Statistical mechanics of Coulomb gases as a quantum theory on Riemann surfaces

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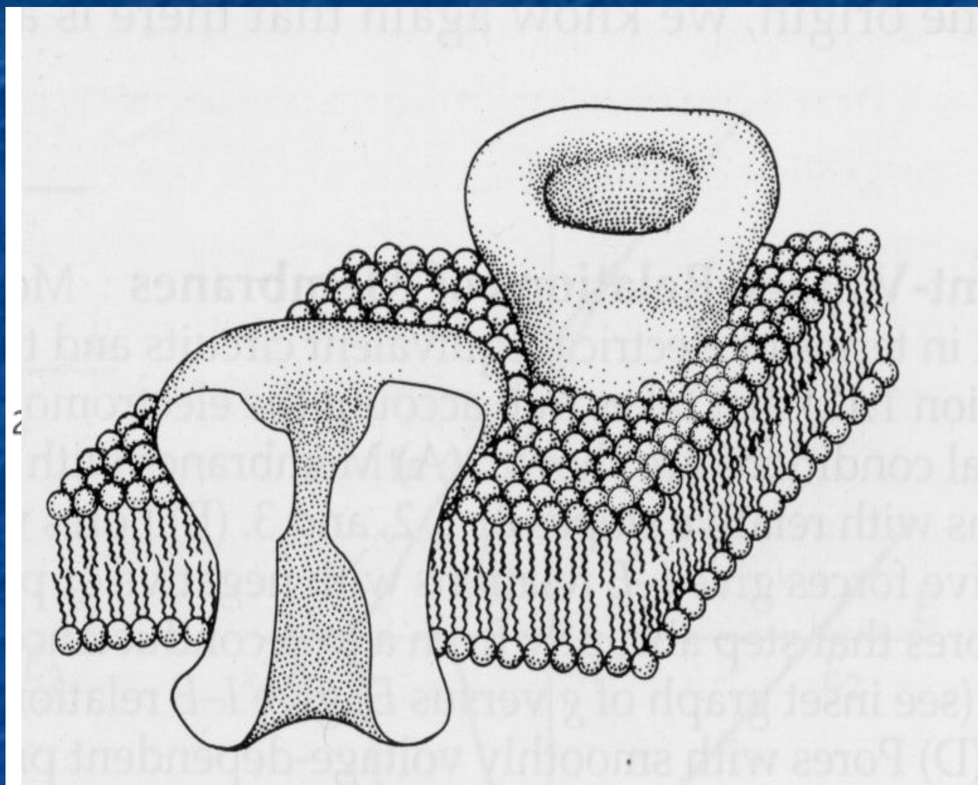
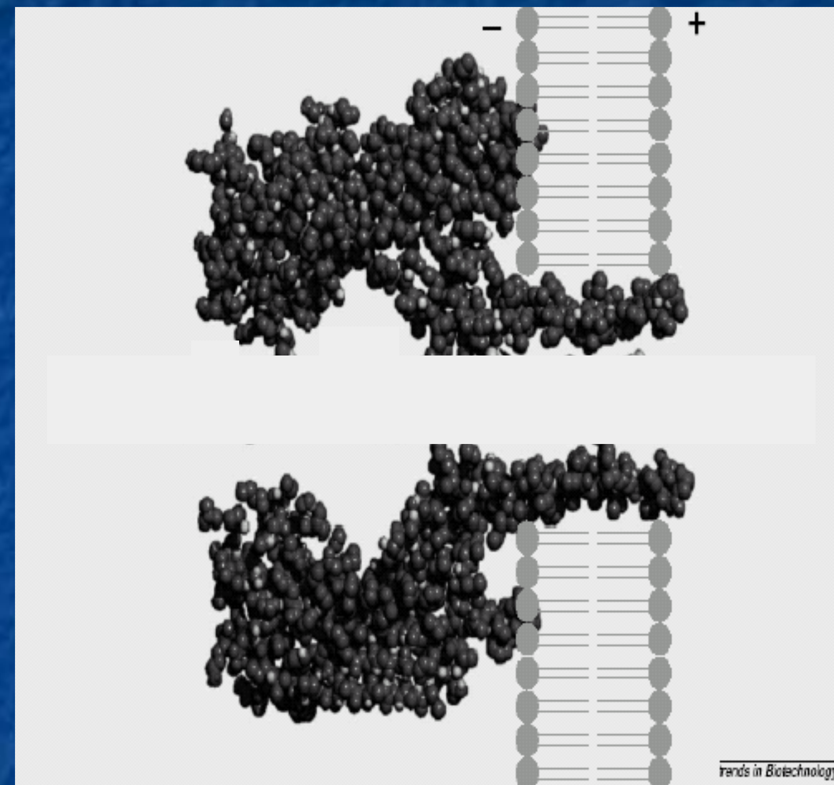
NSF

BSF United States - Israel Binational Science Foundation

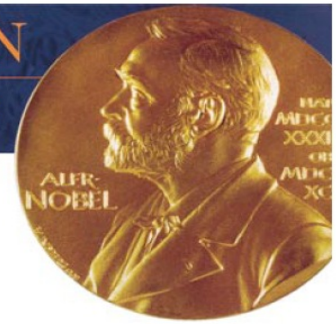
Ion channels of cell membranes



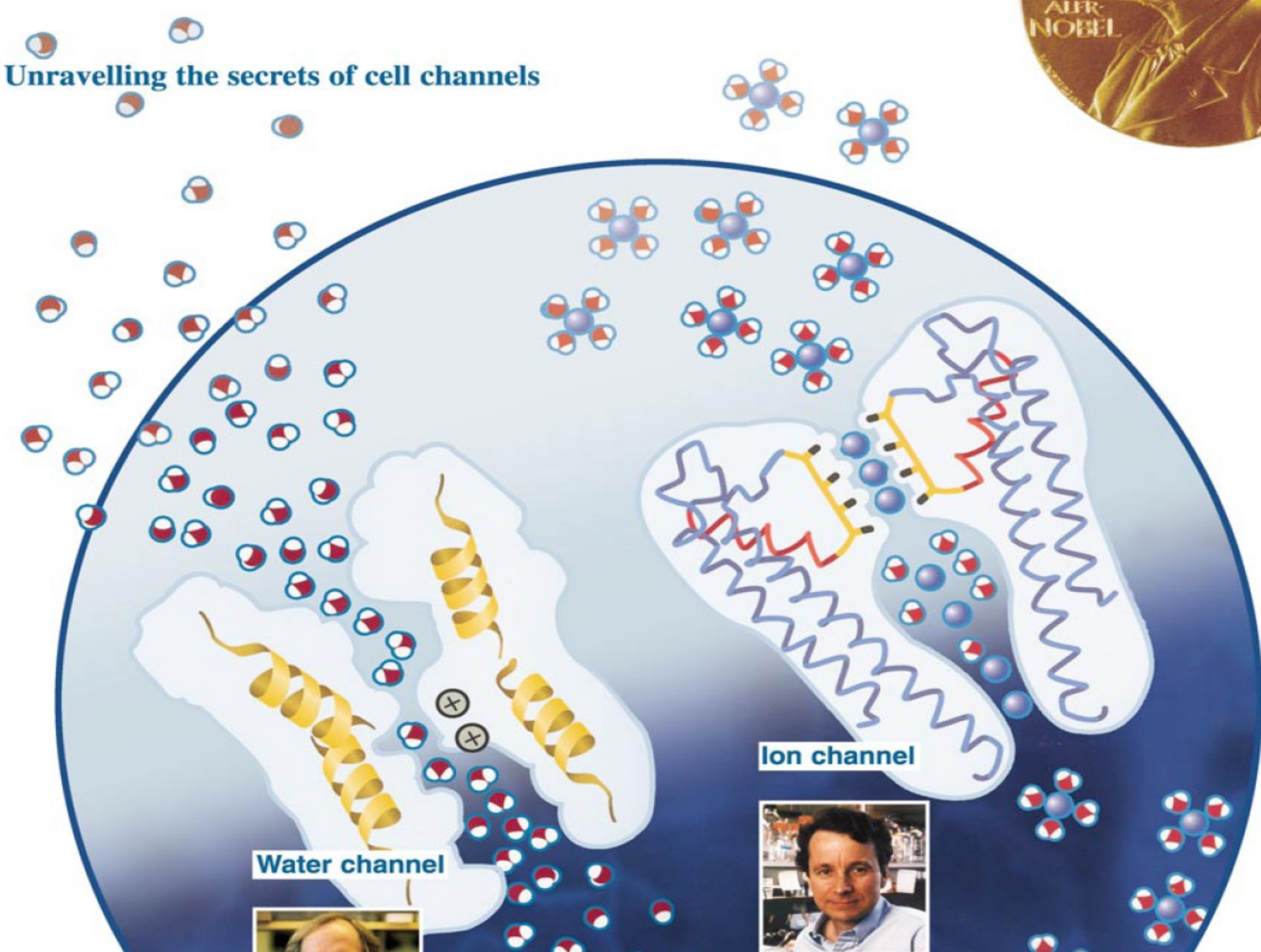


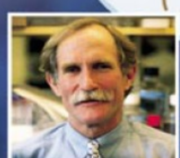
α-Hemolysin

THE NOBEL PRIZE IN CHEMISTRY 2003



Unravelling the secrets of cell channels



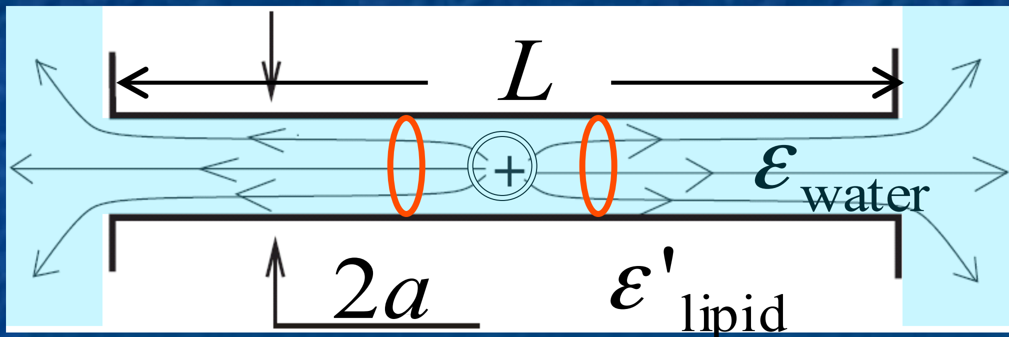


How does water actually pass through the cell membrane? The answer eluded researchers for over a hundred years. It was Peter Agre who finally unravelled the secret. By a happy chance he found a protein that is needed for water to pass in and out. He had discovered the elusive water channel.

In 1998 Roderick MacKinnon determined for the first time at high resolution the structure of an ion channel. As so often in biochemistry, form and function are intimately connected. By showing what the protein looked like at the atomic level, he also realized how it functions.

Angewandte Chemie

Simple Approximation



$$\varepsilon_{water} \approx 81$$

$$\varepsilon'_{lipid} \approx 2 << \varepsilon_{water}$$

Gauss theorem:

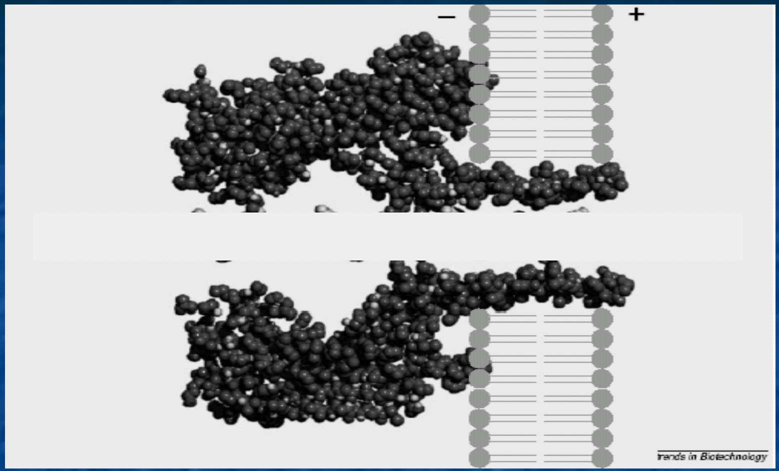
$$2\pi a^2 \varepsilon_{water} E_0 = 4\pi e$$

$$E_0 = \frac{2e}{\varepsilon a^2}$$

Energy:

$$U_L = \frac{\varepsilon E_0^2}{8\pi} \pi a^2 L \approx 4 k_B T$$

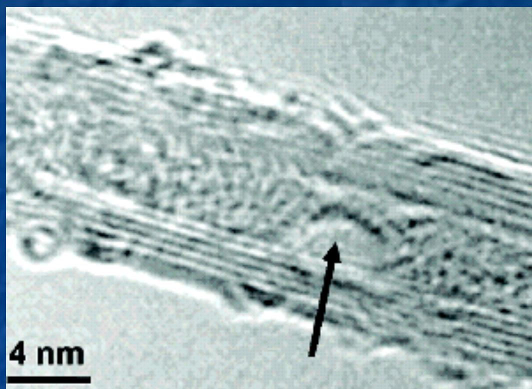
Why narrow channels ?

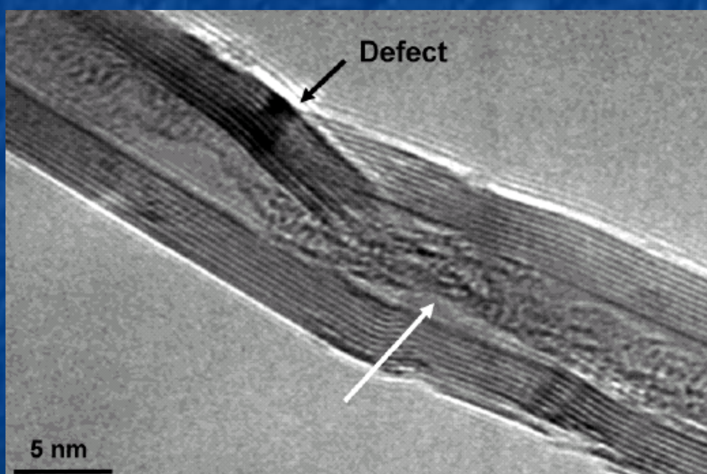


$$\frac{U_L}{k_B T} = \frac{e^2}{\varepsilon k_B T}\frac{L}{2a^2} = \frac{l_B L}{2a^2}$$

$$l_{\text{Bjerrum}} = 0.7\text{nm}$$

Water-filled carbon nanotubes

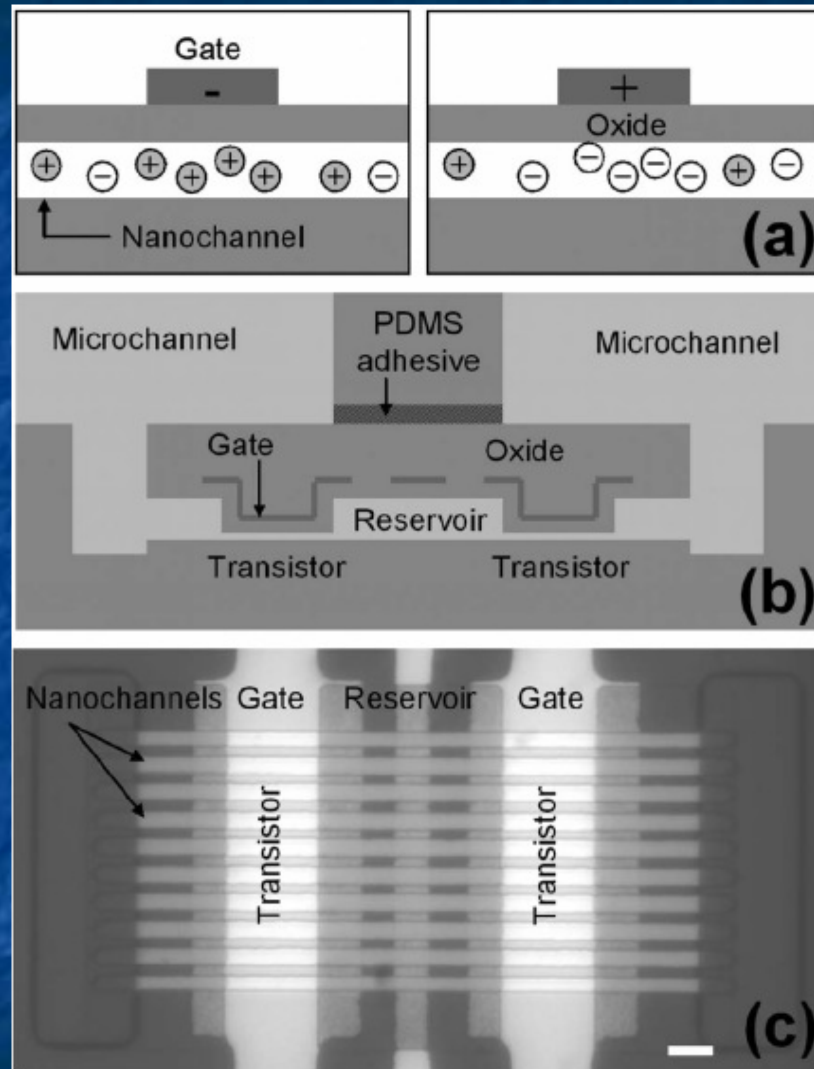




Nevin Naguib,[†] Haihui Ye,[†] Yury Gogotsi,[*,†] Almila G. Yazicioglu,[‡] Constantine M. Megaridis,[‡] and Masahiro Yoshimura[§]

Nanoletters, 2004

NanoFluidics

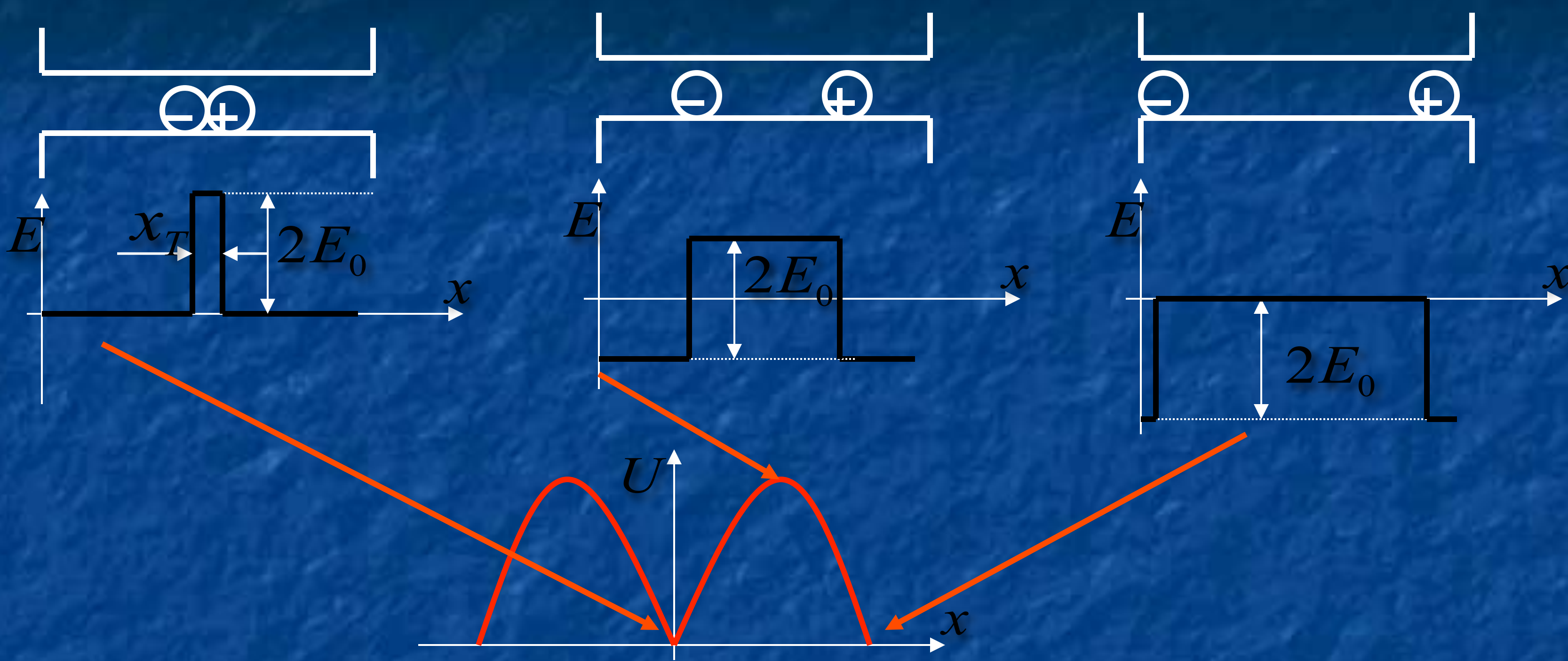


1. Nanofluidic transistor. (a) Schematic of a nanofluidic transistor

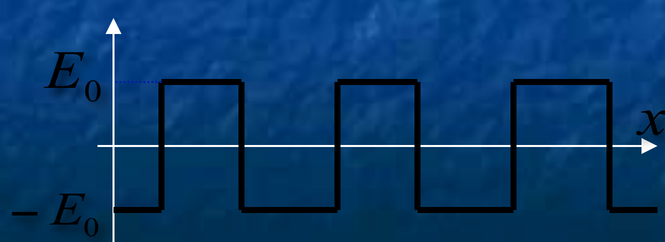
Rohit Karnik and Kenneth Castelino Arun Majumdar

APPLIED PHYSICS LETTERS 88, 123114 (2006)

1D Coulomb Interactions

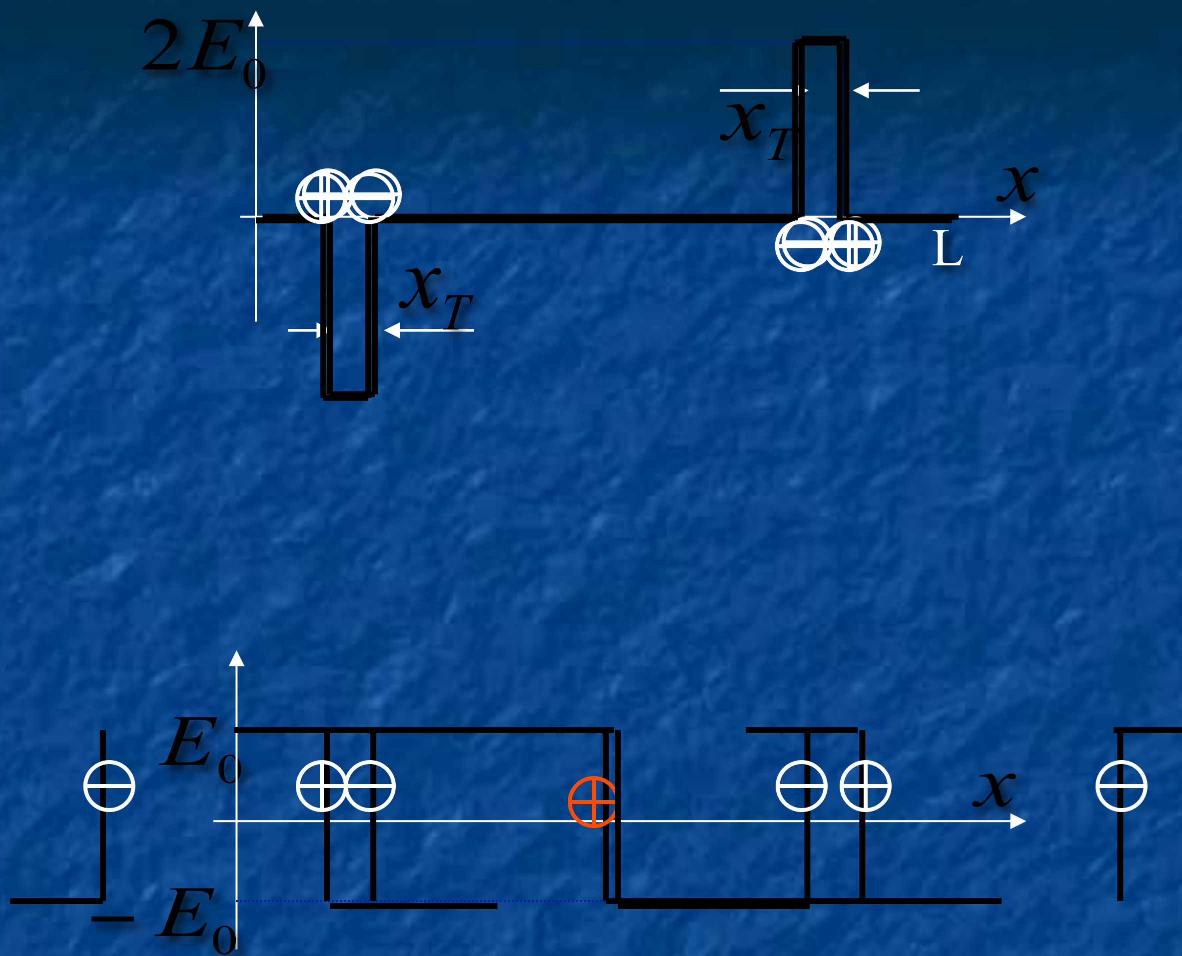


➢ Maximum energy does **NOT** depend on the number of ions.



$$U_L = \frac{\varepsilon E_0^2}{8\pi} \pi a^2 L$$

Entropy !



Free ions enter the channel, increasing the entropy !

Statistical Mechanics of 1D Coulomb gas:

$$\mathcal{Z}_L = \sum_{N_1, N_2 = 0}^{\infty} \frac{f_1^{N_1} f_2^{N_2}}{N_1! N_2!} \prod_{i=1}^{N_1} \int_0^L dx_i \prod_{j=1}^{N_2} \int_0^L dx_j \; e^{-U/k_B T}$$

$$\equiv \int \mathcal{D}\theta(x) \; e^{-\frac{x_T}{2} \int dx \left[\frac{1}{2} (\partial_x \theta)^2 - \frac{4\alpha}{x_T^2} \cos\theta(x) \right]}$$

"Sine-Gordon" quantum mechanics:

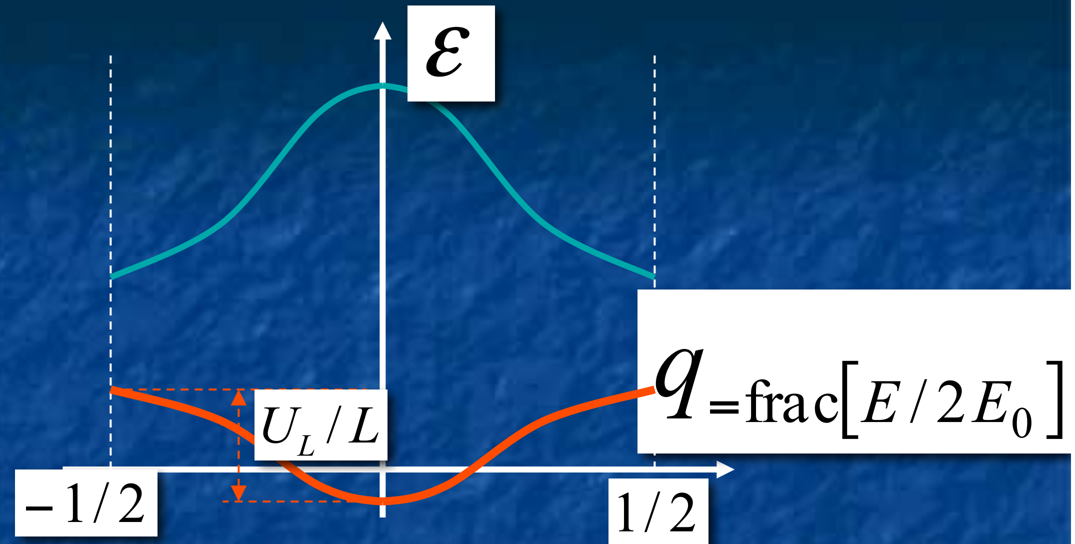
$$\hat{H} = -\partial_\theta^2 - 2\alpha \cos\theta$$

Bare coupling constant (concentration)

Quantum mechanics:

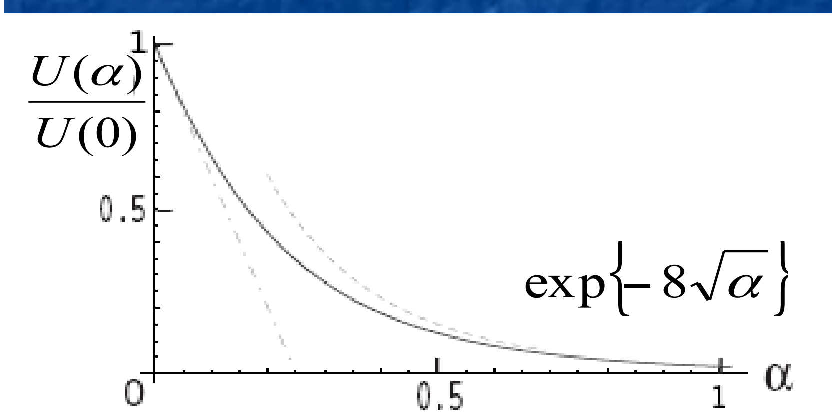
$$\hat{H} = -\partial_\theta^2 - 2\alpha\cos\theta$$

$$Z = \mathrm{Tr}\left\{ e^{-\hat{H}L} \right\} \approx e^{-\varepsilon_0(q)L}$$



Pressure = groundstate energy

Transport barrier = width of the lowest Bloch band



Electric field is conserved modulo $2E_0$

Multi-valent ions:

$\mathbf{Ca^{2+},\ Ba^{2+},\ Fe^{3+}}$

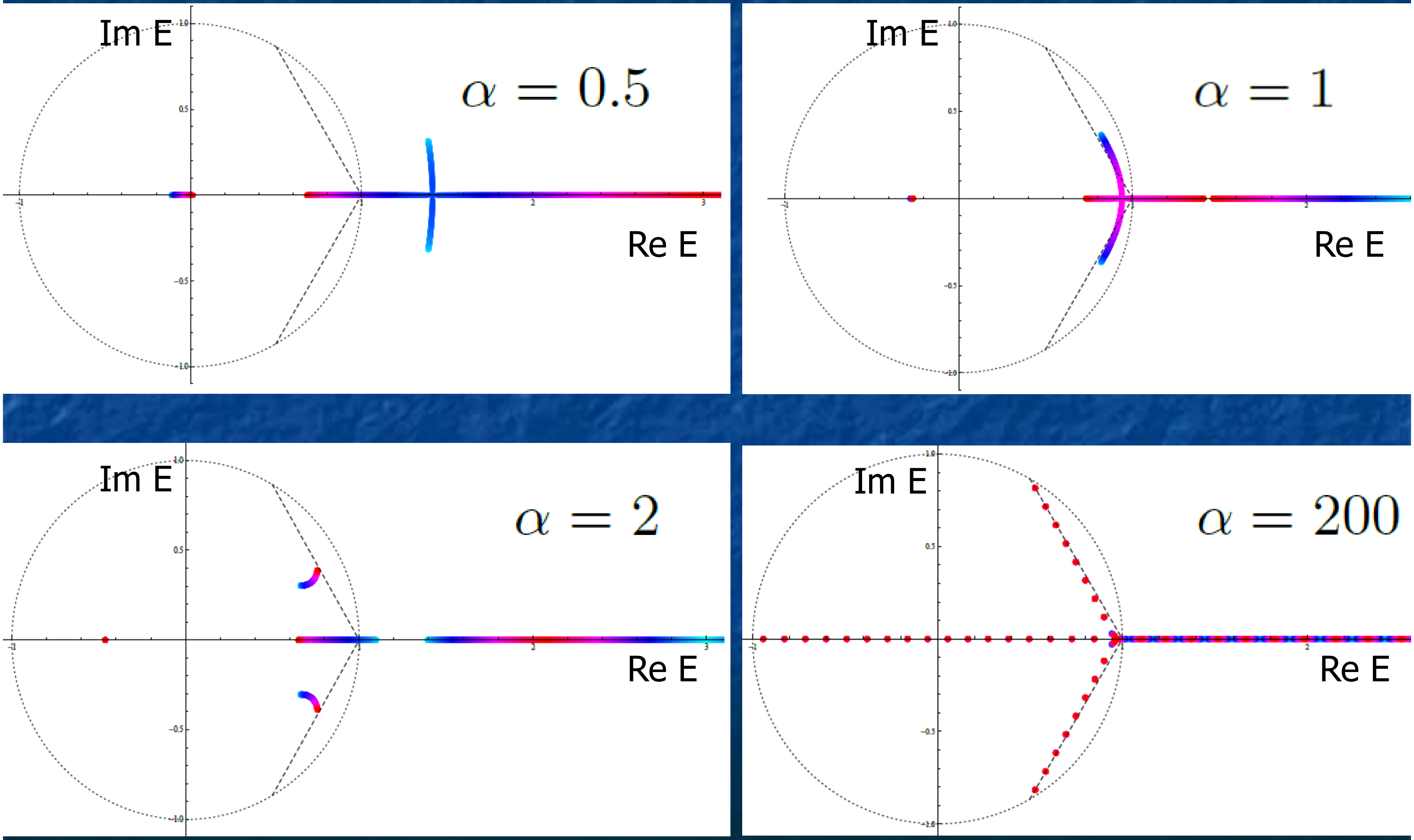
$$\hat{H}_{(2,1)} = -\partial_\theta^2 - \alpha\left(e^{2i\theta} + 2e^{-i\theta}\right);$$

$$\hat{H}_{(3,1)} = -\partial_\theta^2 - \alpha\left(e^{3i\theta} + 3e^{-i\theta}\right);$$

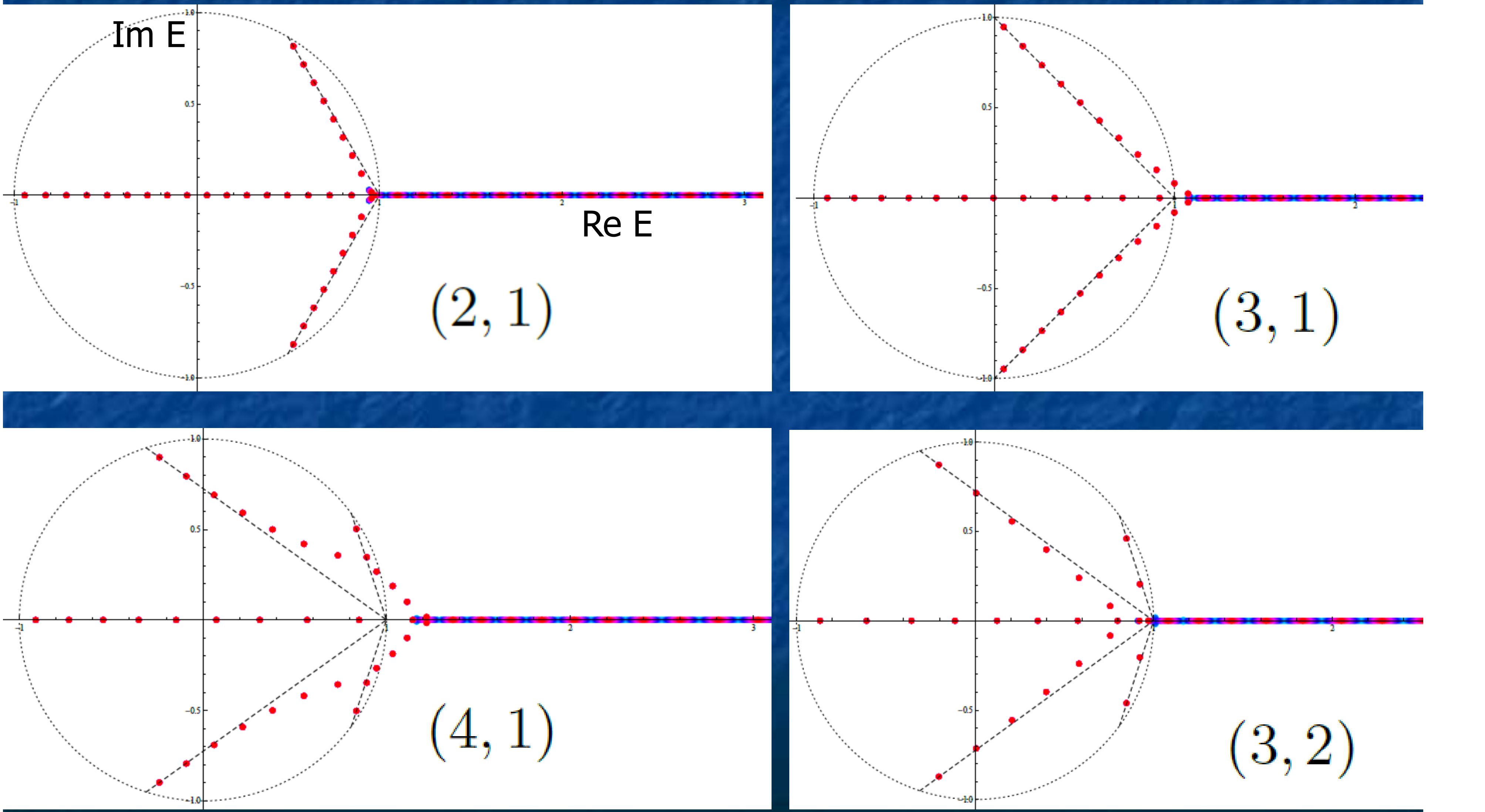
$\mathcal{PT}$ **Symmetry** $\theta \to -\theta$ $i \to -i$

- Eigenvalues are either real or complex-conjugated pairs

Spectra of $\hat{H}_{(2,1)} = -\partial_\theta^2 - \alpha\left(e^{2i\theta} + 2e^{-i\theta}\right);$



More Spectra $\alpha = 200$



Semiclassical constant energy surfaces

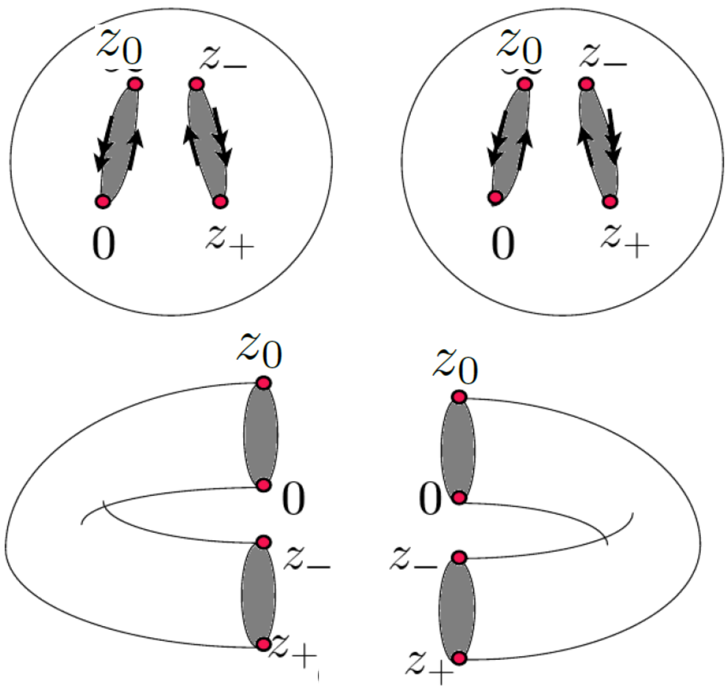
$$z = e^{i\theta}$$

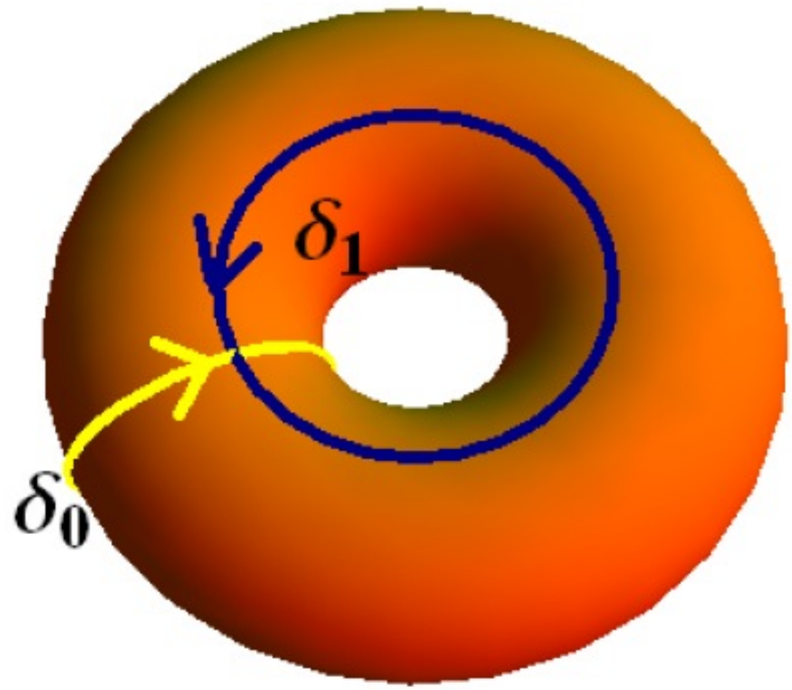
$$u = 2\epsilon/3\alpha$$

$$\frac{3}{2}u = p^2 - \left(\frac{z^2}{2} + \frac{1}{z}\right)$$

Ca^{2+} Cl^{1-}

Family of complex algebraic curves, parameterized by moduli u



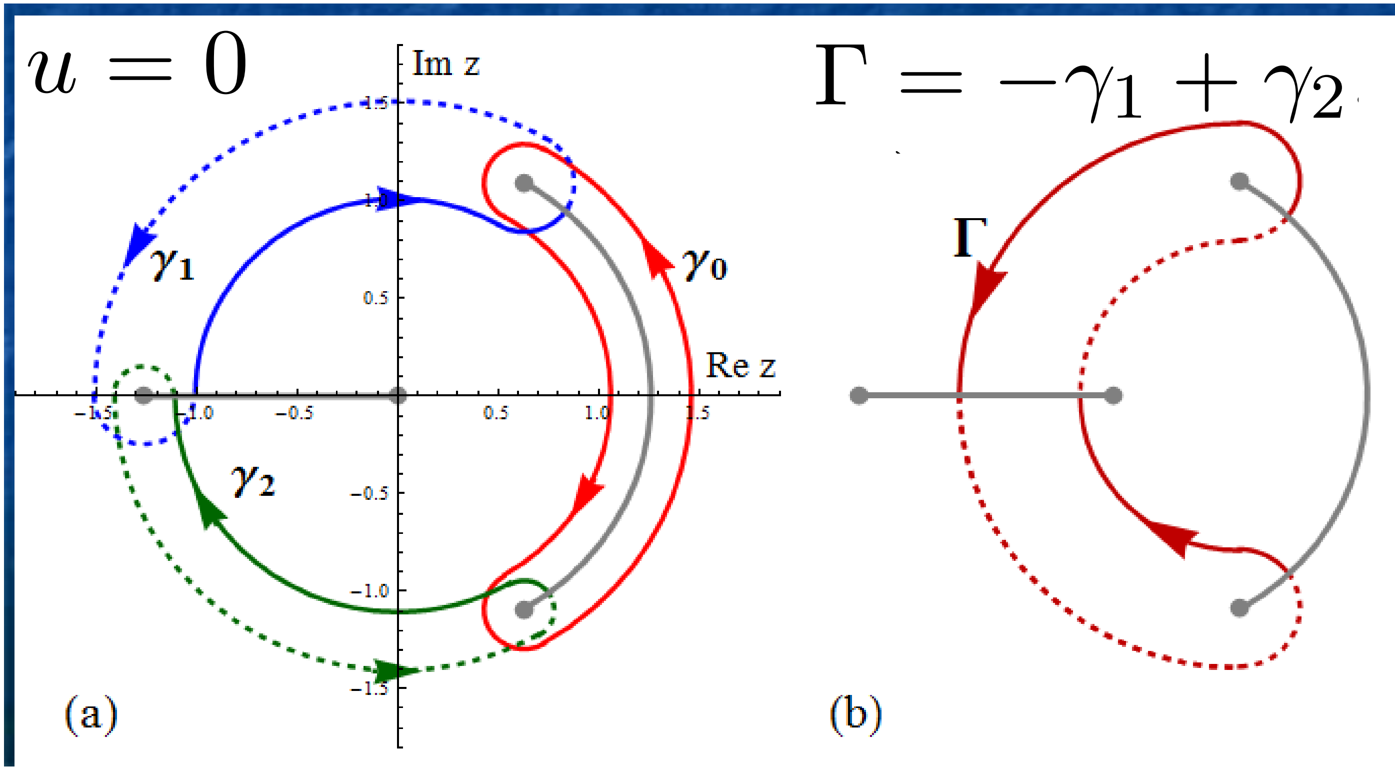


Semiclassical actions and their monodromies

No need to know classical trajectory: action along any periodic orbit is a superposition of two basic cycles.

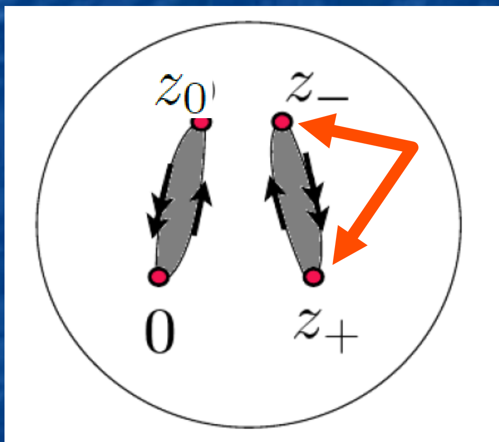
$$S_j(u) = \oint_{\gamma_j} \lambda(u)$$

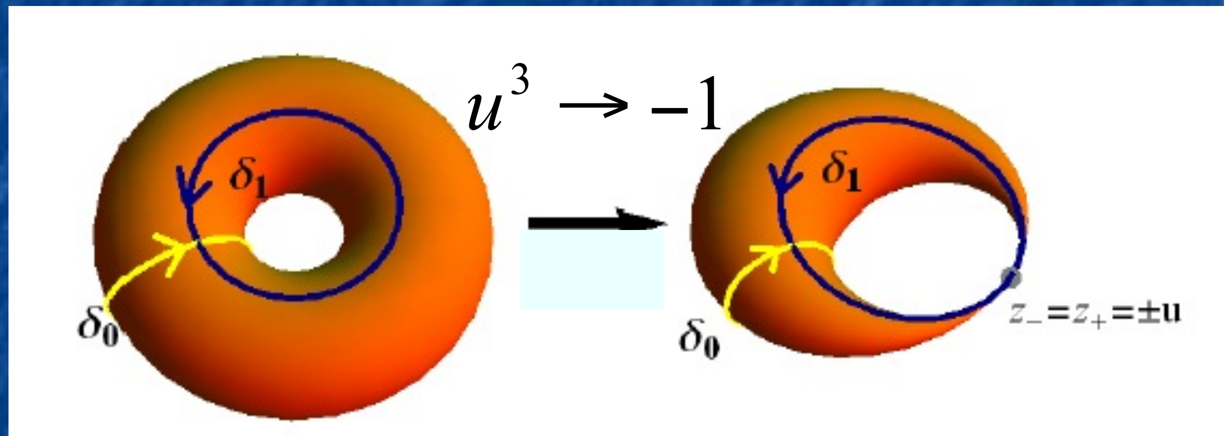
$$\lambda(u) = p(\theta)\, d\theta = p(z)\frac{dz}{iz} = \frac{i}{z^{3/2}}\left(\frac{1}{2}z^3 + \frac{3}{2}uz + 1\right)^{1/2} dz$$



Semiclassical actions and their monodromies

Singular points in the moduli space, where cuts collide





$$(u+1) \to (u+1)e^{2\pi i}$$

$$\begin{pmatrix} S_0(u) \\ S_1(u) \end{pmatrix} \to \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} S_0(u) \\ S_1(u) \end{pmatrix}$$

$$S_{1,2}(u) = Q_{1,2}(u) \mp \frac{i}{2\pi} S_0(u) \ln(1+u)$$

$$Q_1 + Q_2 = S_0$$

Picard – Fuchs Equation

Since there are only two linearly independent holomorphic forms on genus one surface (de Rahm theorem),

$$\{\lambda''(u), \lambda'(u), \lambda(u)\}$$

are linearly dependent forms!

$$\mathcal{L} = (u^3+1)\partial_u^2 + u/4$$

$$\mathcal{L}\lambda(u) = \frac{d}{dz}\left[\frac{i}{4\sqrt{2}}\frac{-3z^2+u(z^3-4)}{z^{1/2}(2+3uz+z^3)^{1/2}}\right]dz$$

$$\oint_{\gamma_j}\mathcal{L}\lambda(u) = \mathcal{L}S_j(u) = 0$$

Picard – Fuchs Equation

The actions satisfy second order ODE:

$$(u^3+1)S_j''(u)+\frac{u}{4}S_j(u)=0$$

Two independent solutions are given by hypergeometric functions:

$F_0(u^3)$ and $uF_1(u^3)$,

$$F_0(u^3)={}_2F_1\left(-\frac{1}{6},-\frac{1}{6};\frac{2}{3};-u^3\right),\quad F_1(u^3)={}_2F_1\left(+\frac{1}{6},+\frac{1}{6};\frac{4}{3};-u^3\right)$$

Solutions of Picard – Fuchs Equation

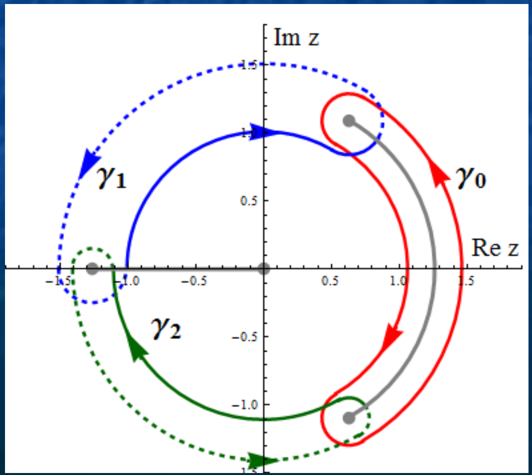
Classical action at ANY energy along ANY (almost) closed orbit may be written as a linear combination:

$$S_j(u) = C_{j0}F_0(u^3) + C_{j1}uF_1(u^3)$$

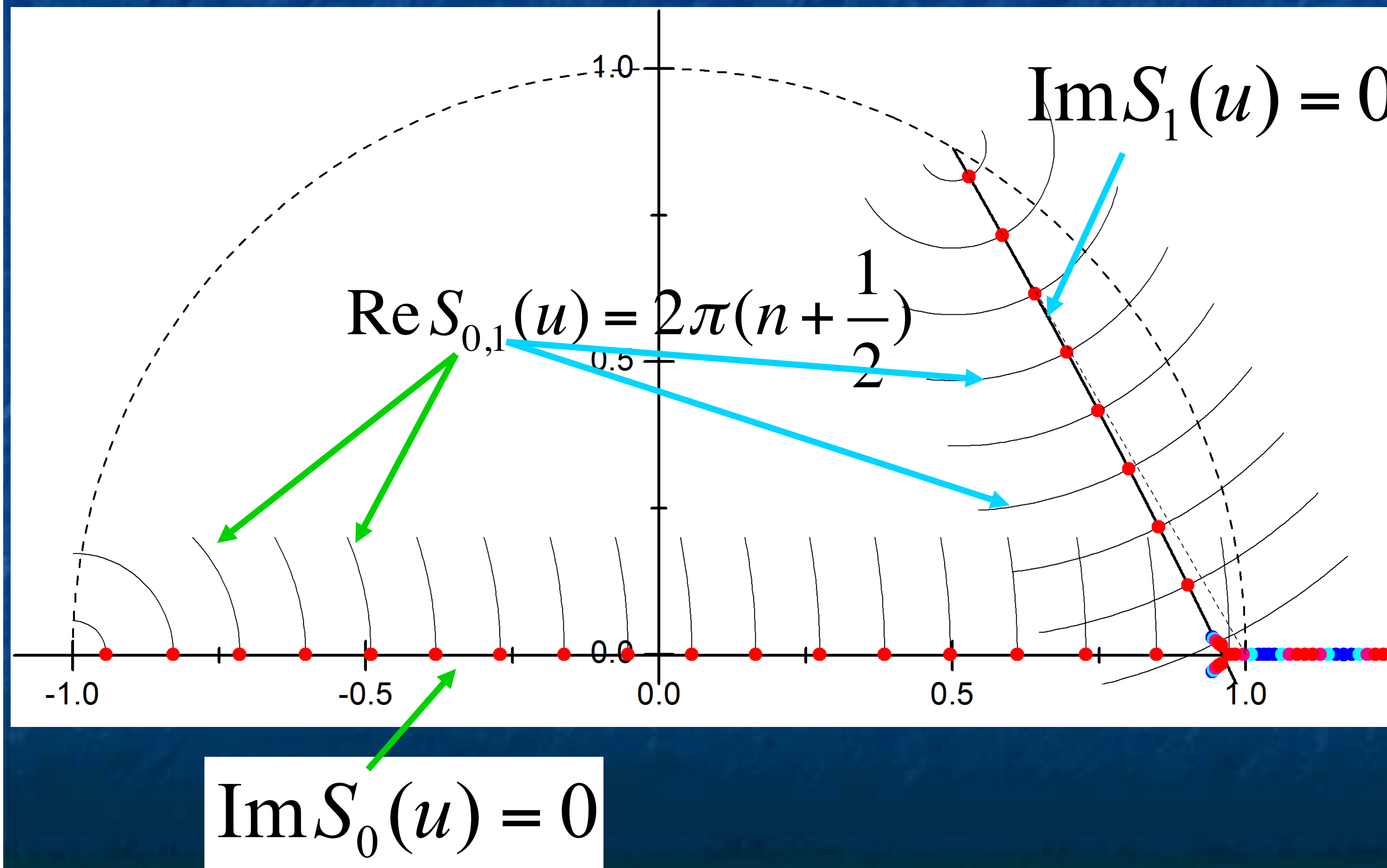
The coefficients may be determined by doing brut-force integration at one (e.g. u=0) specific energy:

$$C_{00} = C_{10}e^{\pi i/3} = C_{20}e^{-\pi i/3} = \frac{2^{11/6}3\pi^{3/2}}{\Gamma(\frac{1}{6})\Gamma(\frac{1}{3})},$$

$$C_{01} = C_{11}e^{-\pi i/3} = C_{21}e^{\pi i/3} = \frac{3^{1/2}\Gamma(\frac{1}{6})\Gamma(\frac{1}{3})}{2^{11/6}\pi^{1/2}}.$$

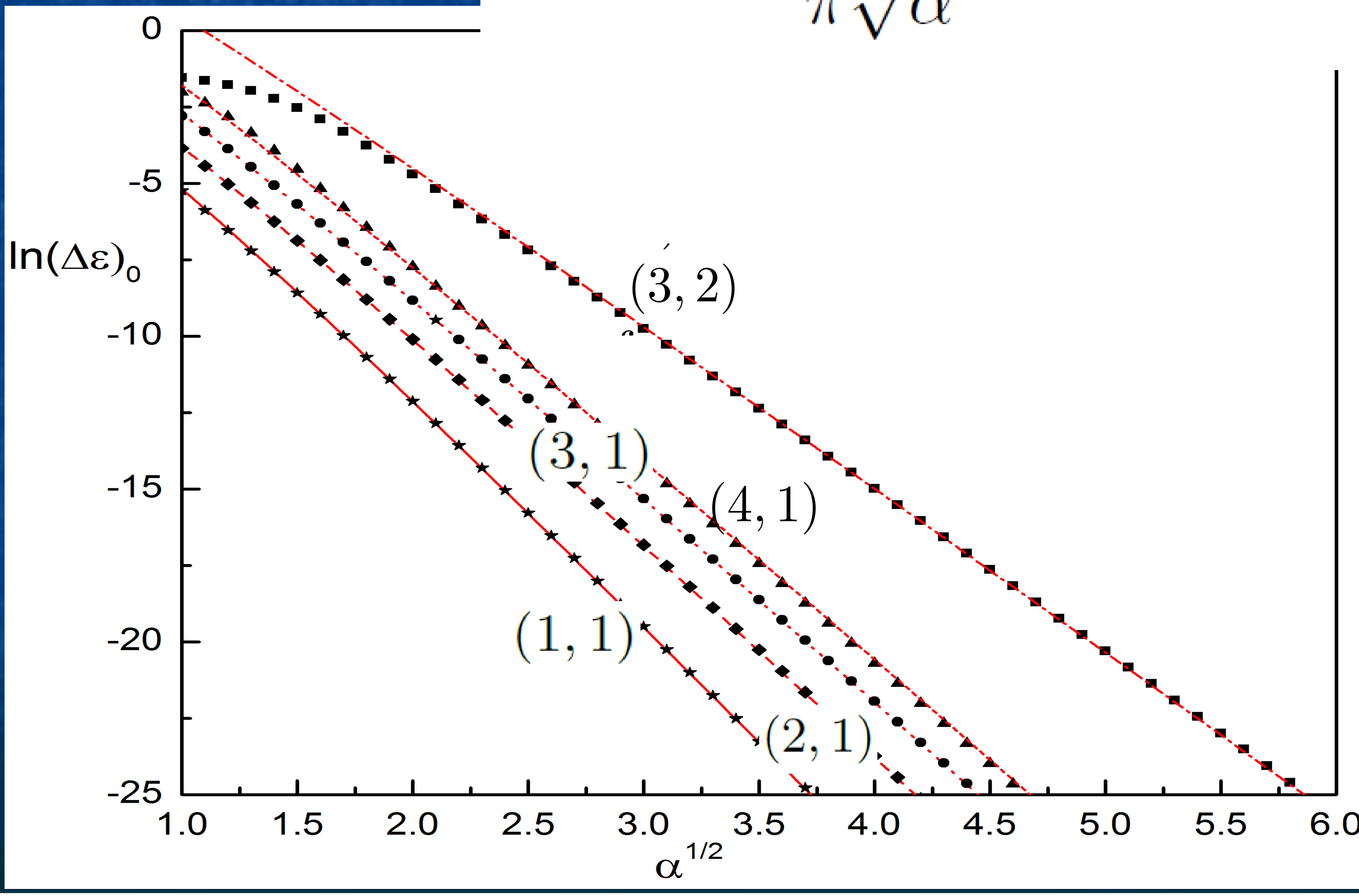


Semiclassical Quantization



Bloch bandwidth = transport barrier

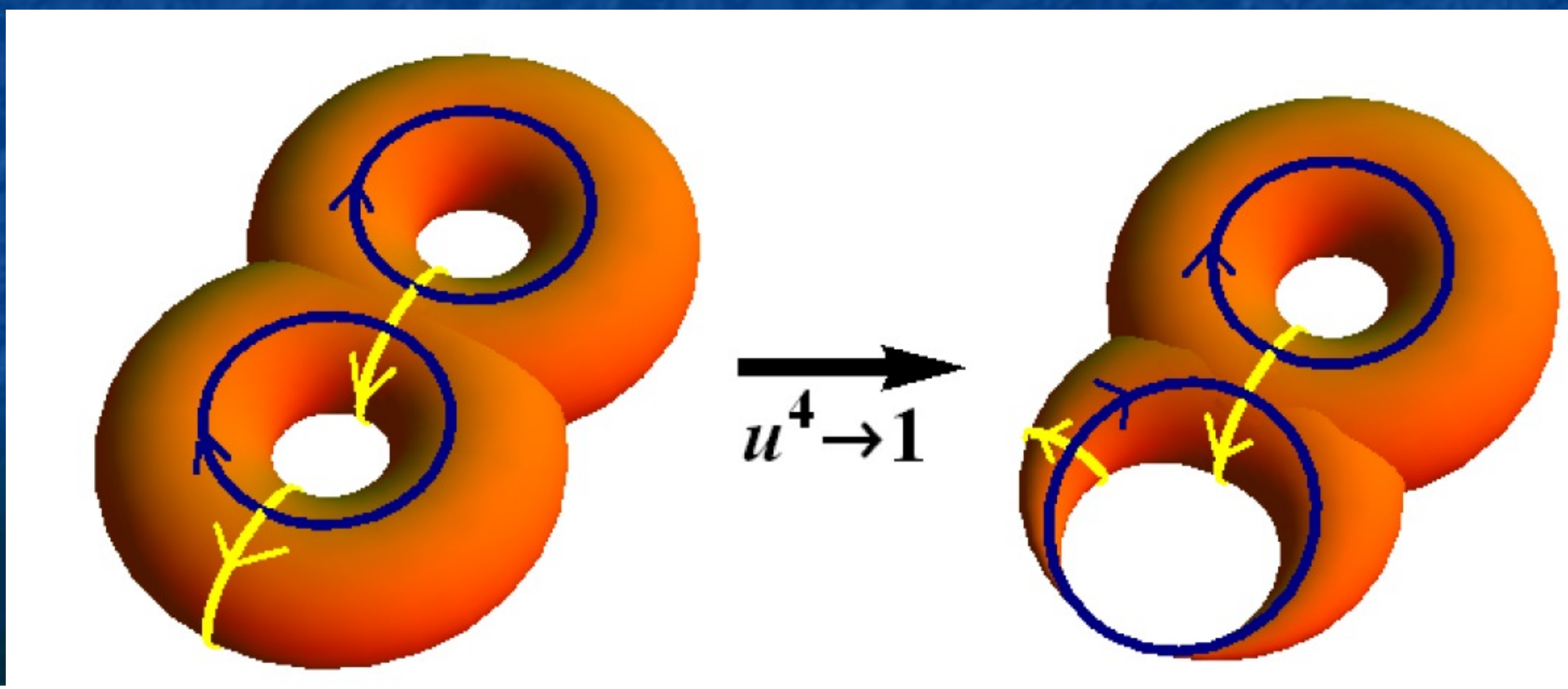
$$(\Delta u)_m = \frac{\omega}{\pi\sqrt{\alpha}} e^{i\alpha^{1/2} S_1(u_m)/2}$$



Trivalent salts: $Fe^{3+} \quad Cl_3^{1-}$

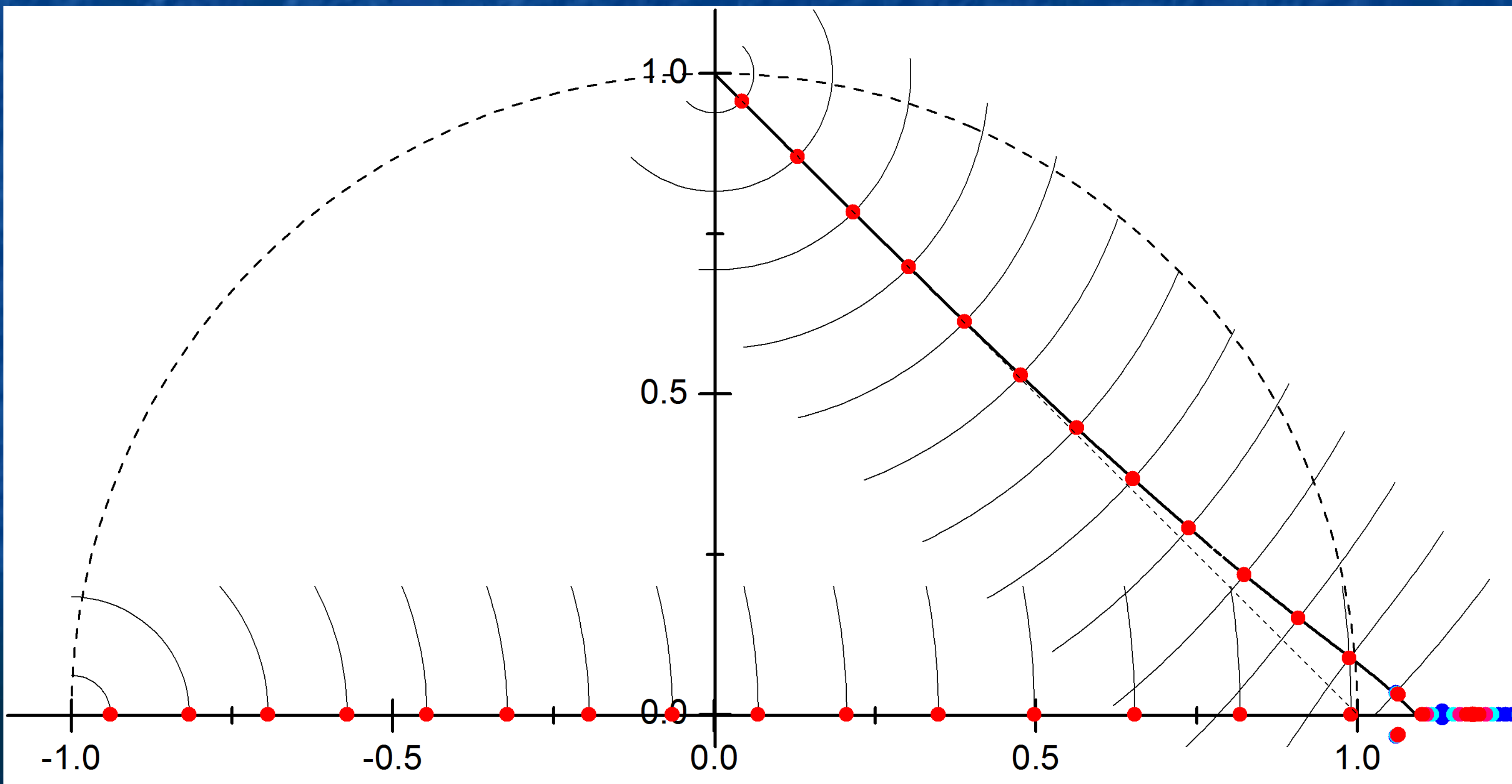
$$\hat{H}_{(3,1)} = -\partial_\theta^2 - \alpha \left(e^{3i\theta} + 3e^{-i\theta} \right);$$

$$\frac{4}{3} u = p^2 - \left(\frac{z^3}{3} + \frac{1}{z} \right)$$



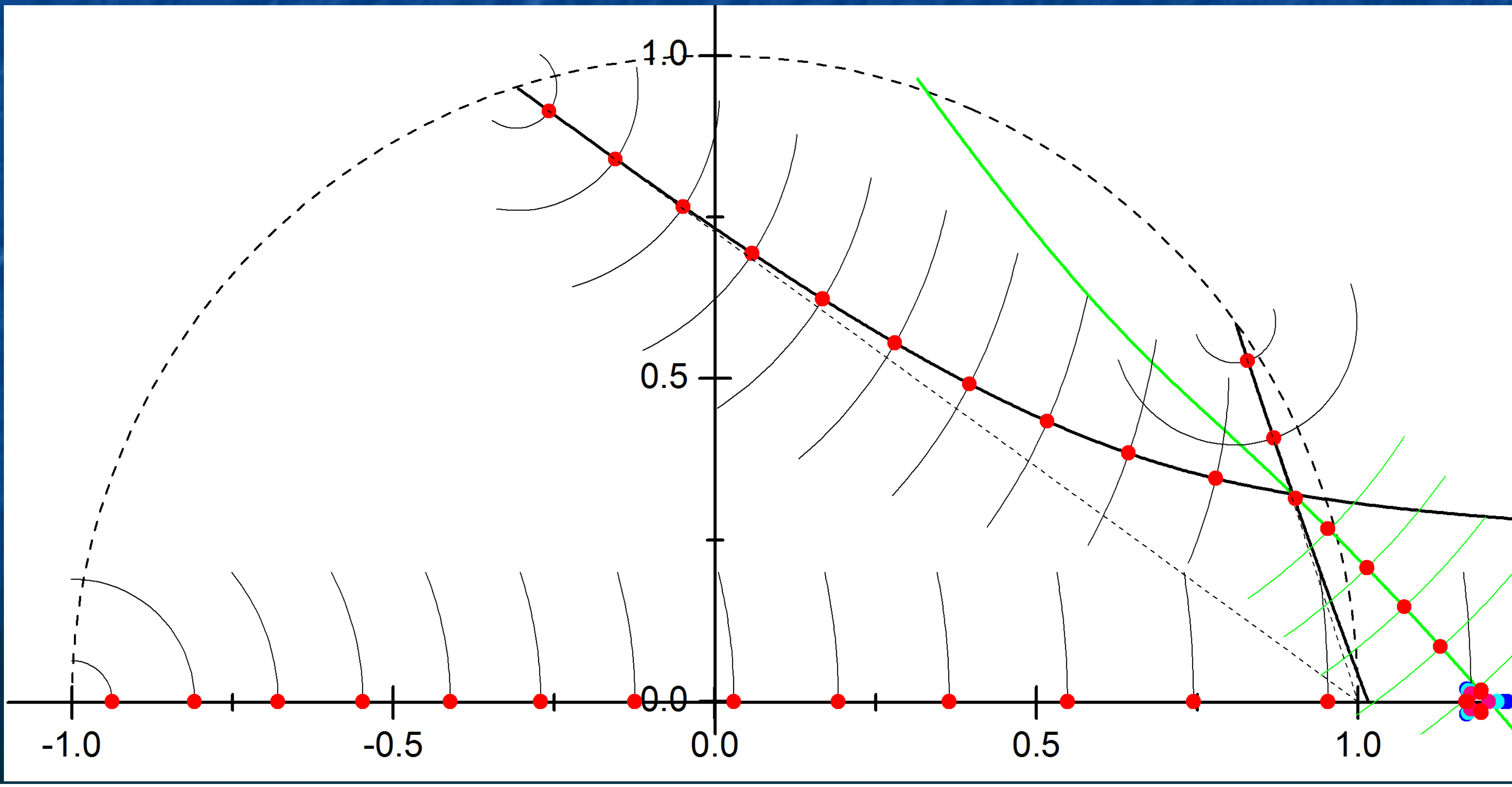
Picard – Fuchs equation and its solutions

$$(u^4-1)S^{(4)}+8u^3S^{(3)}+\frac{217}{18}u^2S''+uS'+\frac{65}{144}S=0$$



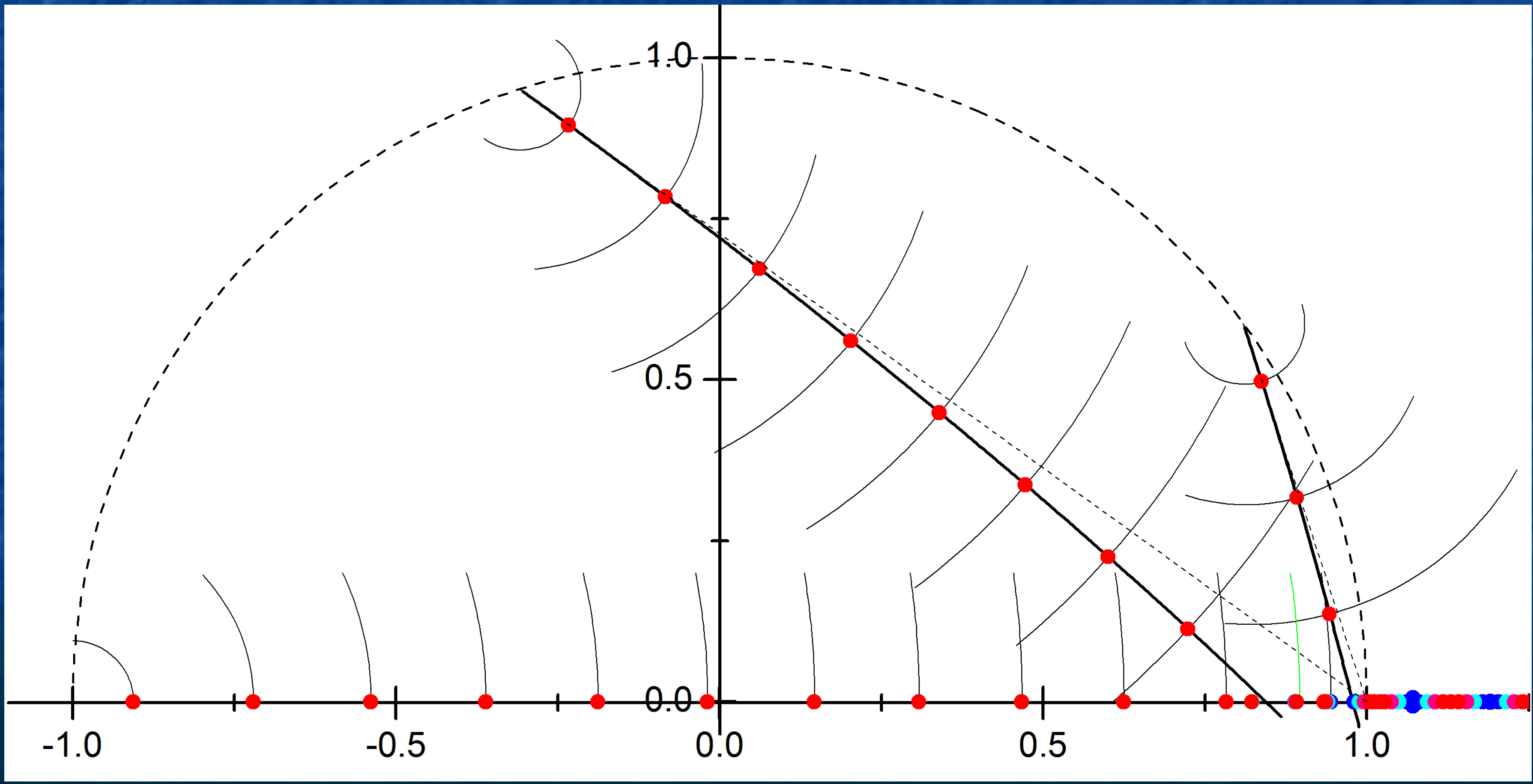
(4,1) Gas

$$(u^5+1)S^{(4)}(u)+\frac{9u^5-1}{u}\,S^{(3)}(u)+\frac{235}{16}\,u^3S''(u)+\frac{5}{4}\,u^2S'(u)+\frac{39}{64}\,uS(u)=0.$$

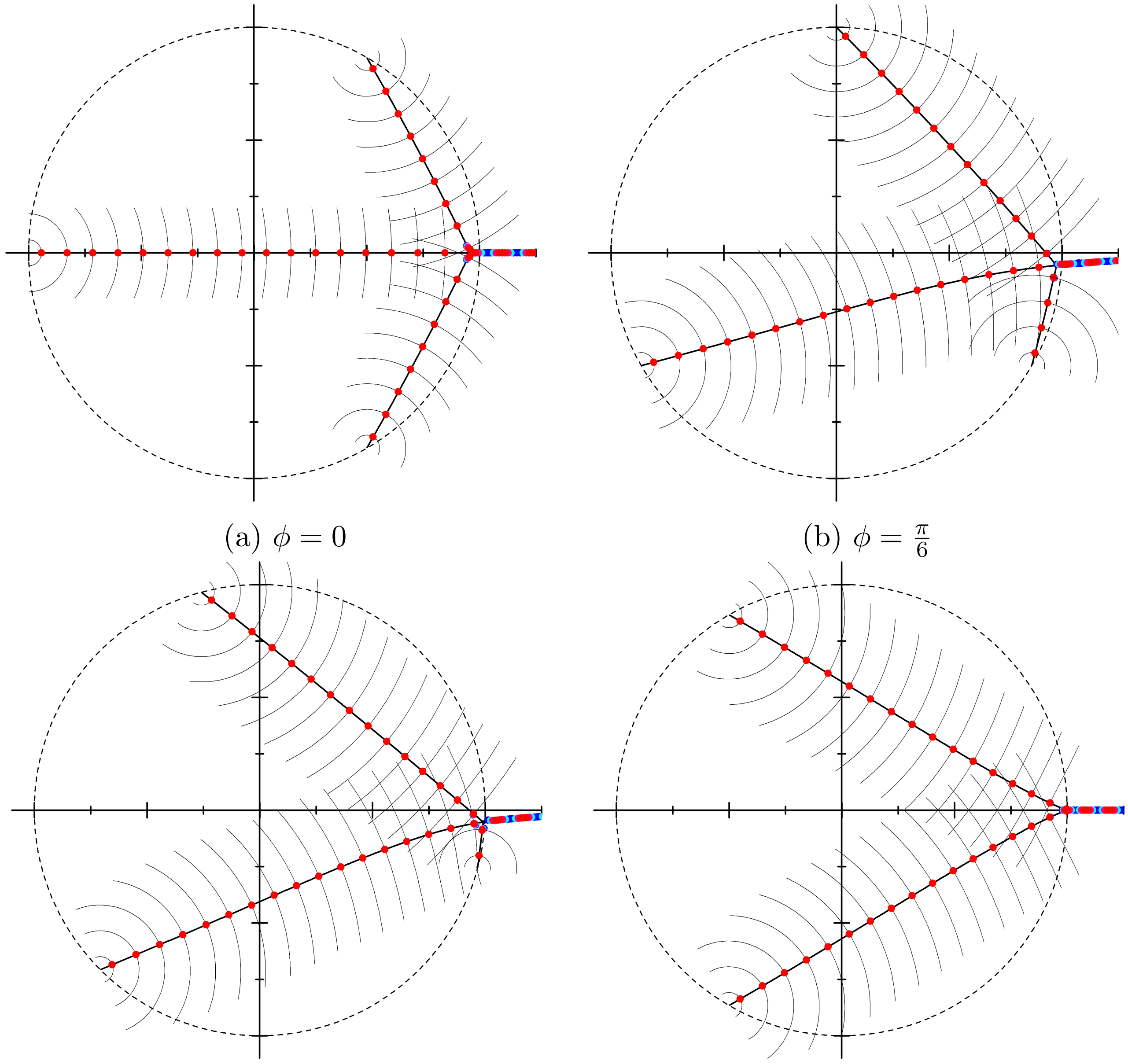


(3,2) Gas

$$(u^5+1)S^{(4)}(u)+\frac{9u^5-1}{u}S^{(3)}(u)+\frac{140}{9}u^3S''(u)+\frac{5}{4}u^2S'(u)+\frac{119}{144}uS(u)=0.$$

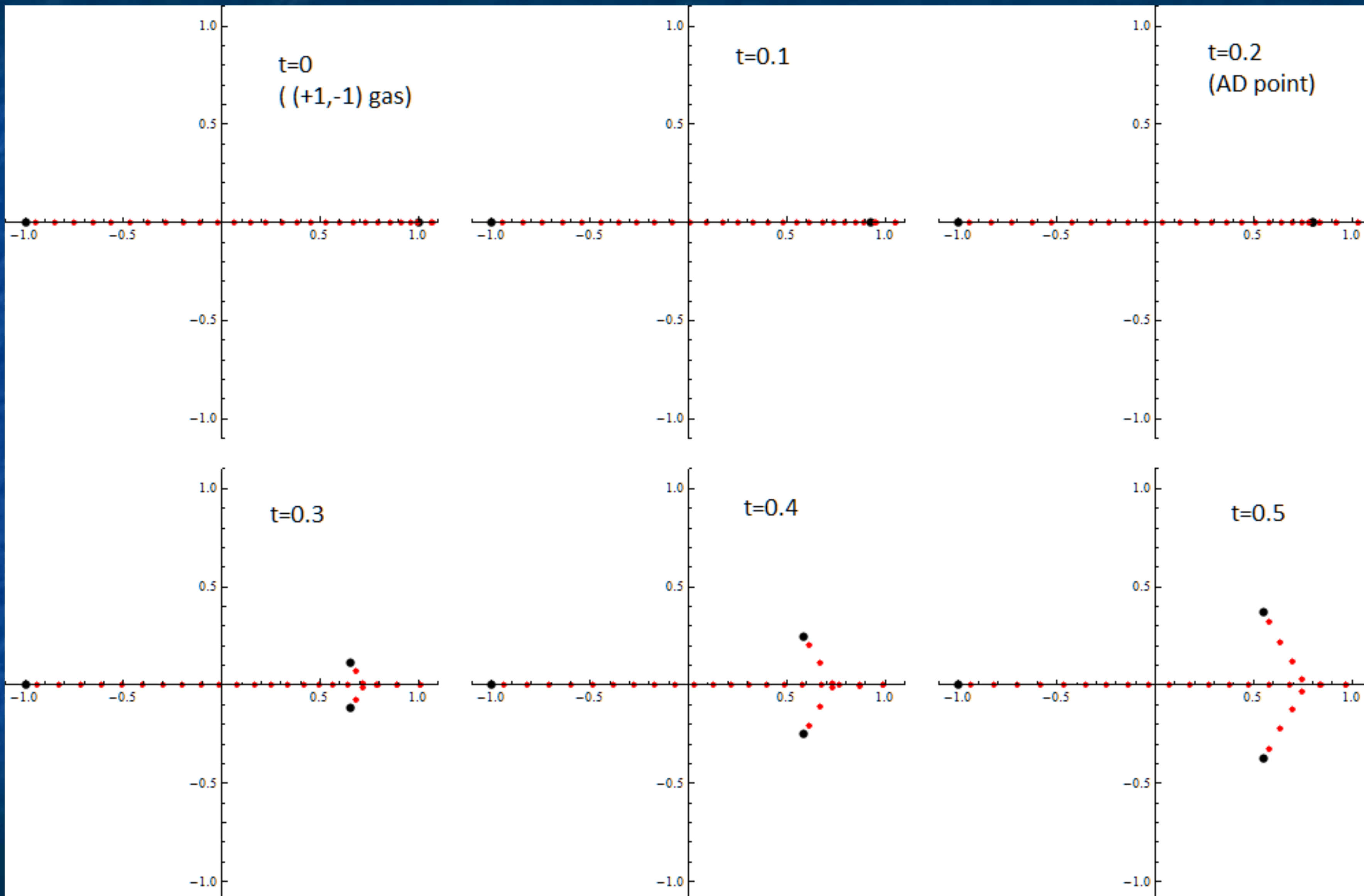


(2,1) Complex fugacity $\alpha = 200e^{i\phi}$



(a) $\phi = 0$ (b) $\phi = \frac{\pi}{6}$ (c) $\phi = \frac{\pi}{4}$ (d) $\phi = \frac{\pi}{3}$

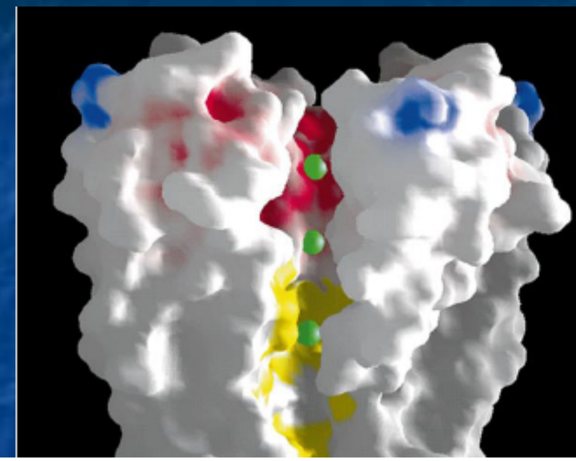
Mixture of (1,1) and (2,1) Coulomb gases

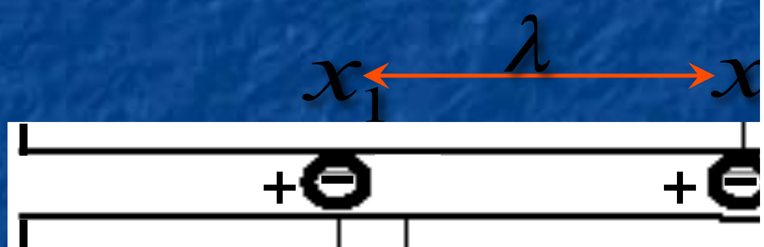


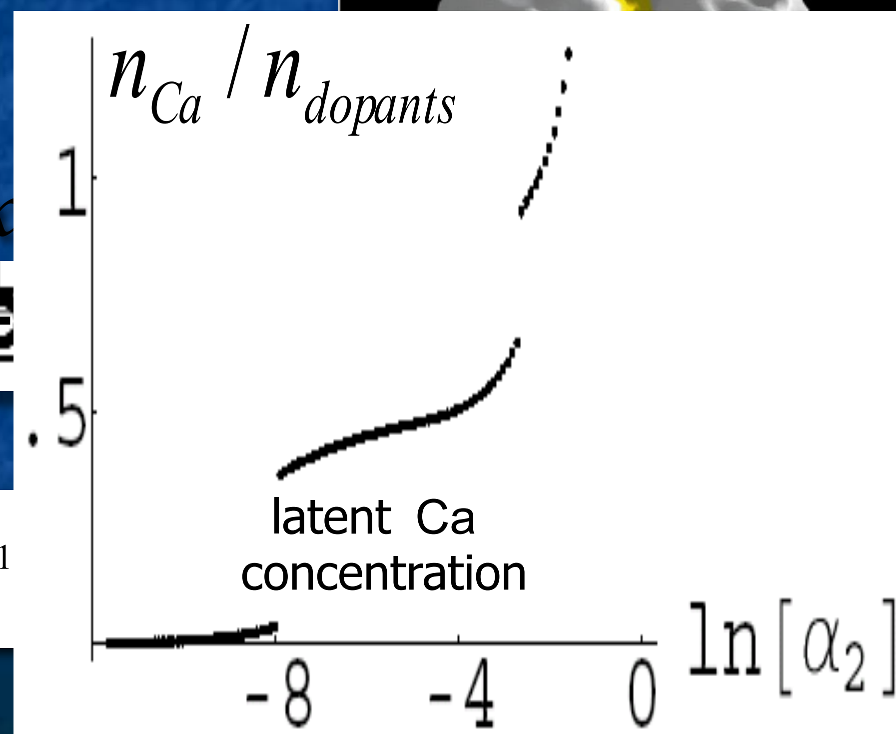
Channels are ``doped'' -fixed wall charges

Potassium Channels and the Atomic Basis of Selective Ion Conduction (Nobel Lecture)**

*Roderick MacKinnon**







$$Z = \mathrm{Tr}\left\{ e^{-\hat{H}\ (x_1-0)} e^{-i\theta} e^{-\hat{H}\ (x_2-x_1}\right.$$

Only one slide to go

- Statistical mechanics of Coulomb gases may be mapped onto NON-HERMITIAN Sine-Gordon quantum mechanics (or QFT, is it integrable?)

- This complex QM is described as a Hamiltonian dynamics on Riemann surfaces with genus > 1

- Tackled by Seiberg-Witten machinery of holomorphic differentials

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