz}\frac{r}{\sqrt{1+r'^2}}\frac{d}{dz}-\frac{n^2}{r^2}\right]\varphi_n(z)$$

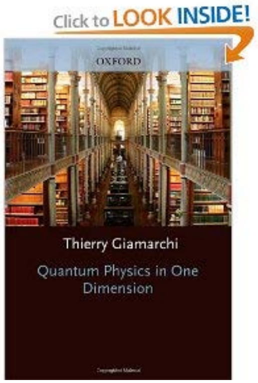
$$-\frac{\hbar^2}{8m}(\kappa_1-\kappa_2)^2\varphi_n(z) \quad = \quad E\varphi_n(z)$$



8. Tomonaga-Luttinger Liquid

> *… In 1D interacting electron systems, single-particle excitations do not exist but are converted into collective excitations. This is why the* **Fermi liquid theory breaks down** *for 1D.*

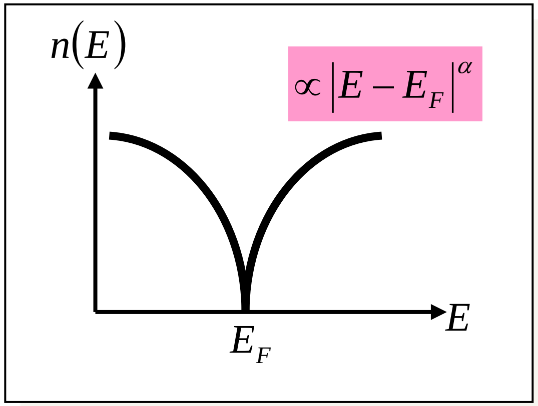
Giamarchi.,"*Quantum Physics in One Dimension*" (Oxford Univ Pub)



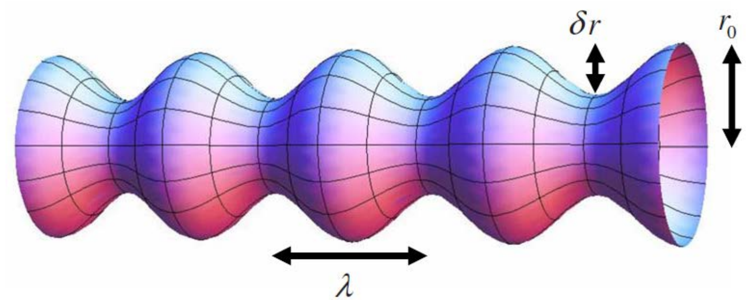
Single-particle density of states :

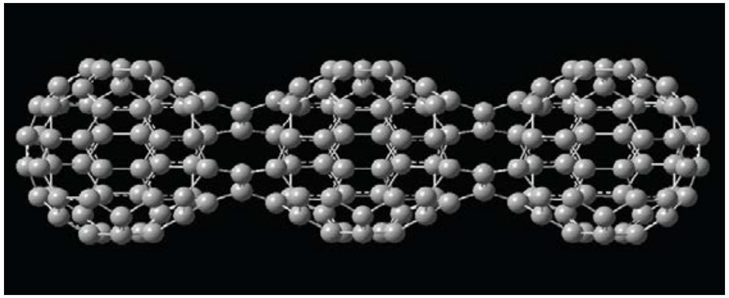
$$n(E) \propto |E - E_F|^{\alpha}$$

α : TLL exponent:



$$-\frac{\hbar^2}{2m}\left[\frac{1}{r\sqrt{1+r'^2}}\frac{d}{dz}\frac{r}{\sqrt{1+r'^2}}\frac{d}{dz}-\frac{n^2}{r^2}\right]\varphi_n(z) - \frac{\hbar^2}{8m}(\kappa_1-\kappa_2)^2\varphi_n(z) = E\varphi_n(z)$$





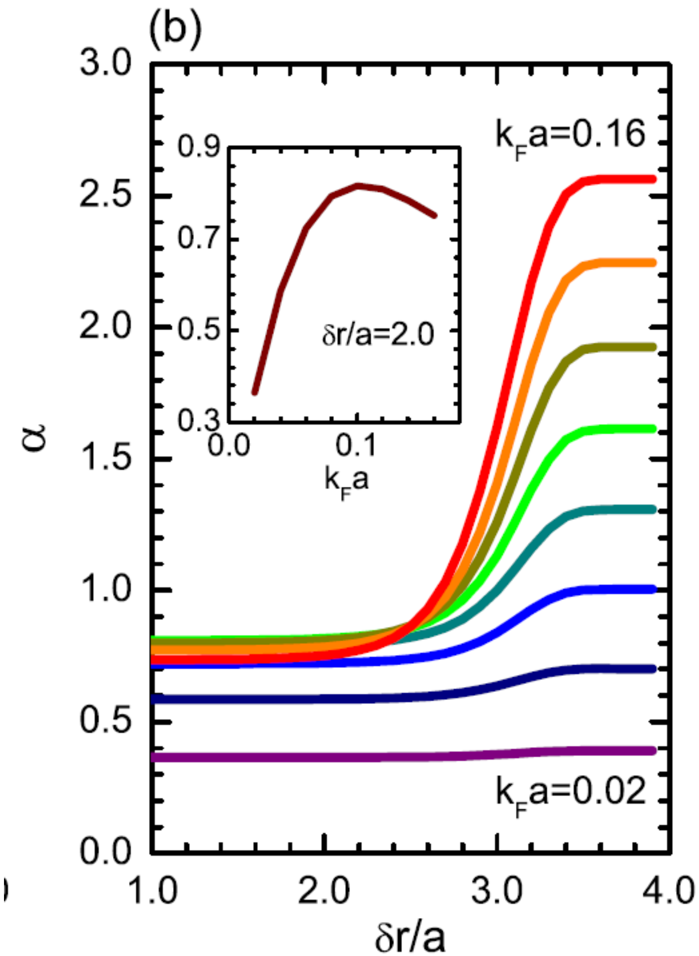
Question

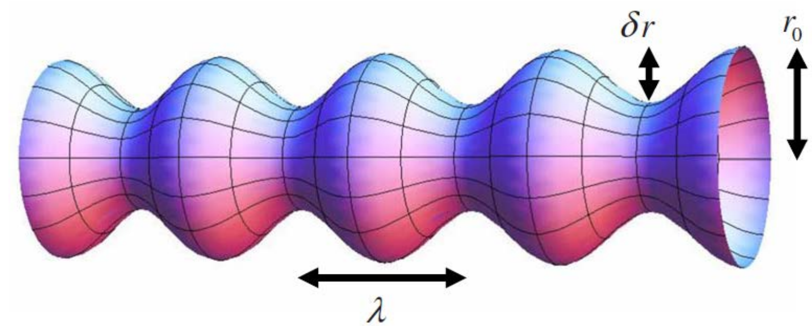
Does curved geometry induce a quantitative change in the TLL exponent α ?

9. Numerical result of the TLL exponent α

Increase in δr enhances α remarkably!

H. Shima et al., Phys. Rev. B **79** (2009) 201401.

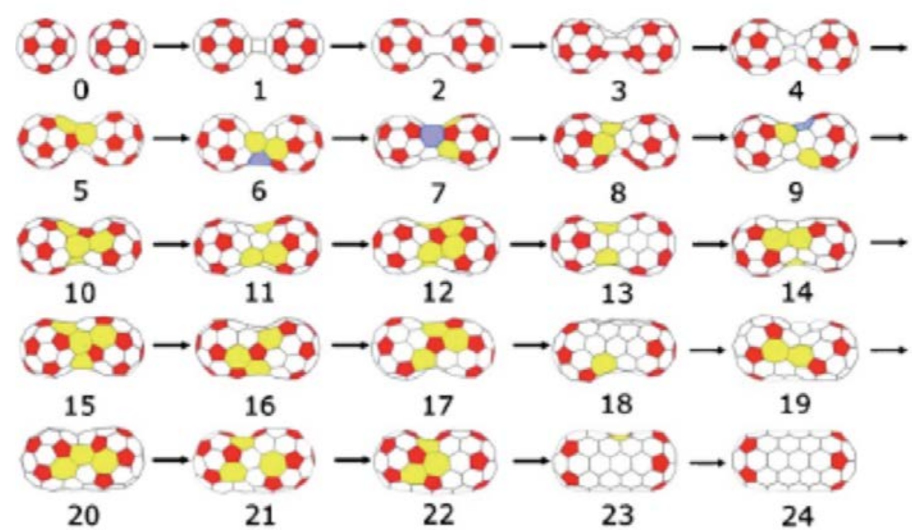




Consistent with the experiment done by:

J. Onoe *et al.*, Europhys.Lett. **98** (2012) 27001.

Tuning α by EB irradiation time (?)



H. Ueno *et al.,* Fullerene Sci. Technol. **6**, 319 (1998).

10. Summary on QM topics

Quantum mechancis on curved surface

-Geometric effects on quantum particles confined to curved surfaces are demonstrated

-Non-zero surface curvature yields effective scalar (P) and vector (A_μ) potentials

$$H = -\frac{1}{2\sqrt{g}}\left(\partial_\mu - iA_\mu\right)g^{\mu\nu}\sqrt{g}\left(\partial_\nu - iA_\nu\right) + P$$

Scalar potential (curvature-induced)

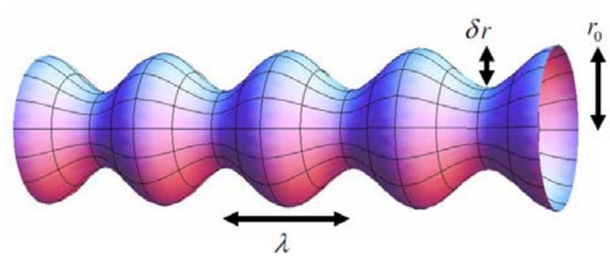
$$P = \frac{1}{8}g^{\mu\nu}g^{\rho\sigma}\left(\alpha^i_{\mu\nu}\alpha^i_{\rho\sigma} - 2\alpha^i_{\mu\rho}\alpha^i_{\nu\sigma}\right)I$$

Vector potential (torsion-induced)

$$A_\mu = \frac{1}{2}S_\mu^{rs}L_{sr}$$

Curvature-induced scalar potential

- P produces quantum localized states at locally deformed regions
- P causes a quantitative change in the Tomonaga-Luttinger liquids (TLL) exponent



Torsion-induced vector potential

- A_μ yields presistent current oscillation in a twisted quantum ring
- A_μ implies the possibility of novel MEMS and NEMS devices