# Discrete scale invariance in charged particles

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INT program "Quantum Few- and
Many-Body Systems in Universal Regimes"

October 29 (2024)

# Plan of this talk



0. Introduction
   - Efimov effect & discrete scale invariance

1. Non-relativistic charged particles
   - Efimovian states in hydrogen molecular ion

   Y. Nishida, Phys. Rev. A 105, L010802 (2022)

2. Relativistic charged particles
   - Atomic collapse resonances & vacuum polarization in graphene

   Y. Nishida, Phys. Rev. B 90, 165414 (2014); 94, 085430 (2016)

3. Coulomb + short-range potentials
   - Universality & generalized Bethe-Peierls

   S. Mochizuki & Y. Nishida, arXiv:2408.06011

# Efimov effect & discrete scale inv.

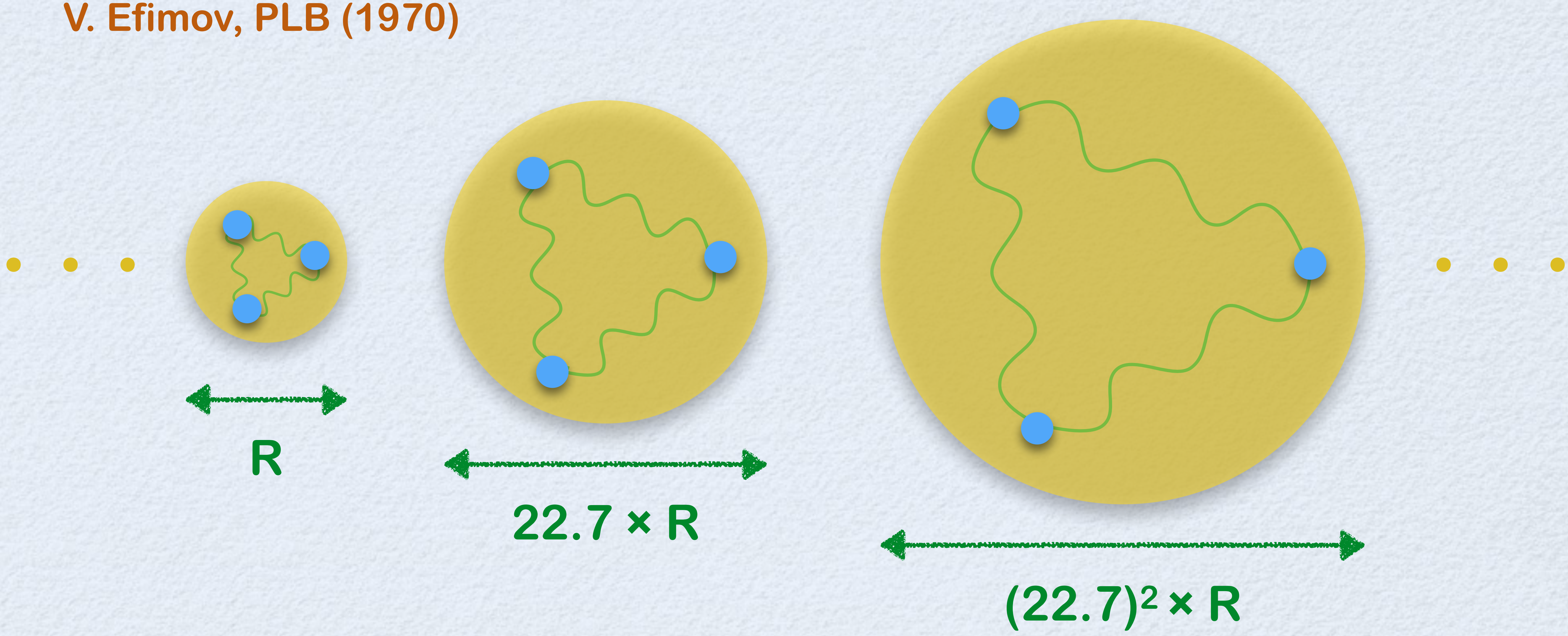
# Efimov effect

- ✓ 3 bosons
- ✓ 3 dimensions
- ✓ s-wave resonance

→ Infinite bound states with universal scaling

$$E_n \sim (22.7)^{-2n} E_0$$

V. Efimov, PLB (1970)




**Discrete scale invariance**

# Efimov effect

## 3-body Schrodinger equation

$$[T_1 + T_2 + T_3 + V_{12} + V_{23} + V_{31}]\, \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = E\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$$

Zero-range and infinite scattering length

## Hyperradial motion

$$\left[-\frac{1}{2m}\left(\frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R}\right) + \frac{s^2}{2mR^2}\right]\psi(R) = -\frac{\kappa^2}{2m}\psi(R)$$

Scale invariant potential with $s^2 = -1.013 < 0$

induced by hyperangular motion

Its solution $\psi(R) \propto K_{i|s|}(\kappa R)$

# Efimov effect

Its solution $\psi(R) \propto K_{i|s|}(\kappa R) \to \sin\left[|s| \ln(\kappa r_0) + \delta\right]$

$\psi'/\psi|_{R=r_0}$ has to be fixed by short-range B.C.

If $\kappa = \kappa_*$ is a solution for $\kappa r_0 \ll 1$,

$\kappa = (e^{\pi/|s|})^{-n} \kappa_*$ are also solutions

$$\left[ -\frac{1}{2m} \left( \frac{\partial^2}{\partial R^2} + \frac{1}{R} \frac{\partial}{\partial R} \right) + \frac{s^2}{2mR^2} \right] \psi(R) = E \psi(R)$$

- Scale invariance is broken by short-range B.C. down to discrete scale invariance
- Long-range Coulomb potential is usually obstacle

⇒ Discrete scale invariance in charged particles

# Non-relativistic charged particles

L. D. Landau & E. M. Lifshitz, “Quantum Mechanics”

# Hydrogen molecular ion




V(R) ~ $R^{-1}$ ⇒ $R^{-2}$

Born-Oppenheimer approximation (M≫m)

- Schrodinger equation for a light particle

$$\left[-\frac{\nabla_3^2}{2m} - \frac{kq^2}{|\vec{R}_1 - \vec{r}_3|} - \frac{kq^2}{|\vec{R}_2 - \vec{r}_3|}\right]\phi(\vec{r}_3) = \mathcal{E}_{\vec{R}_1\vec{R}_2}\phi(\vec{r}_3)$$

- Schrodinger equation for two heavy particles

$$\left[-\frac{\nabla_1^2}{2M} - \frac{\nabla_2^2}{2M} + \frac{kq^2}{|\vec{R}_1 - \vec{R}_2|} + \mathcal{E}_{\vec{R}_1\vec{R}_2}\right]\Phi(\vec{R}_1, \vec{R}_2)$$

$$= E\Phi(\vec{R}_1, \vec{R}_2)$$

# Hydrogen molecular ion


V(R) ~ $R^{-1}$ ⇒ $R^{-2}$

Hydrogen-like atom $\mathcal{E}_n = -\frac{1}{2ma_B^2 n^2} \quad (n = 1, 2, \ldots)$

under electric field produced by far separated charge

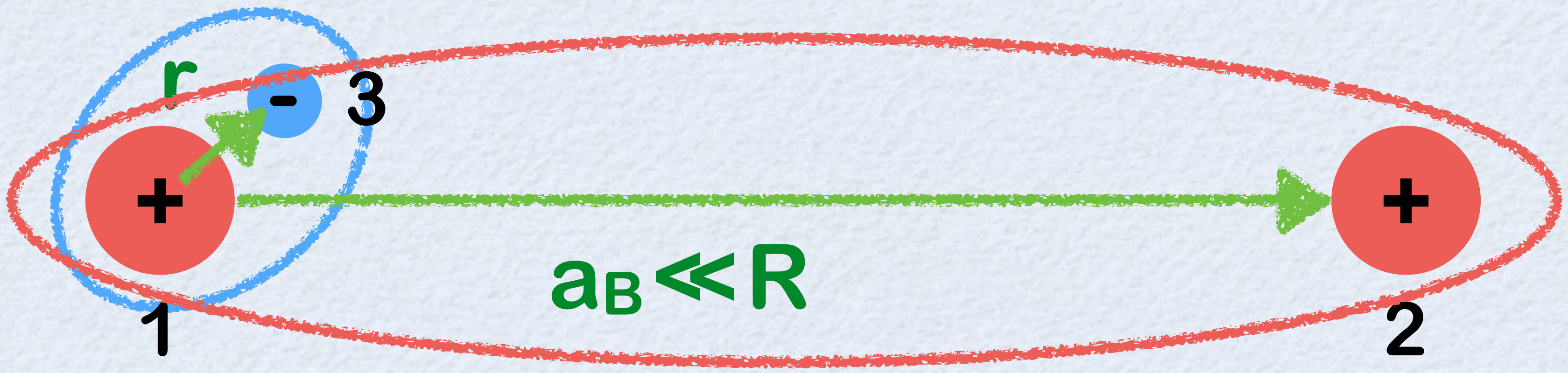
$$V(\vec{r}) = \frac{kq^2}{R} - \frac{kq^2}{|\vec{R} - \vec{r}|} \simeq -\frac{kq^2}{R^2}\hat{R}\cdot\vec{r}$$

1st-order perturbation $\Delta\mathcal{E}_n = \langle V(\vec{r})\rangle_n = 0 \quad (n = 1)$

$$\Delta\mathcal{E}_n = \langle V(\vec{r})\rangle_n = \pm\frac{3}{mR^2}, 0(\times 2) \quad (n = 2)$$

Scale invariant attraction for n=2,3,...

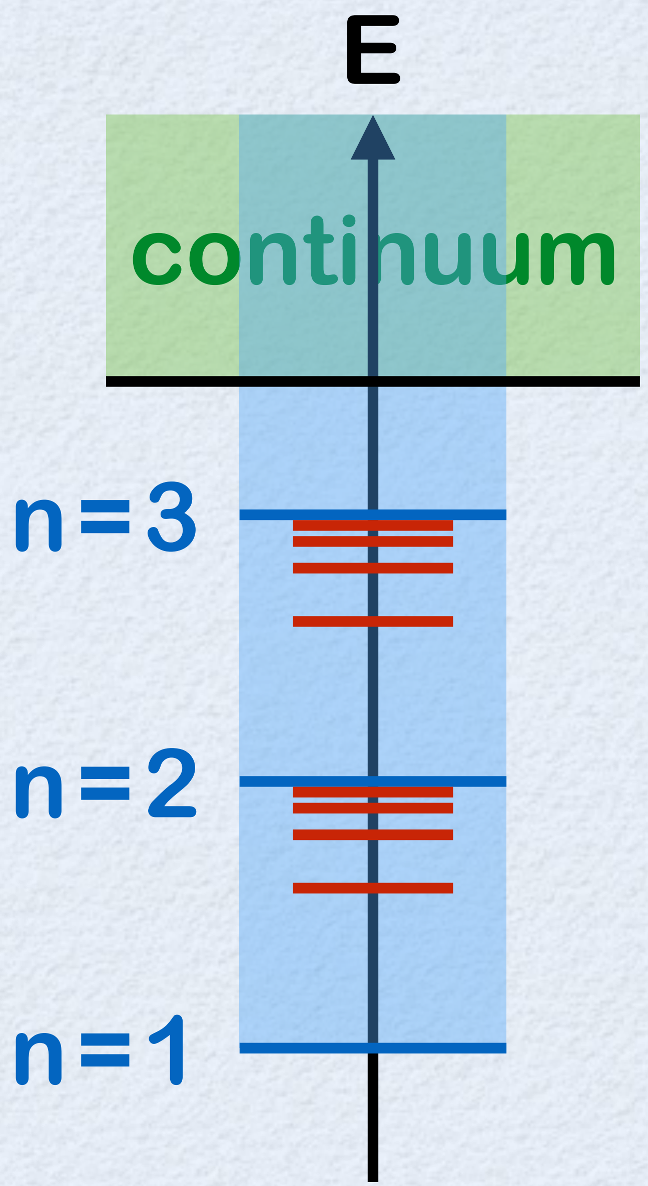
# Hydrogen molecular ion




$V(R) \sim R^{-1} \Rightarrow R^{-2}$

**Infinite bound states obeying discrete scale invariance**

toward thresholds of $(H)_{n=2,3,\ldots}$




- Efimovian states are resonances embedded into continuum of $(H)_{n=1}$
- Relevant to $H_2^+$ ions or trions (nuclear systems?)
- Generalization to 2D, 1D & logarithmic Coulomb potential

Y. Nishida, Phys. Rev. A 105, L010802 (2022)

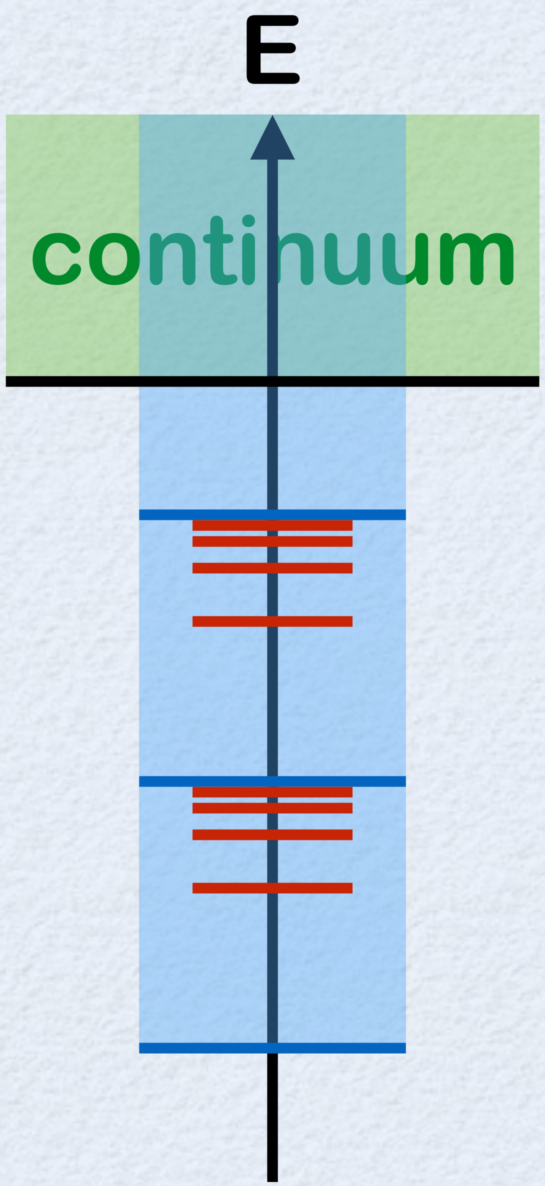
# Experimental observation

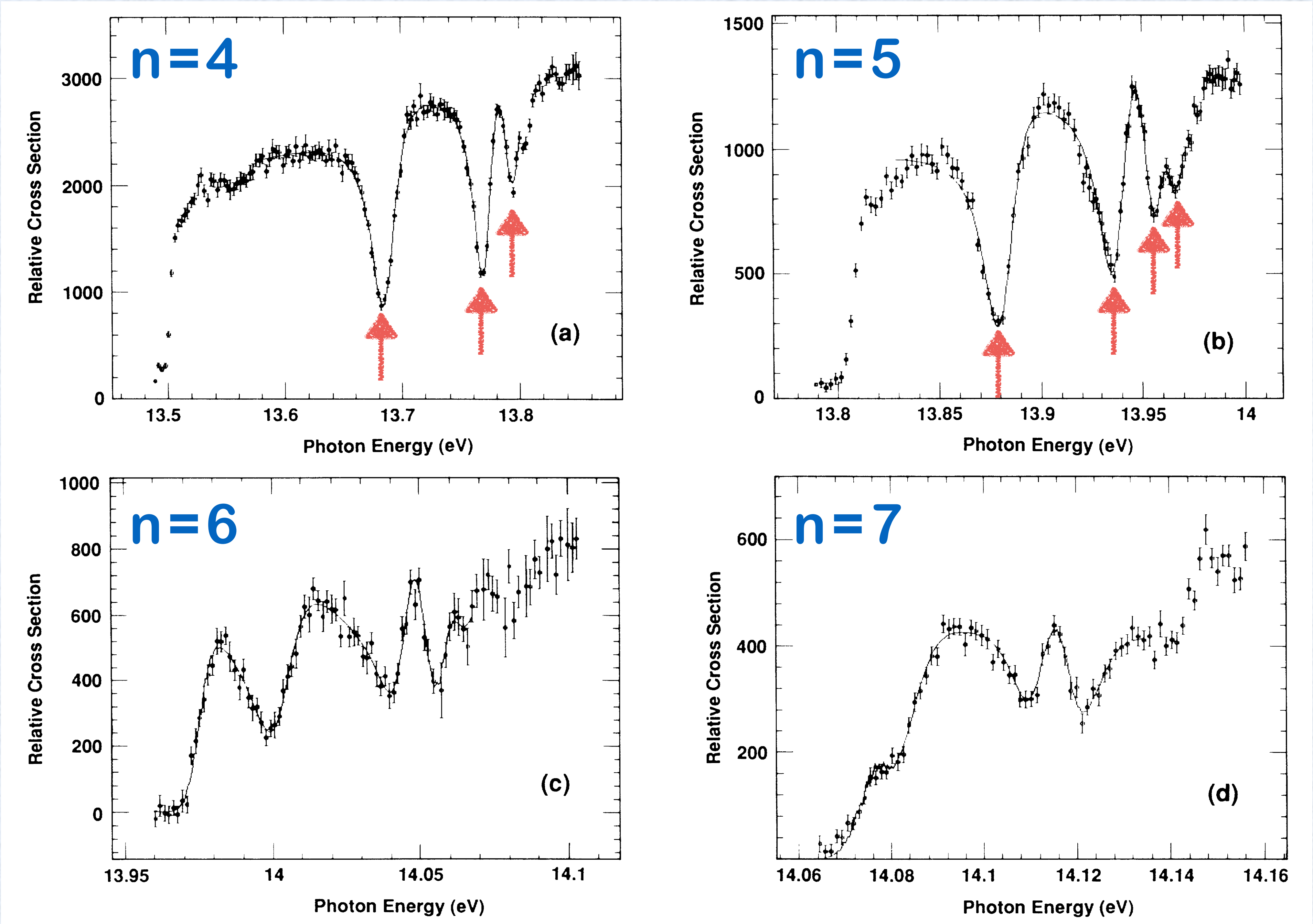


## Doubly excited resonances via photo detachment

$$H^- + \gamma \rightarrow H^{-**} \rightarrow H^{0*}(\leq n) + e^-$$

P. G. Harris et al.
PRL 65, 309 (1990)



# Relativistic charged particles

# Atomic collapse



## Hydrogen-like atom from Dirac equation

$$\left[\vec{\alpha}\cdot\vec{p}+\beta m-\frac{Z\alpha}{r}\right]\psi(\vec{r})=E\psi(\vec{r})$$

Coulomb potential is scale invariant

$$E_{n'j}=\frac{m}{\sqrt{1+\frac{(Z\alpha)^2}{[n'+\sqrt{(j+\frac{1}{2})^2-(Z\alpha)^2}]^2}}}$$

becomes complex for $Z>\dfrac{j+\frac{1}{2}}{\alpha}>137$

"Atomic collapse" Y. B. Zeldovich & V. S. Popov (1971)

$$\psi(\vec{r})\sim e^{\pm i\sqrt{(Z\alpha)^2-(j+\frac{1}{2})^2}\,\ln r}\qquad(r\ll a_B)$$

signals discrete scale invariance

# Atomic collapse



## Hydrogen-like atom from Dirac equation

$$\left[\vec{\alpha}\cdot\vec{p}+\beta m-\frac{Z\alpha}{r}\right]\psi(\vec{r})=E\psi(\vec{r})$$

Coulomb potential is scale invariant

- Z>137 is not yet achieved with a single nucleus but may be realized by colliding two heavy nuclei

W. Greiner, B. Muller & J. Rafelski, "Quantum Electrodynamics of Strong Fields"

- Because $v_F/c$~O(0.01), $\alpha_{\mathrm{eff}}=\frac{ke^2}{\hbar\text{“}v_{\mathrm{F}}\text{”}}\sim O(1)$

  "superheavy nucleus" can be realized by a charged impurity with Z~O(1) on graphene

V. M. Pereira, J. Nilsson & A. H. Castro Neto, PRL (2007)

A. V. Shytov, M. I. Katsnelson & L. S. Levitov, PRL (2007)

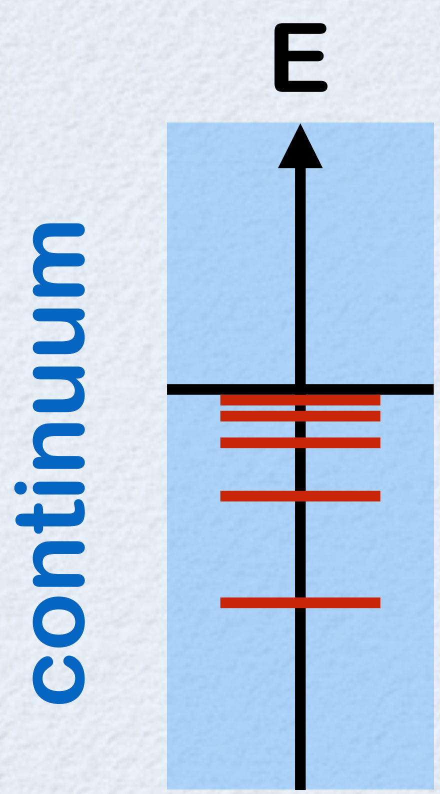
# Graphene

**2D massless Dirac equation with a charged impurity**

$$\left[\vec{\sigma}\cdot\vec{p} - \frac{Z\alpha_{\mathrm{eff}}}{r}\right]\psi(\vec{r}) = E\psi(\vec{r})$$

**Scale invariance is broken by short-range B.C.**

**down to discrete scale invariance for $Z\alpha_{\mathrm{eff}}>1$**




**Infinite ~~bound states~~ resonances**

**"Atomic collapse resonances"**

**⇒ DoS peaks probed by STM**

# Graphene

**Scale invariance is broken by short-range B.C.**

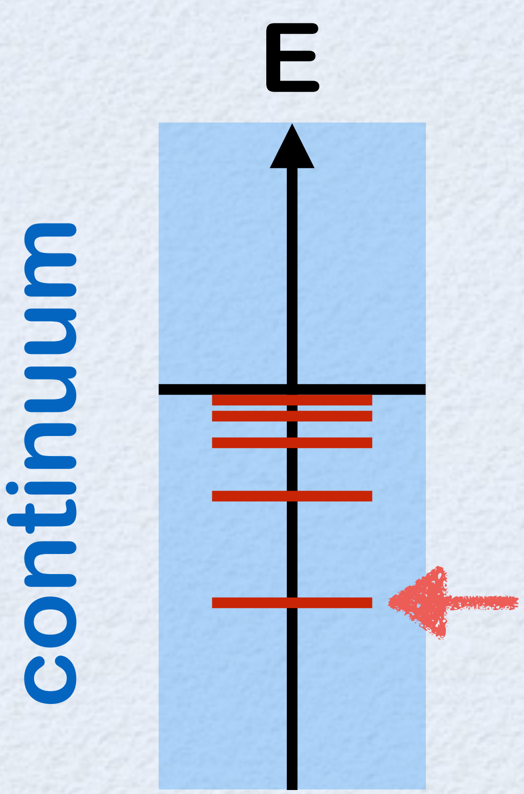
**down to discrete scale invariance for $Za_{eff}>1$**

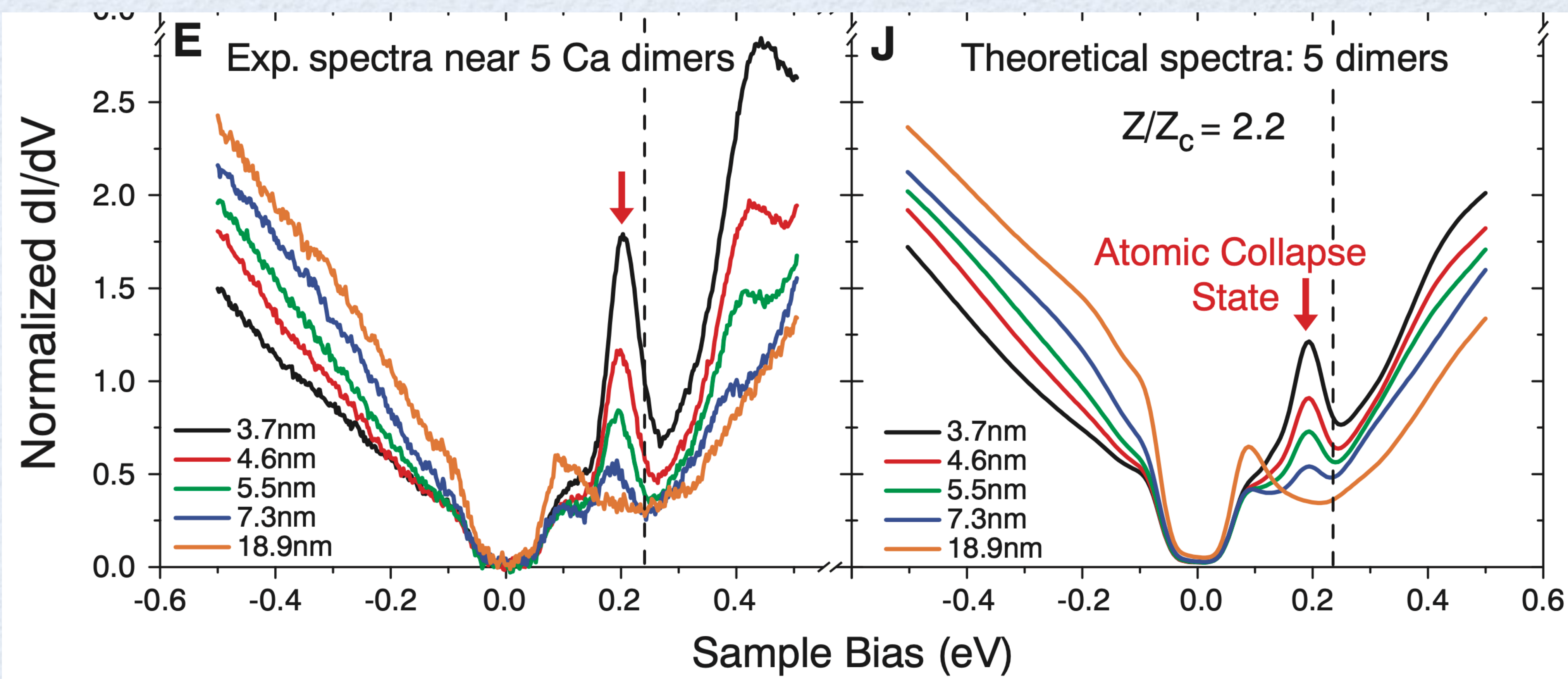
**Infinite ~~bound states~~ resonances**

**"Atomic collapse resonances"**

**⇒ DoS peaks probed by STM**

M. F. Crommie et al.
Science 340, 734 (2013)




**Cond-mat realization of "superheavy nucleus"**

# Vacuum polarization


Charge distribution of electrons $n(r) = \sum_{E<0} |\psi_E(\vec{r})|^2$

- Scale invariance ⇒ $n(r) = \frac{C}{r^2}$ Power law
- Discrete scale invariance ⇒ $n(r) = \frac{F(\ln r)}{r^2}$

Power law + log-periodic oscillation

$$F_j(r/r_j^*) = \frac{\gamma}{2\pi^2} \mathrm{Re} \int_0^\infty dz \frac{\Gamma(1-ig+i\gamma)\Gamma(1-ig-i\gamma)}{\Gamma(1+2i\gamma)\Gamma(1-2i\gamma)} \left[ \frac{1 + \frac{(j-ig+i\gamma)\Gamma(1+2i\gamma)\Gamma(1-ig-i\gamma)}{(j-ig-i\gamma)\Gamma(1-2i\gamma)\Gamma(1-ig+i\gamma)} \left(\frac{r}{zr_j^*}\right)^{2i\gamma}}{1 - \frac{(j-ig+i\gamma)\Gamma(1+2i\gamma)\Gamma(1-ig-i\gamma)}{(j-ig-i\gamma)\Gamma(1-2i\gamma)\Gamma(1-ig+i\gamma)} \left(\frac{r}{zr_j^*}\right)^{2i\gamma}} \right] \times e^{-z} U(-ig+i\gamma, 1+2i\gamma, z) U(1-ig-i\gamma, 1-2i\gamma, z)$$

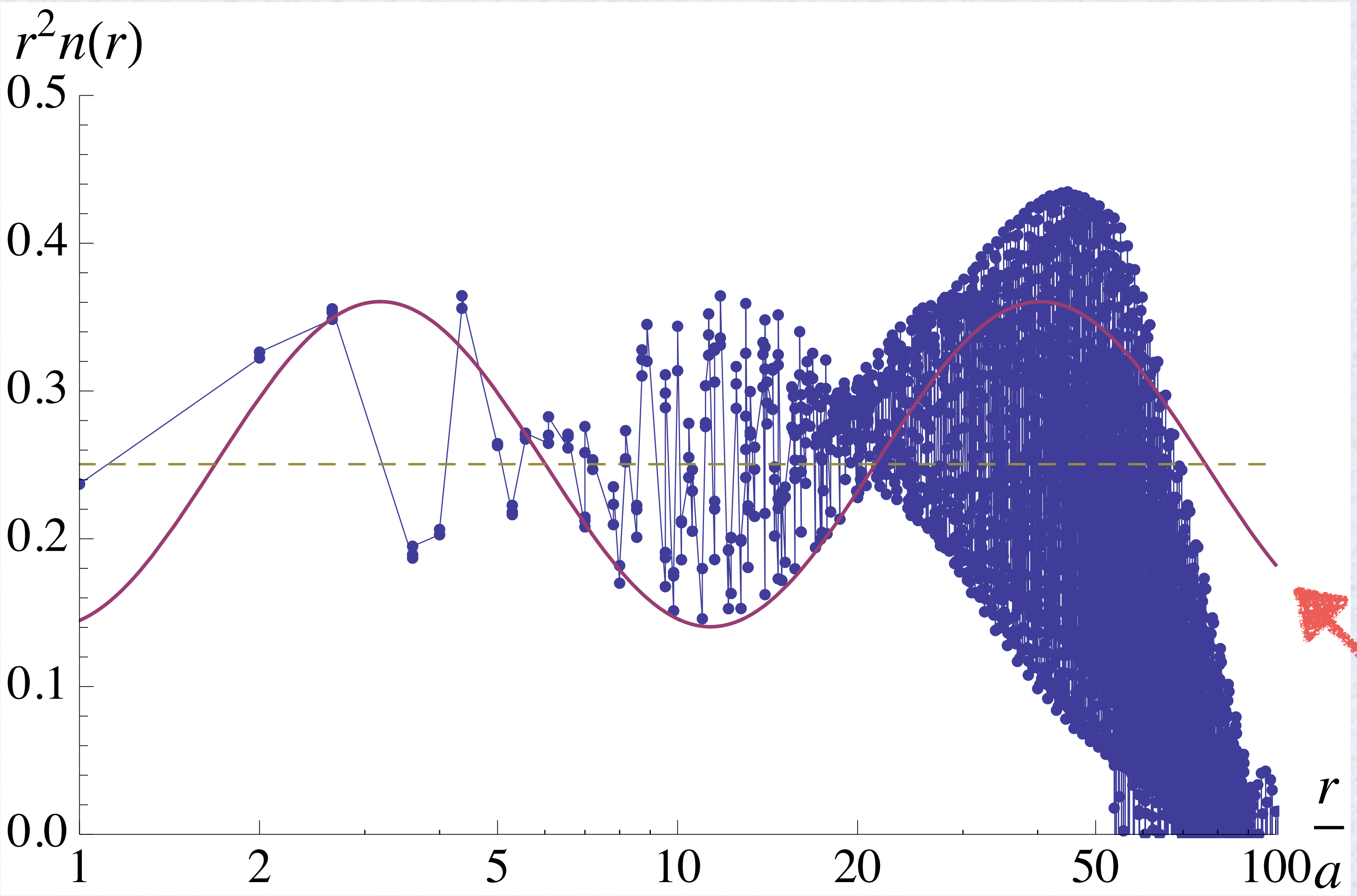
Y. Nishida, Phys. Rev. B 90, 165414 (2014); Phys. Rev. B 94, 085430 (2016)

# Vacuum polarization

## Comparison to lattice data for Za$_{eff}$=4/3

(exact diagonalization on honeycomb lattice with 124x124 sites)

V. M. Pereira, J. Nilsson & A. H. Castro Neto, PRL (2007)




Shape & period are predictions

Amplitude & phase are fit parameters

$$n(r) = \frac{F(\ln r)}{r^2}$$

- Envelop fits well our prediction but fast oscillation exists with its origin unknown

# Coulomb + short-range potentials

# Short-range universality

Short-range universality arises when R ≪ a, $k^{-1}$


- Universal physics is described by zero-range interaction with R~0 under fixed a
- Bethe-Peierls B.C. is its direct implementation

$$\lim_{r\to 0}\psi(r) \propto \frac{1}{r} - \frac{1}{a} + O(r)$$

H. Bethe and R. Peierls
Proc. R. Soc. Lond. A (1935)

- Bethe-Peierls B.C. + Born-Oppenheimer approx. provides intuitive understanding of Efimov effect

⇒ Generalization to charged particles

# Generalized Bethe-Peierls B.C.

**S-wave radial Hamiltonian** $\hat{H} = -\frac{1}{2m}\frac{d^2}{dr^2} \pm \frac{1}{ma_0 r}$

**has to be not only hermitian but also self-adjoint**

$$\int_0^\infty dr\, \varphi(r)^* \hat{H} \chi(r) = \int_0^\infty dr\, [\hat{H}\varphi(r)]^* \chi(r)$$

$\lim_{r\to 0} \chi(r) = \lim_{r\to 0} \varphi(r) = 0$ **is usually imposed, but**

$\lim_{r\to 0} W[\chi(r), f(r)\cos\delta - g(r)\sin\delta] = 0$ **is possible**

**Generalized Bethe-Peierls boundary condition**

$$\lim_{r\to 0} \chi(r) \propto 1 - \frac{r}{\tilde{a}} \pm \frac{2r}{a_0} \ln\left(e^{2\gamma-1}\frac{2r}{a_0}\right) + O(r^2 \ln r)$$

**(Coulomb modified) scattering length** $\cot\delta = -\frac{a_0}{2\tilde{a}}$

# Generalized Bethe-Peierls B.C.



$$\lim_{r\to 0}\chi(r) \propto 1 - \frac{r}{\tilde{a}} \pm \frac{2r}{a_0}\ln\left(e^{2\gamma-1}\frac{2r}{a_0}\right) + O(r^2\ln r)$$

- Information of short-range potential enters only through (Coulomb modified) scattering length
- (Coulomb modified) effective ranges are all zero

⇒ Suitable to directly describe universal physics

for R ≪ a, $a_0$, $k^{-1}$

2-body bound-state solution

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} \pm \frac{1}{ma_0 r}\right]\chi(r) = -\frac{\kappa^2}{2m}\chi(r)$$

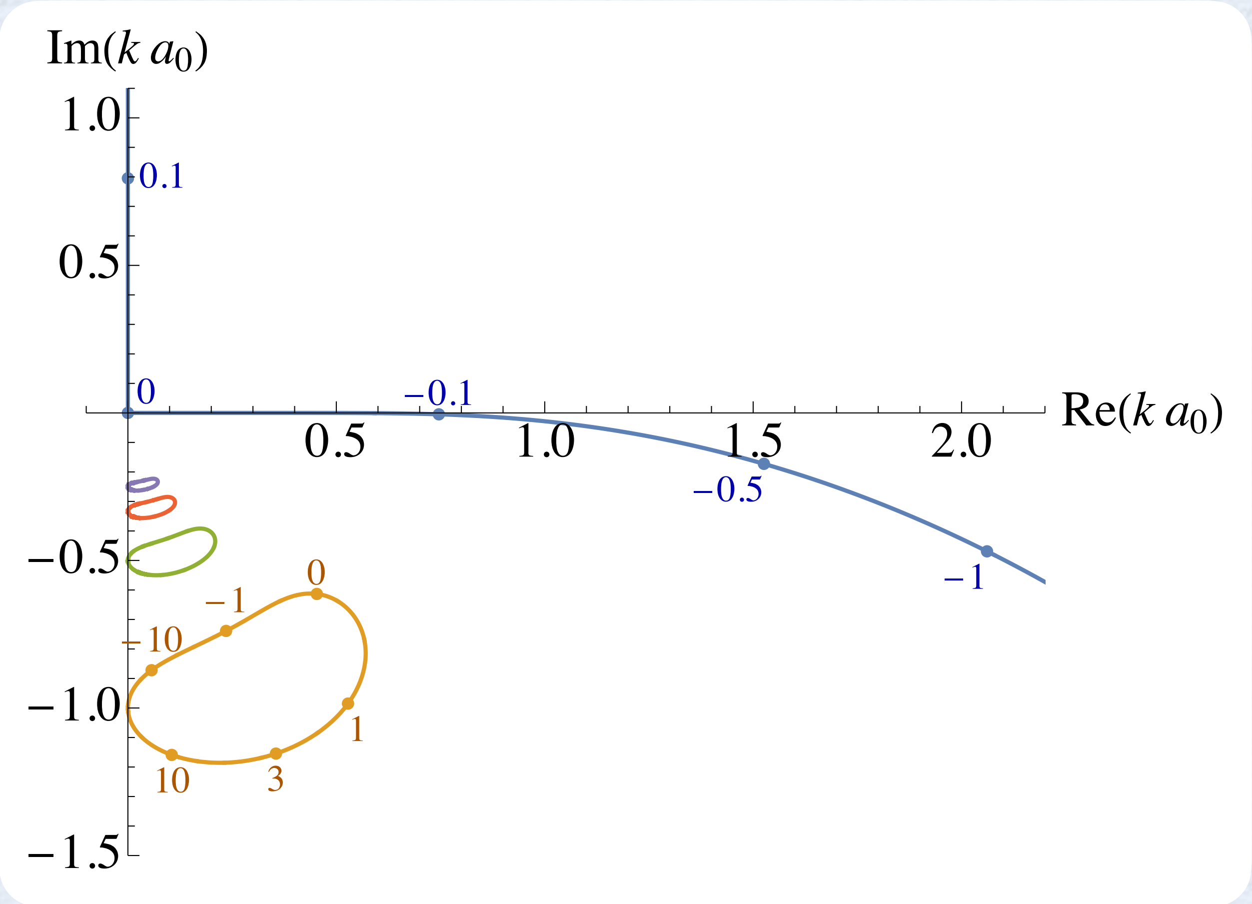
$$\Rightarrow \quad \chi(r) = H^+_\eta(i\kappa r)$$

B.C. $\Rightarrow \quad \kappa = \frac{1}{\tilde{a}} \pm \frac{2}{a_0}\left[\Psi\left(1 \pm \frac{1}{\kappa a_0}\right) + \ln\left(\kappa a_0\right)\right]$

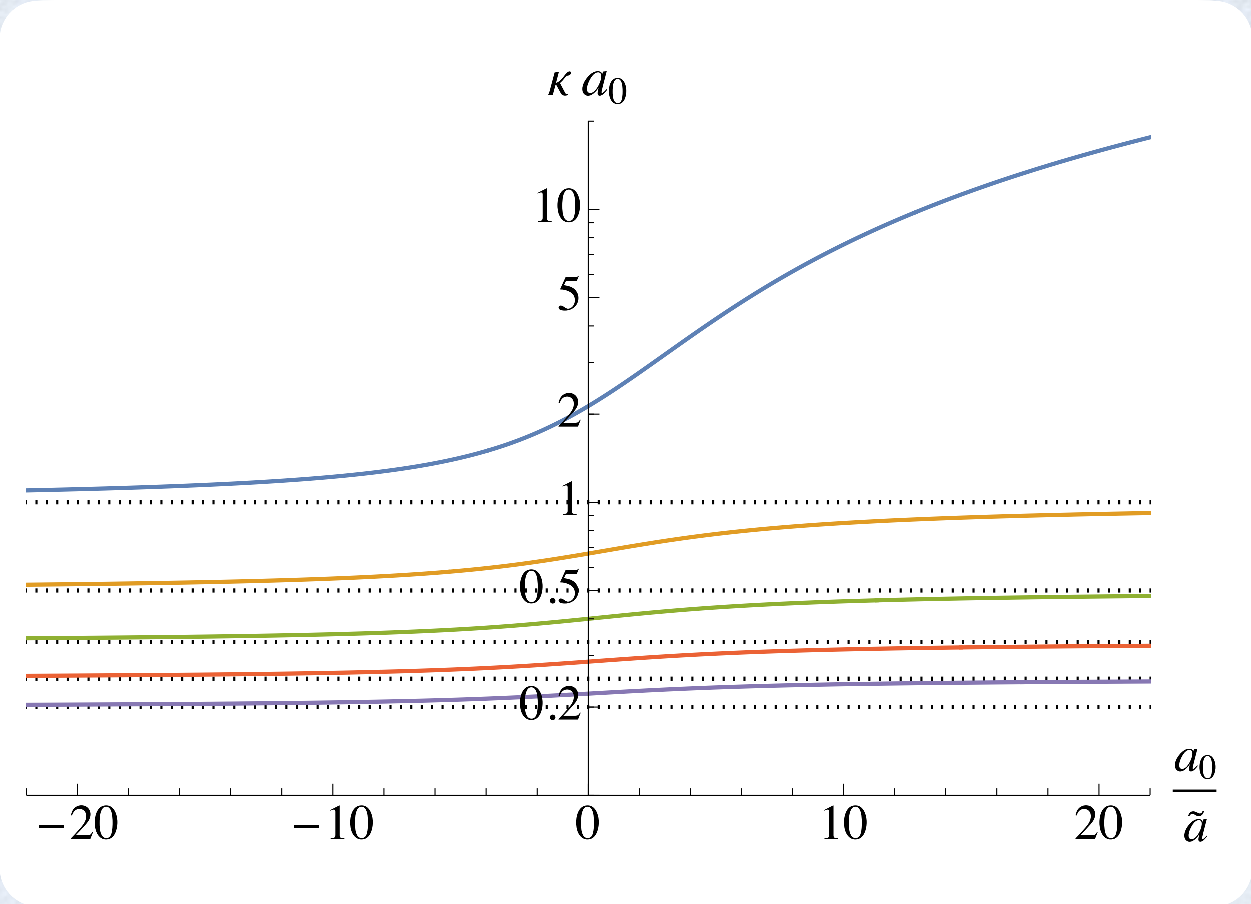
# Generalized Bethe-Peierls B.C.



## Repulsive Coulomb




## Attractive Coulomb




- Infinite resonances
- One of them turns into a bound state for a > 0

- Infinite bound states
- No resonances

See also, C. H. Schmickler, H.-W. Hammer & A. G. Volosniev, PLB (2019)

# Born-Oppenheimer approx.



3 equally charged heavy-heavy-light particles at a=∞

$$\hat{H}_{\text{light}} = -\frac{\nabla_r^2}{2m} + \sum_{i=1,2} \frac{1}{m a_0 |r - R_i|}$$


Trial wave function for a light particle

$$\psi(r) = \sum_{i=1,2} \frac{H_\eta^+(i\kappa|r - R_i|)}{|r - R_i|}$$

$$\Rightarrow \quad \kappa = \frac{2}{a_0}\left[\Psi\left(1 + \frac{1}{\kappa a_0}\right) + \ln(\kappa a_0)\right] + \frac{C_\eta H_\eta^+(i\kappa R)}{R}$$

B.C.

# Born-Oppenheimer approx.

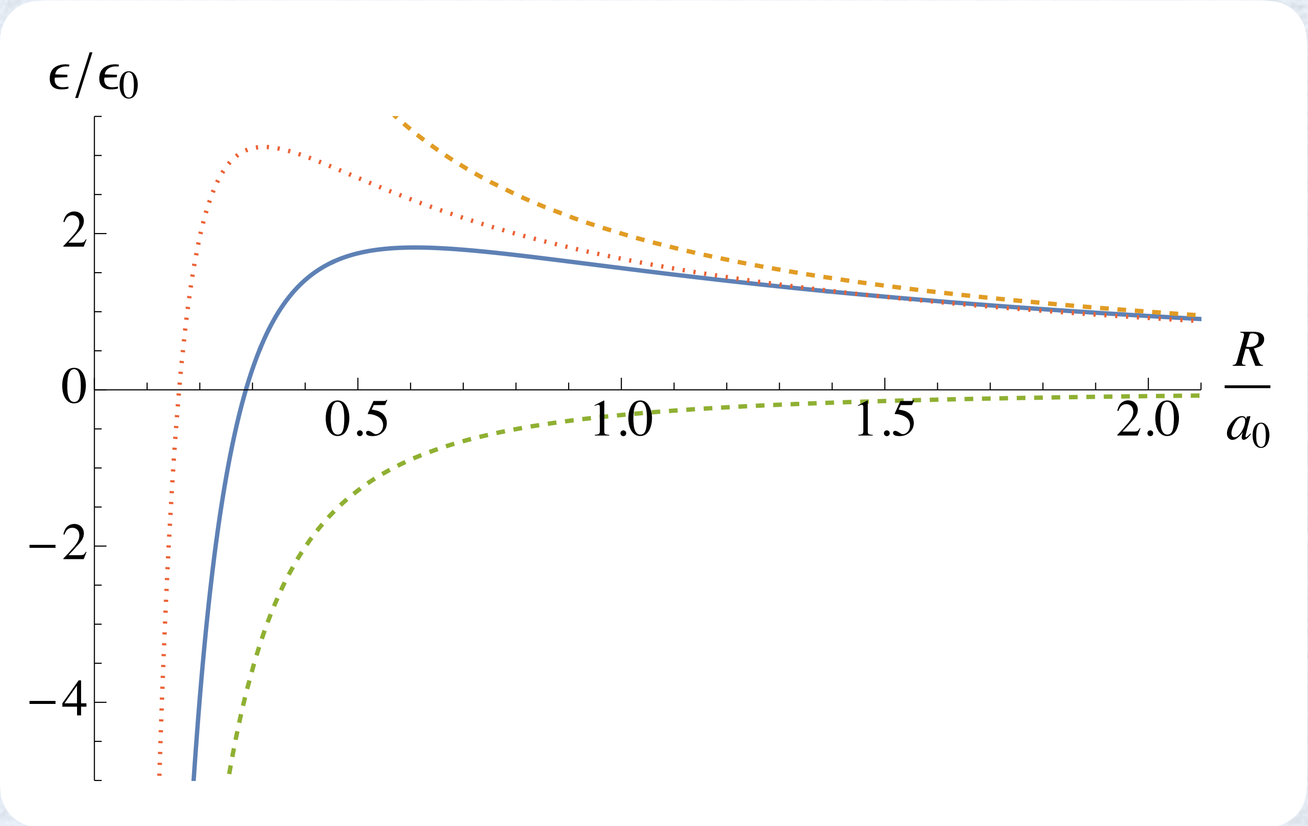
## Energy expectation value of a light particle

$$E(R) = \langle\psi|\hat{H}_{\text{light}}|\psi\rangle$$

$$\to -\frac{(0.567)^2}{2mR^2} \quad (R \to 0)$$

$$\to +\frac{1}{ma_0 R} \quad (R \to \infty)$$

$$\approx -\frac{(0.567)^2}{2mR^2} + \frac{1}{ma_0 R}$$




## Heavy-heavy Schrodinger equation

$$\left[-\frac{1}{M}\frac{d^2}{dR^2} - \frac{1/4 + s^2}{MR^2} + \frac{2}{Ma_0' R}\right]\chi(R) = -\frac{\kappa^2}{M}\chi(R)$$

scale invariant attraction  Coulomb repulsion

# Born-Oppenheimer approx.

Heavy-heavy Schrodinger equation

$$\left[-\frac{1}{M}\frac{d^2}{dR^2}-\frac{1/4+s^2}{MR^2}+\frac{2}{Ma_0'R}\right]\chi(R)=-\frac{\kappa^2}{M}\chi(R)$$

scale invariant attraction   Coulomb repulsion

$$\Rightarrow \quad \left(\frac{\kappa}{\kappa_*}\right)^{2is}=\frac{\Gamma\left(\frac{1}{2}+is\right)\Gamma\left(\frac{1}{2}-is+\frac{1}{\kappa a_0'}\right)}{\Gamma\left(\frac{1}{2}-is\right)\Gamma\left(\frac{1}{2}+is+\frac{1}{\kappa a_0'}\right)}$$

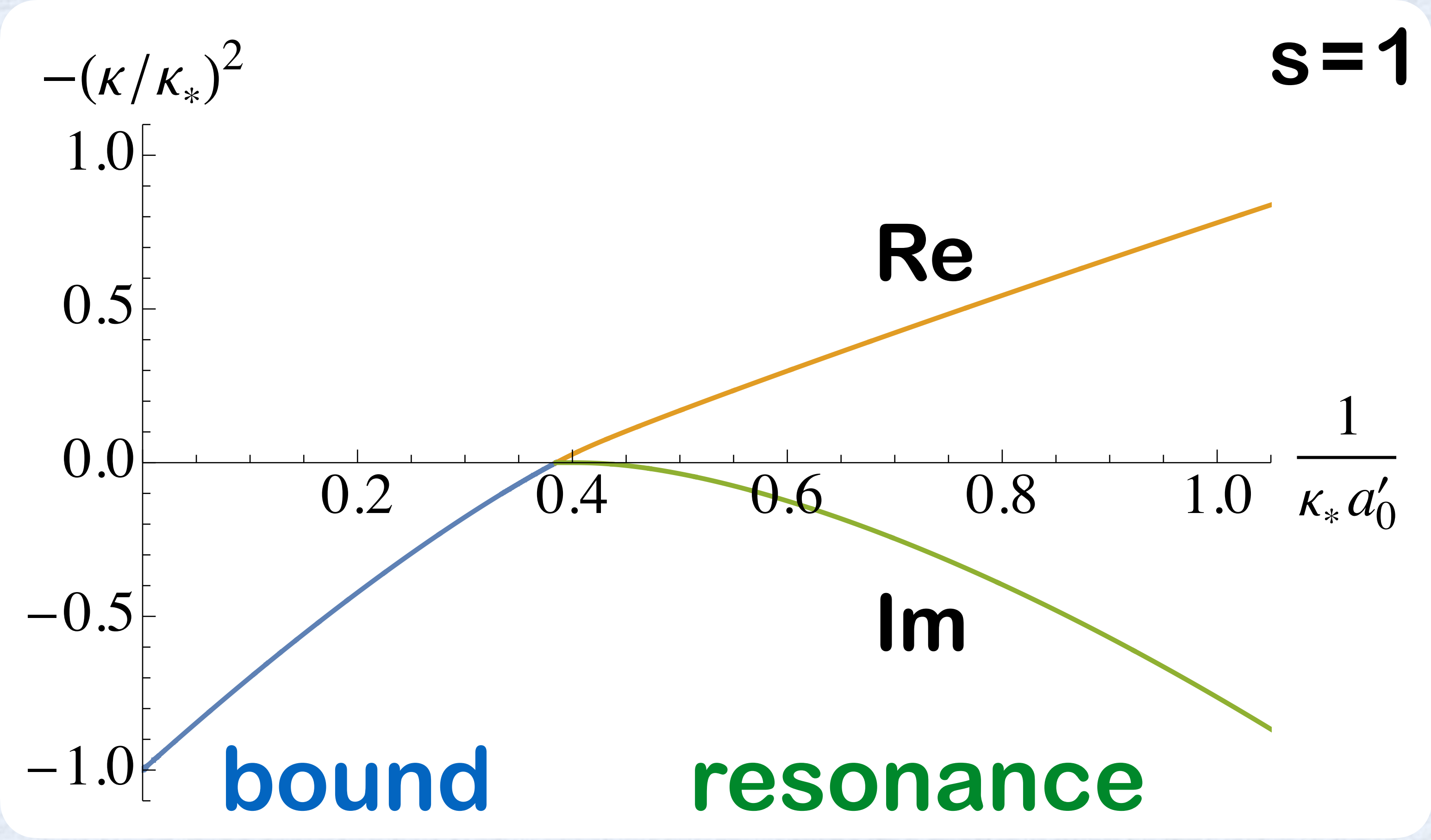
- Three-body parameter $\kappa_*$ fixes the phase at R~0
- This equation is invariant under $\kappa_* \to e^{-n\pi/s}\kappa_*$ , so that one solution generates infinite solutions

⇒ Consequence of discrete scale invariance

# Born-Oppenheimer approx.

## 3-body bound states & resonances

$$\Rightarrow \quad \left(\frac{\kappa}{\kappa_*}\right)^{2is} = \frac{\Gamma\left(\frac{1}{2}+is\right)\Gamma\left(\frac{1}{2}-is+\frac{1}{\kappa a_0'}\right)}{\Gamma\left(\frac{1}{2}-is\right)\Gamma\left(\frac{1}{2}+is+\frac{1}{\kappa a_0'}\right)}$$




S. Mochizuki & Y. Nishida

arXiv:2408.06011

- Bound state turns resonance by Coulomb repulsion
- Infinite solutions are obtained by $\kappa_* \to e^{-n\pi/s}\kappa_*$

# Summary and future work



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2. Relativistic charged particles
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⇒ Applications to nuclear systems ?