Mass dependence of instanton determinant in QCD: part I

Gerald Dunne (UConn)

Hyunsoo Min (Univ. Seoul and UConn)

- determinants in quantum field theory
- semiclassical "instanton" background
- 1 dimensional (ODE) computational method : Levit & Smilansky
- higher dimensional radial extension
- renormalization
- results

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with: Jin Hur and Choonkyu Lee (SNU) PLB (hepth/0407222/0410190)

Computing Determinants of Partial Differential Operators

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problem: determinant of a (partial) differential operator

Many applications in quantum field theory:

- **effective action**
- **tunneling rates**

$$D_\mu = \partial_\mu - g A_\mu$$

Quantum field theory functional integral

$$Z = \int \mathcal{D}\psi\, \mathcal{D}\bar{\psi}\, \mathcal{D}A\, exp\left[\int d^4x \left(tr F^2 + \bar{\psi}\left[i \not{D} - m\right]\psi\right)\right]$$

$$= \int \mathcal{D}A\, exp\left[\int d^4x\, tr F^2\right] det\left[i\not{D} - m\right]$$

Effective action : $S[A] = log\, det\left[i\not{D} - m\right]$

Exact results : covariantly constant $F_{\mu\nu}$

problem: determinant of a (partial) differential operator

Many applications in quantum field theory:

- **effective action**
- **tunneling rates**

$$Z = \int \mathcal{D}\phi \, e^{-S[\phi]} \sim \frac{e^{-S[\phi_b]}}{\sqrt{\det S^{(2)}[\phi_b]}}$$

" bounce" : $S^{(2)}[\phi_b]$ has a negative eigenvalue

tunneling rate : $\Gamma = 2\,\mathcal{I}m\, \ln Z$

$$= \left|\det\left(\frac{S^{(2)}[\phi_b]}{S^{(2)}[\phi_0]}\right)\right|^{-\frac{1}{2}} e^{-S[\phi_b]}$$

problem: determinant of a (partial) differential operator

Many applications in quantum field theory:

- **effective action**
- **tunneling rates**

Few exact results, so need approximation methods

- **derivative expansion**
- **WKB**
- **thin/thick wall approximation for tunneling rates**
- **numerical ?**

Instanton background in QCD

Instantons : semiclassical solutions $F_{\mu\nu} = \pm \tilde{F}_{\mu\nu}$

Stationary points of gauge functional integral : minimize Yang-Mills action for fixed topological charge

e.g. SU(2) single instanton (Belavin et al) :

$$A_\mu(x) = A_\mu^a(x)\frac{\tau^a}{2} = \frac{\eta_{\mu\nu a}\tau^a x_\nu}{r^2 + \rho^2}$$

$$F_{\mu\nu}(x) = F_{\mu\nu}^a(x)\frac{\tau^a}{2} = -\frac{2\rho^2\eta_{\mu\nu a}\tau^a}{(r^2 + \rho^2)^2}$$

Instanton background in QCD

First simplification :

Self-duality ⟹ Dirac and Klein-Gordon operators **isospectral**

$$(i\not{D} - m) \qquad\qquad (-D_\mu D_\mu + m^2)$$

$$\Gamma^F(A;m) = -2\,\Gamma^S(A;m) - \frac{1}{2}\ln\left(\frac{m^2}{\mu^2}\right)$$

⟹ compute **scalar** determinant instead of **spinor** determinant

Instanton background - asymptotics

Renormalized effective action :

function of m only

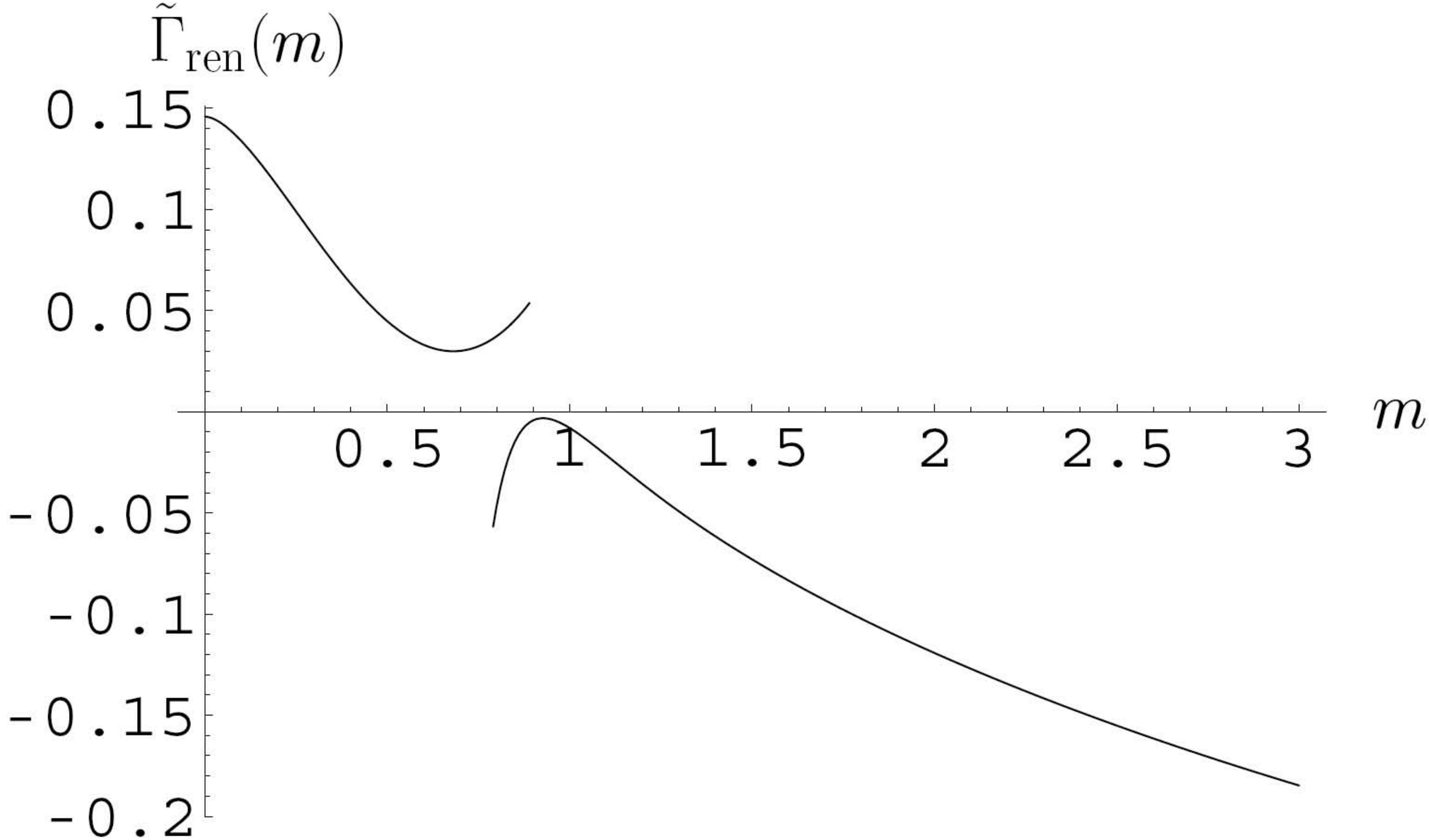
$$\Gamma^S_{\rm ren}(A;m) = \tilde{\Gamma}^S_{\rm ren}(m\rho) + \frac{1}{6}\ln(\mu\rho)$$

- **Small m** limit : exact massless Green's functions known
- **Large m** limit : from heat kernel expansion

$$\tilde{\Gamma}^S_{\rm ren}(m) \sim \begin{cases} \alpha\left(\frac{1}{2}\right) + \frac{1}{2}\left(\ln m + \gamma - \ln 2\right) m^2 + \dots \\ -\frac{\ln m}{6} - \frac{1}{75m^2} - \frac{17}{735m^4} + \frac{232}{2835m^6} - \frac{7916}{148225m^8} + \cdots \end{cases}$$

$$\alpha\left(\frac{1}{2}\right) = -\frac{5}{72} - 2\zeta'(-1) - \frac{1}{6}\ln 2 \simeq 0.145873\ldots$$

Instanton background



Question : how to connect large and small mass limits ?

Computing ODE determinants efficiently

Levit/Smilansky (1976) , Coleman (1977), …

Ordinary differential operator **eigenvalue problems** (i =1, 2):

$$\mathcal{M}_i\, \phi_i = \lambda_i\, \phi_i \qquad\qquad \phi_i(0) = 0 = \phi_i(L)$$

$$x \in [0, L]$$

Solve related **initial value problem** :

$$\mathcal{M}_i\, \phi_i = 0 \qquad\qquad \phi_i(0) = 0 \quad ; \quad \phi_i'(0) = 1$$

Theorem :

$$\boxed{det\left(\frac{\mathcal{M}_1}{\mathcal{M}_2}\right) = \frac{\phi_1(L)}{\phi_2(L)}}$$

- other b.c.'s
- zero modes
- systems of ODE's

Kirsten & McKane

Computing ODE determinants efficiently

Theorem :

$$\det\left(\frac{\mathcal{M}_1}{\mathcal{M}_2}\right) = \frac{\phi_1(L)}{\phi_2(L)}$$

$$\left(\mathcal{M}_i - k^2\right)\,\phi_i = 0 \qquad\qquad \phi_i(0) = 0 \quad ; \quad \phi_i'(0) = 1$$

proof 1 : $\det\left(\frac{\mathcal{M}_1 - k^2}{\mathcal{M}_2 - k^2}\right) = \frac{\phi_1(k^2, L)}{\phi_2(k^2, L)}$ same analytic structure in k^2

proof 2 : zeta function :

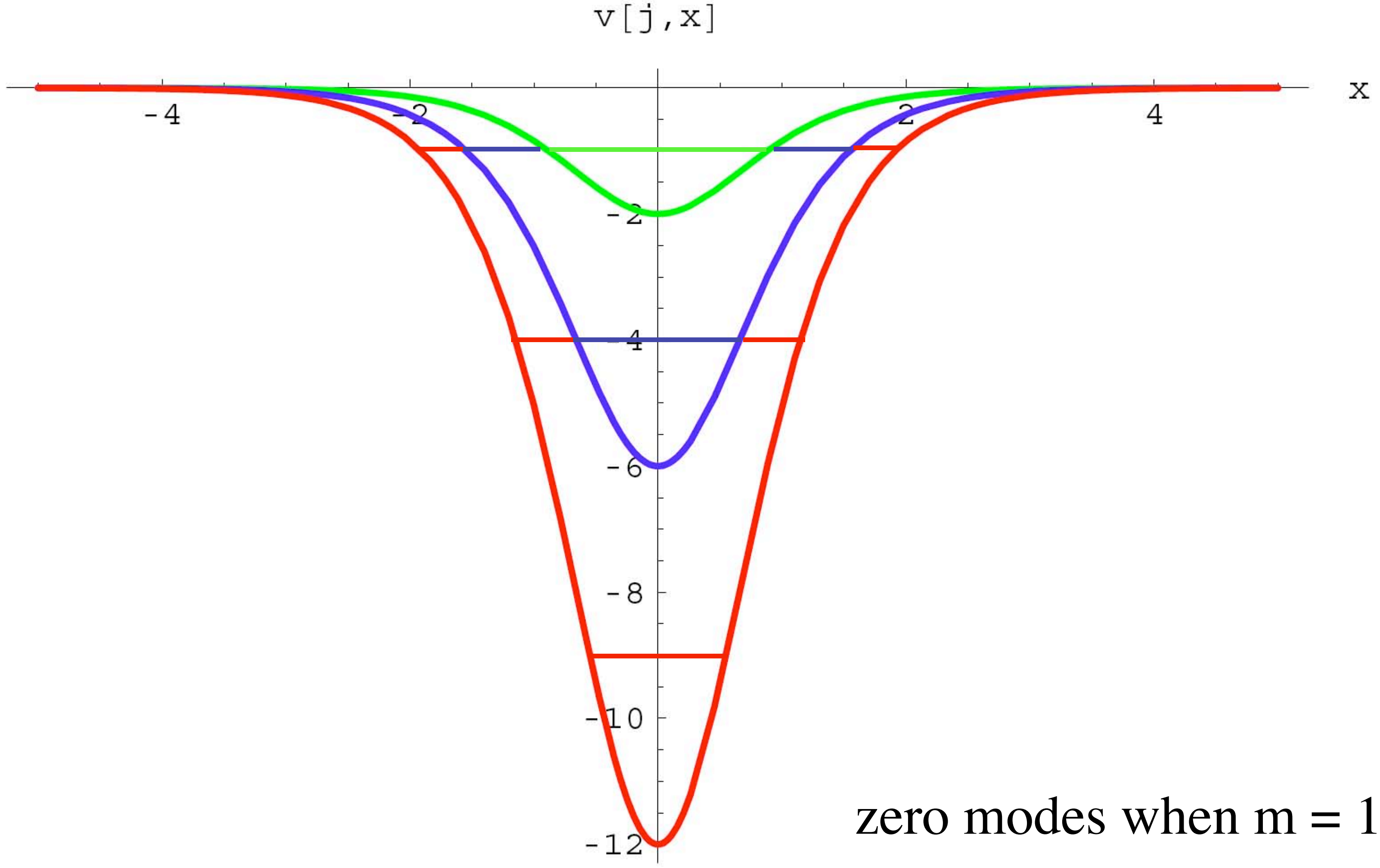
$$\zeta_{\mathcal{M}_1}(s) - \zeta_{\mathcal{M}_2}(s) = \frac{1}{2\pi i}\int_\gamma dk\, k^{-2s}\,\frac{d}{dk}\ln\frac{\phi_1(k^2, L)}{\phi_2(k^2, L)} \qquad \mathcal{R}e(s) > \frac{1}{2}$$

$$\zeta_{\mathcal{M}_1}(s) - \zeta_{\mathcal{M}_2}(s) = \frac{\sin(\pi s)}{\pi}\int_0^\infty dk\, k^{-2s}\,\frac{d}{dk}\ln\frac{\phi_1(-k^2, L)}{\phi_2(-k^2, L)} \qquad -\frac{1}{2} < \mathcal{R}e(s) < \frac{1}{2}$$

$$\Longrightarrow \quad \zeta'_{\mathcal{M}_1}(0) - \zeta'_{\mathcal{M}_2}(0) = -\ln\frac{\phi_1(0, L)}{\phi_2(0, L)}$$

Example : Poschl-Teller potentials

$$\mathcal{M}_1 = -\frac{d^2}{dx^2} + m^2 - j(j+1)\mathrm{sech}^2(x) \qquad \mathcal{M}_2 = -\frac{d^2}{dx^2} + m^2$$



j = 1

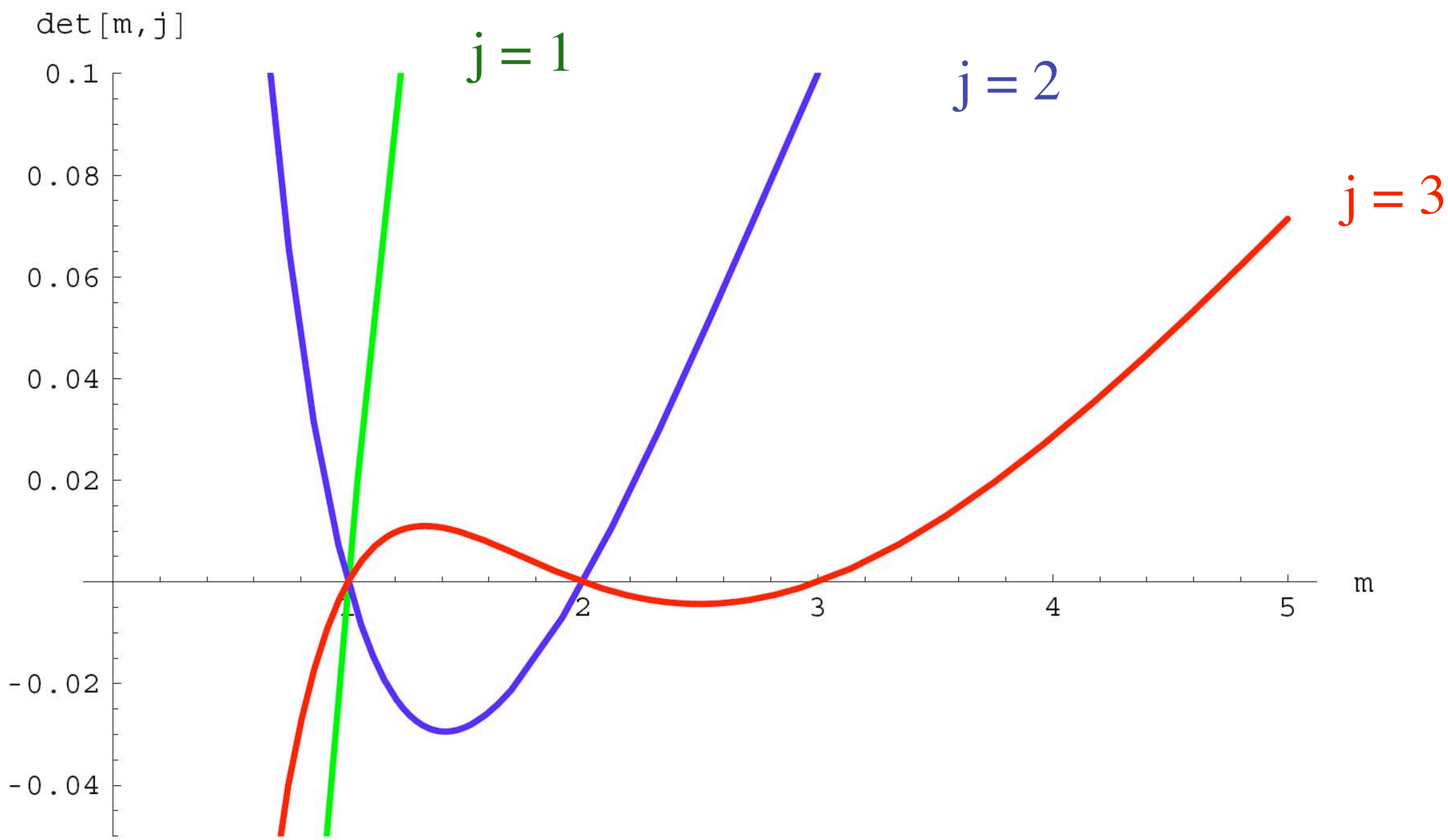
j = 2

j = 3

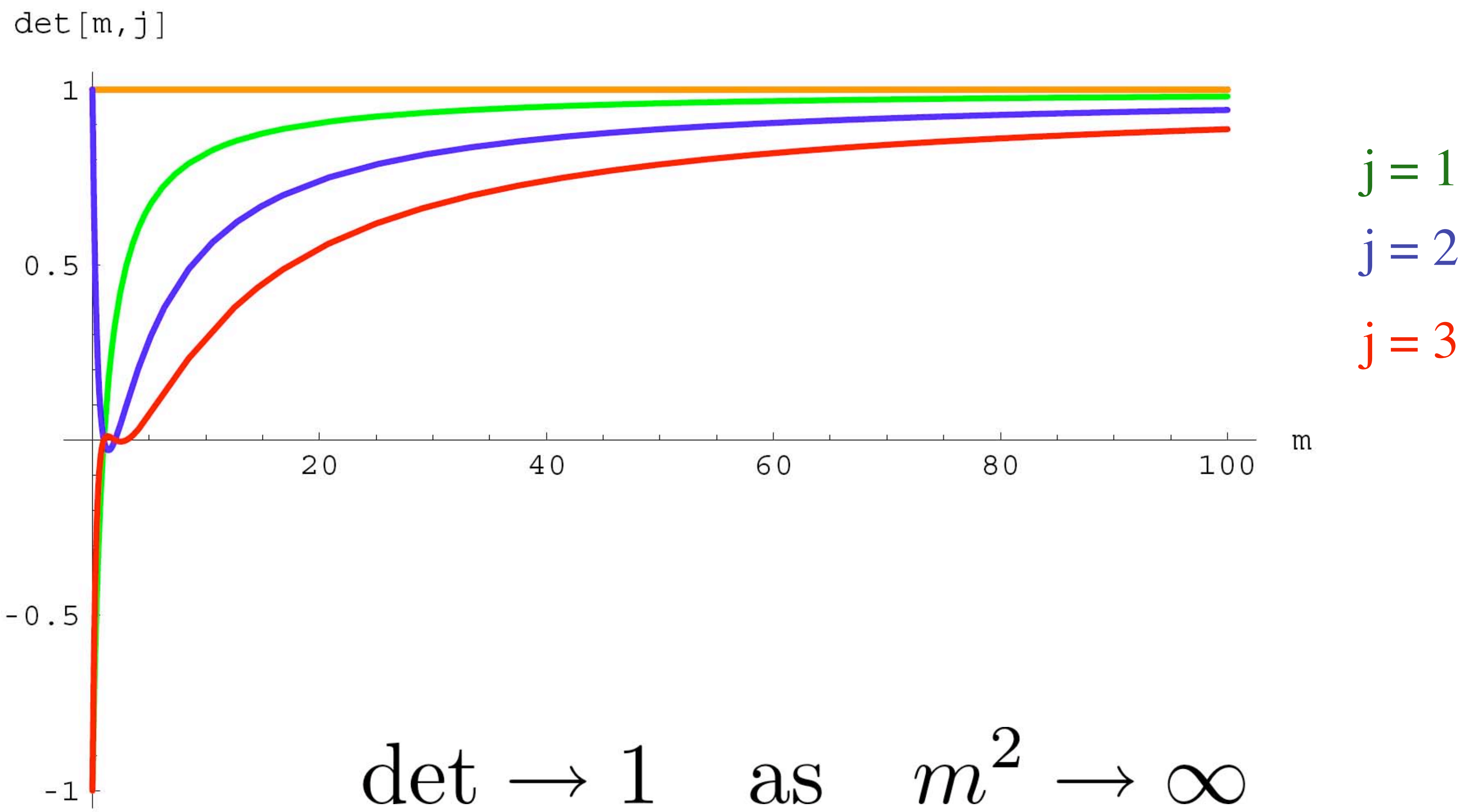
zero modes when m = 1, …, j

Example : Poschl-Teller potentials

analytically : $$\det\left(\frac{\mathcal{M}_1}{\mathcal{M}_2}\right) = \frac{\Gamma(m)\Gamma(m+1)}{\Gamma(m-j)\Gamma(m+j+1)}$$

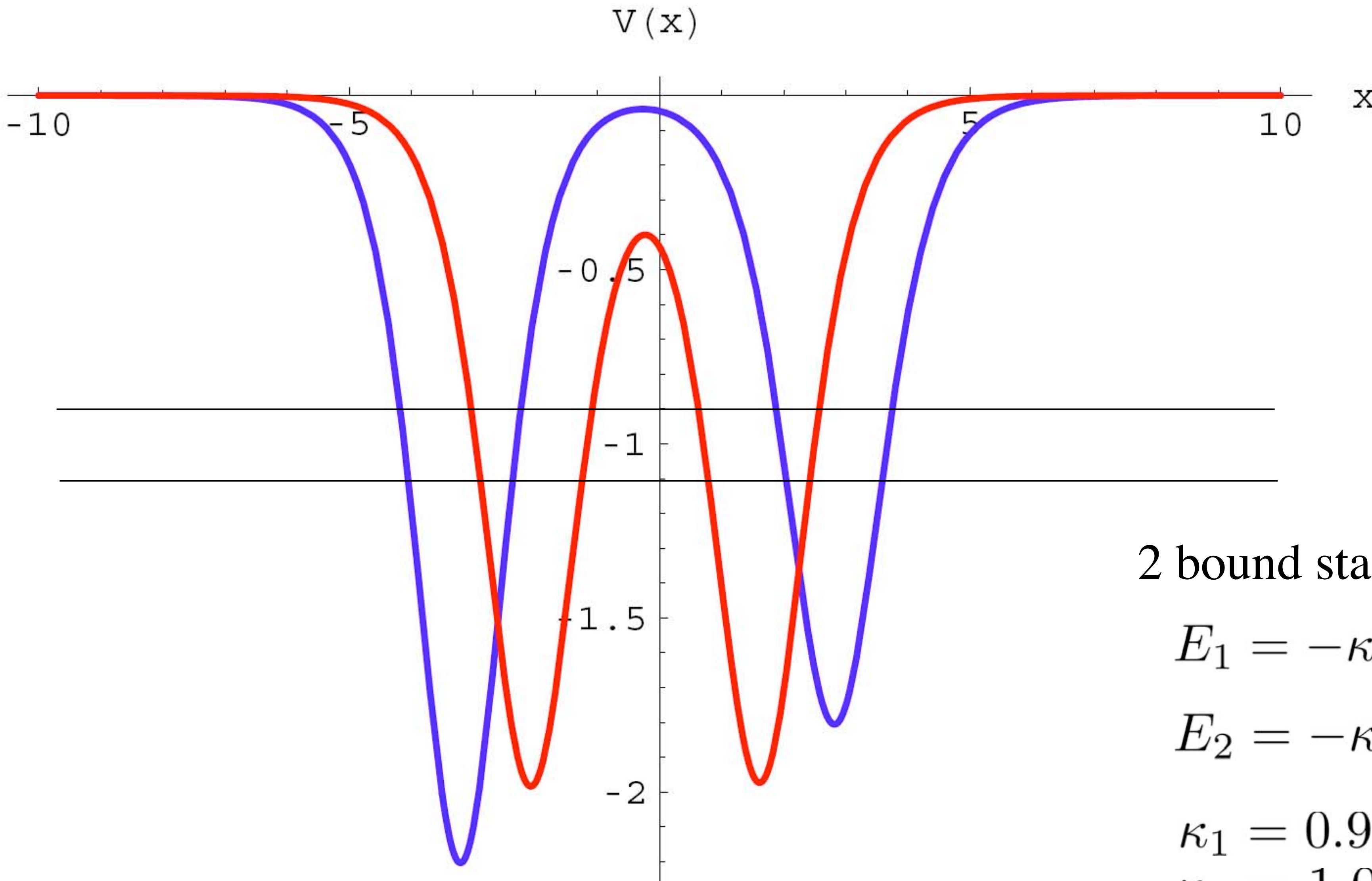


Example : Poschl-Teller potentials



$$\det \to 1 \quad \text{as} \quad m^2 \to \infty$$

Example : isospectral potentials



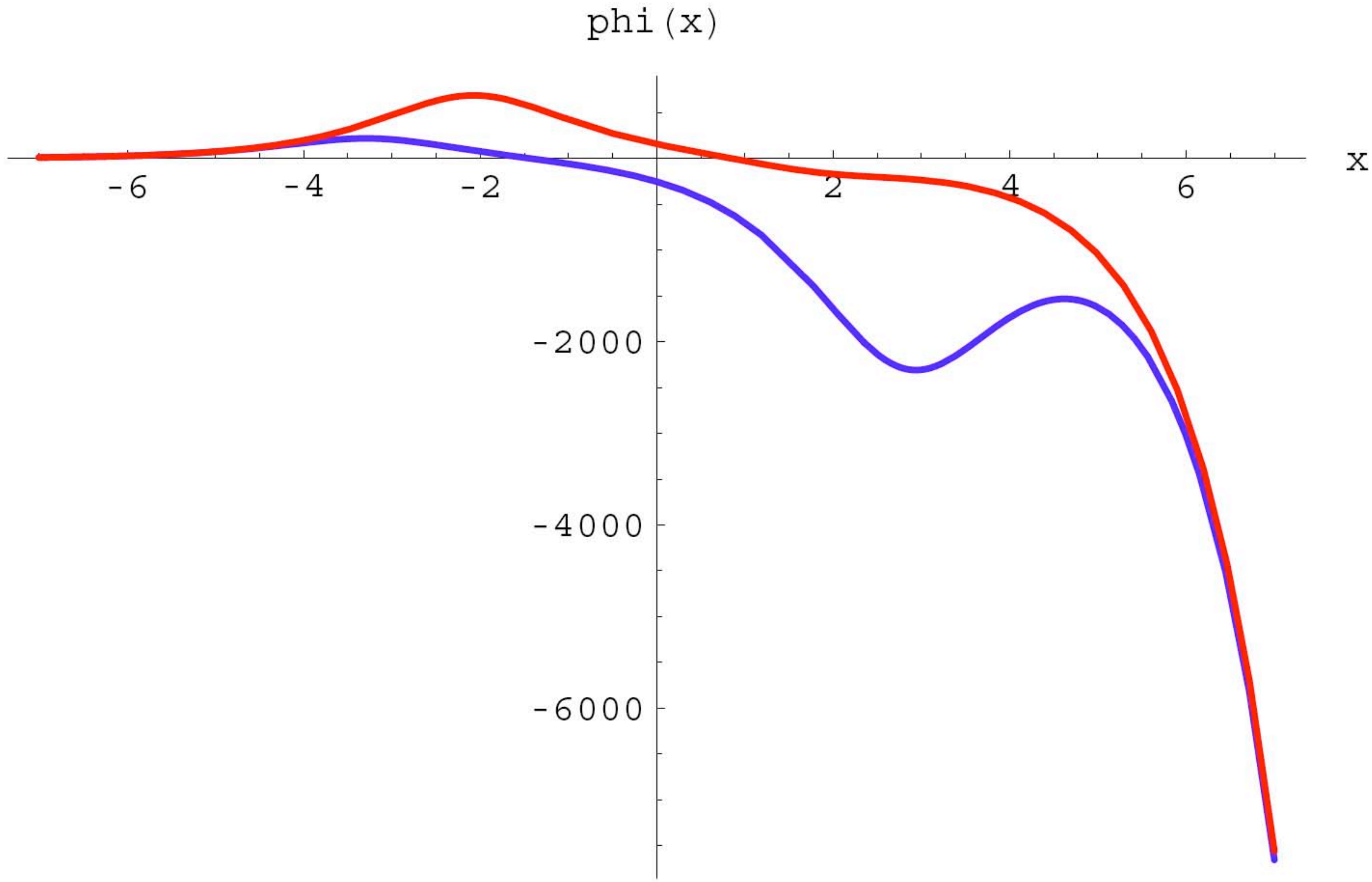
2 bound states

$$E_1 = -\kappa_1^2$$

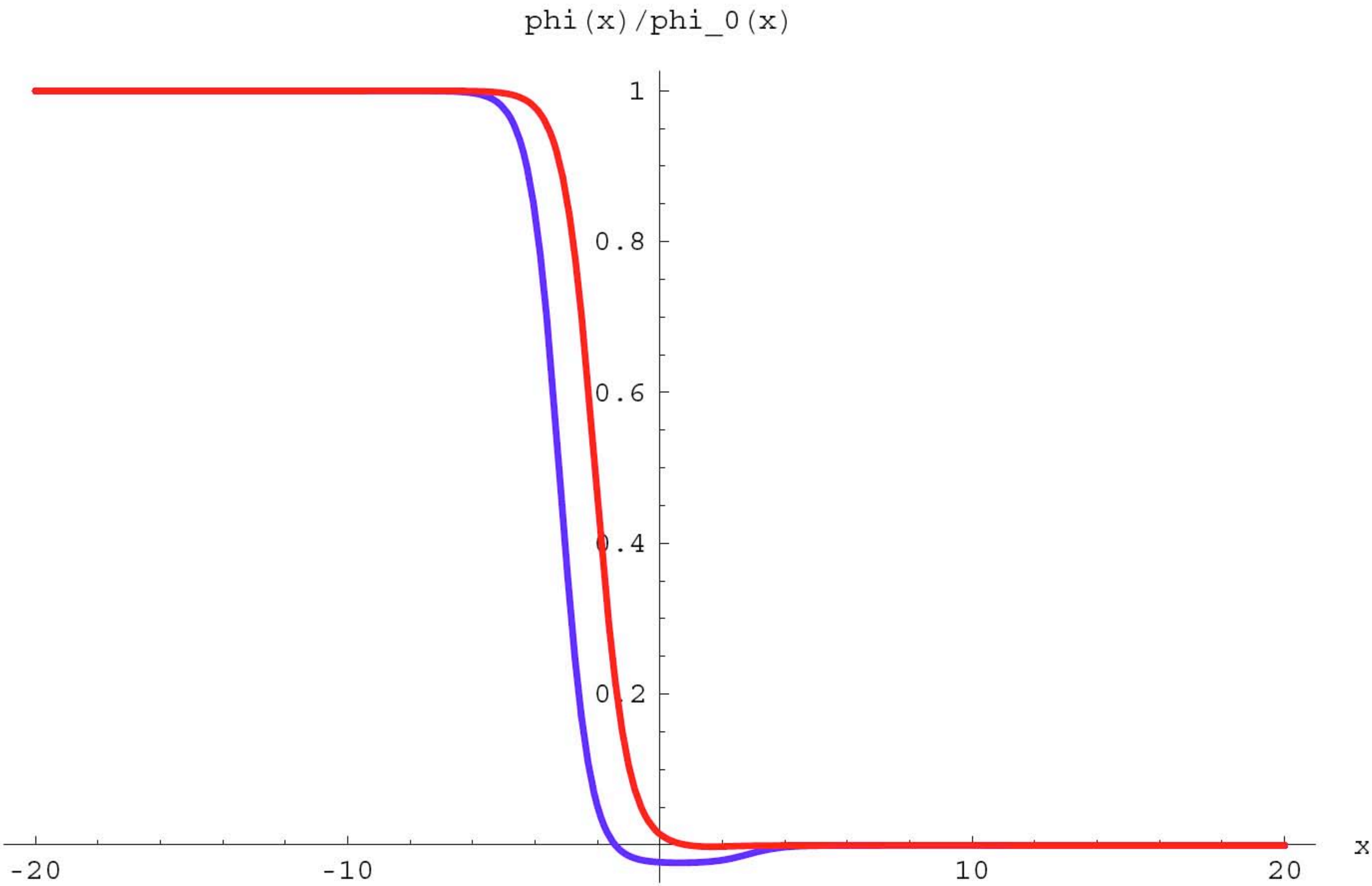
$$E_2 = -\kappa_2^2$$

$$\kappa_1 = 0.95$$
$$\kappa_2 = 1.05$$

Example : isospectral potentials



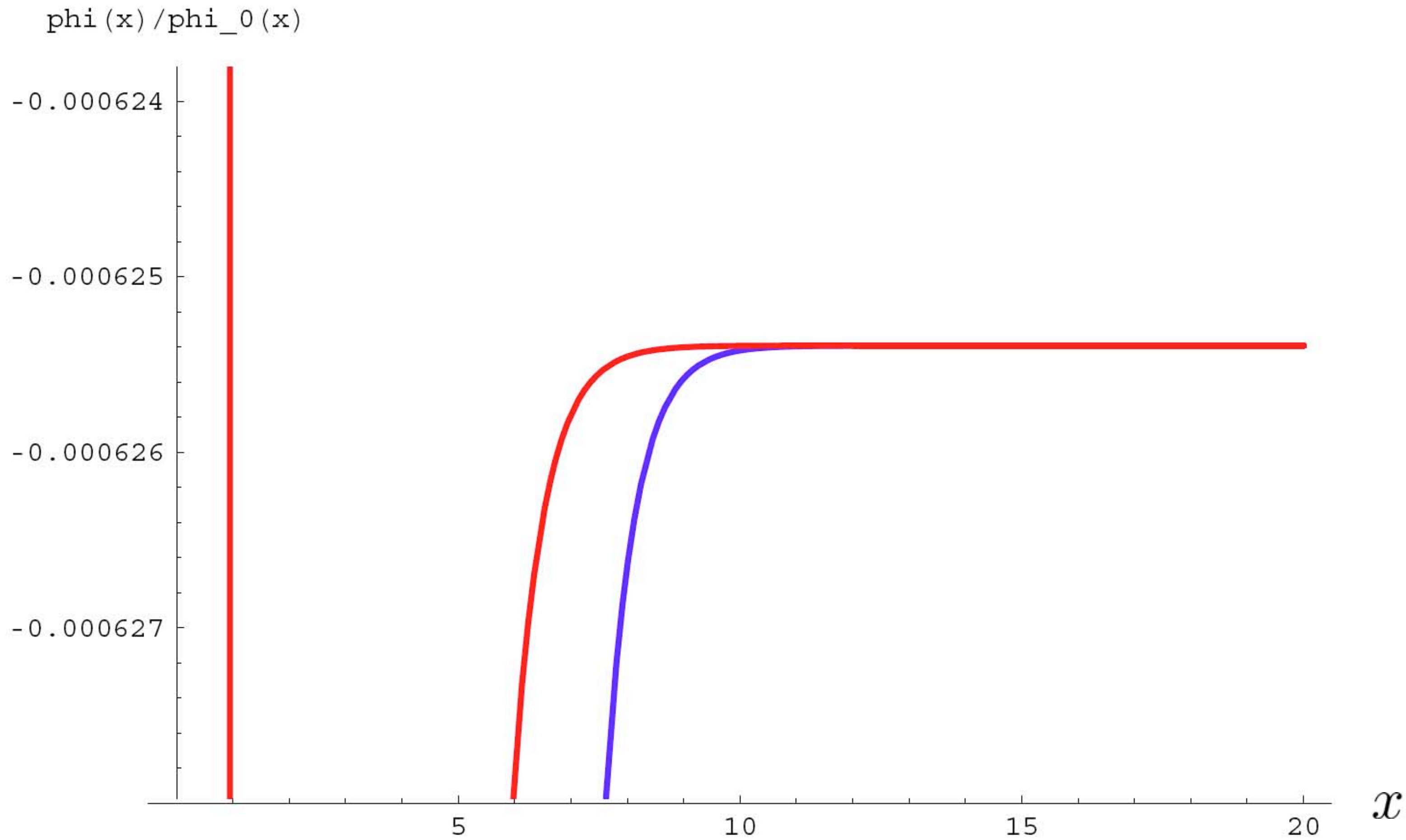
Example : isospectral potentials



Example : isospectral potentials

$$\det(\kappa_1, \kappa_2) = \exp\left\{-2\left(\operatorname{arctanh}(1/\kappa_1) + \operatorname{arctanh}(1/\kappa_2)\right)\right\}$$

$$\det(0.95, 1.05) = -0.000625391$$



Instanton background in QCD

scalar (Klein-Gordon) determinant in an instanton background :

$$\Gamma^S(A;m) = \ln\left[\frac{\mathrm{Det}(-D^2+m^2)}{\mathrm{Det}(-\partial^2+m^2)}\right]$$

now involves **partial** differential operators

radial symmetry reduces problem to a sum over ODEs

Radial symmetry in 4 dim.

Free Klein-Gordon operator :

$$-\partial^2 \to \mathcal{H}^{\rm free}_{(l)} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2}\right]$$

$$l = 0,\ \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ \cdots$$

Instanton Klein-Gordon operator :

$$j = |\, l \pm \tfrac{1}{2}\, |$$

$$-D^2 \to \mathcal{H}_{(l,j)} \equiv \left[-\frac{\partial^2}{\partial r^2} - \frac{3}{r}\frac{\partial}{\partial r} + \frac{4l(l+1)}{r^2} + \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}\right]$$

"angular momenta" : $L_a = -\frac{i}{2}\eta_{\mu\nu a} x_\mu \partial_\nu$ $\qquad J^a = L^a + T^a$

degeneracy : $\quad d_{(l,j)} = (2l+1)(2j+1)$

$$\Gamma = \sum_{l=0,\frac{1}{2},\ldots} d_l \left\{ \ln\det\left(\frac{\mathcal{H}_{(l,l+\frac{1}{2})} + m^2}{\mathcal{H}^{\rm free}_{(l)} + m^2}\right) + \ln\det\left(\frac{\mathcal{H}_{(l+\frac{1}{2},l)} + m^2}{\mathcal{H}^{\rm free}_{(l+\frac{1}{2})} + m^2}\right)\right\}$$

sum of radial (ODE) log determinants $\qquad d_l = (2l+1)(2l+2)$

Two numerical improvements

1. Evaluate **log det of ratio** directly :

$$\mathcal{S}_{(l,j)}(r) = \ln\left(\frac{\psi_{(l,j)}(r)}{\psi_{(l)}^{\text{free}}(r)}\right)$$

$$\boxed{\frac{d^2 S_{(l,j)}}{dr^2} + \left(\frac{dS_{(l,j)}}{dr}\right)^2 + \left(\frac{1}{r} + 2m\frac{I'_{2l+1}(mr)}{I_{2l+1}(mr)}\right)\frac{dS_{(l,j)}}{dr} = U_{(l,j)}(r)}$$

potential : $$U_{(l,j)}(r) = \frac{4(j-l)(j+l+1)}{r^2+1} - \frac{3}{(r^2+1)^2}$$

initial values : $$S_{(l,j)}(r=0) = 0 \quad , \quad S'_{(l,j)}(r=0) = 0$$

exact, but more stable numerically

Two numerical improvements

2. Expand about **approximate** solutions :

$$\frac{d^2 S_{(l,j)}}{dr^2} + \left(\frac{dS_{(l,j)}}{dr}\right)^2 + \left(\frac{1}{r} + 2m\frac{I'_{2l+1}(mr)}{I_{2l+1}(mr)}\right)\frac{dS_{(l,j)}}{dr} = U_{(l,j)}(r)$$

small

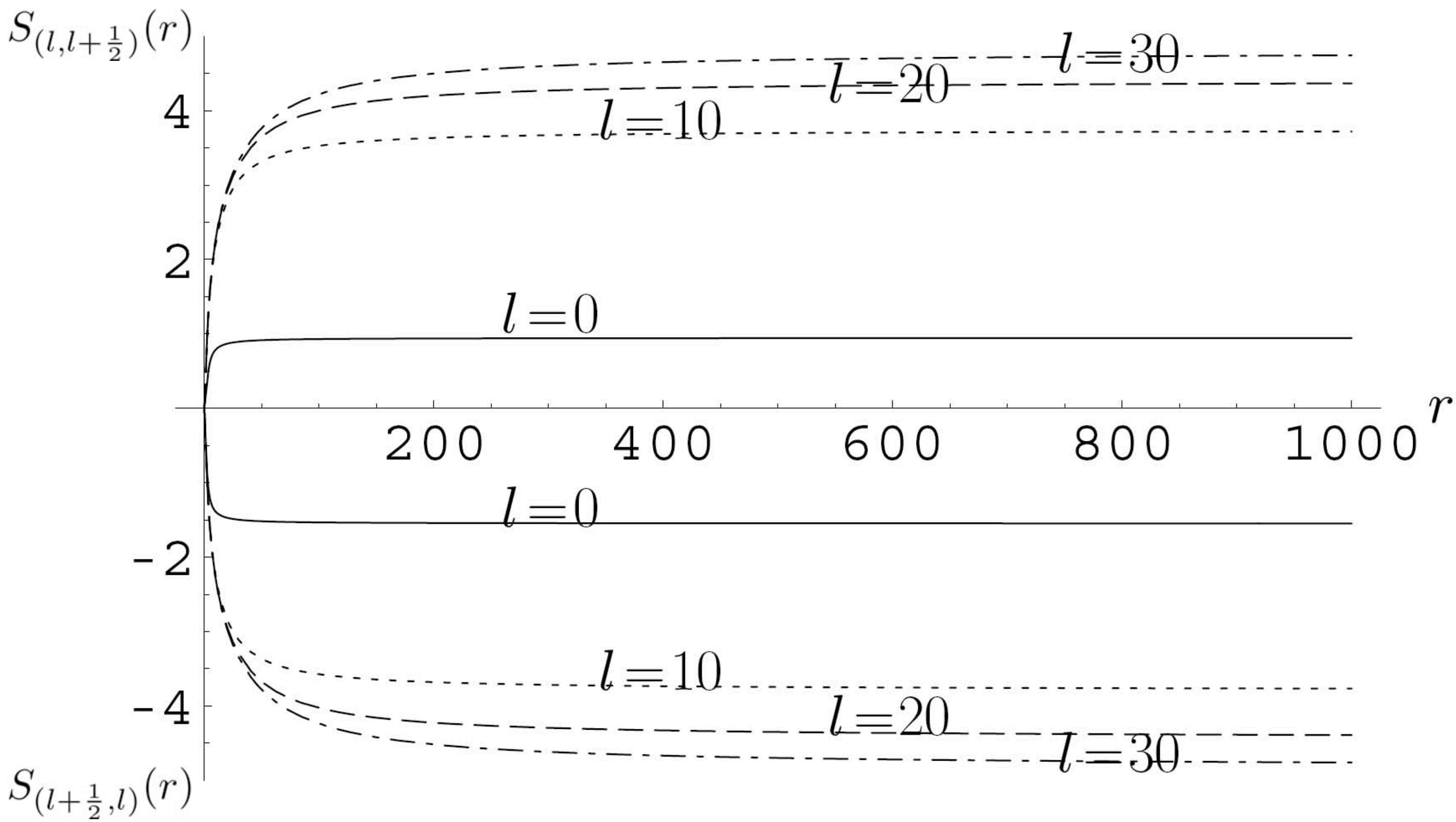
$$S_{(l,j)}(r) = \int_0^r dr' \left(\frac{U_{(l,j)}(r')}{W_l(r')}\right) + T_{(l,j)}(r) \qquad W_l(r) = \frac{1}{r} + 2m\frac{I'_{2l+1}(mr)}{I_{2l+1}(mr)}$$

$$\frac{d^2 T_{(l,j)}}{dr^2} + \left(\frac{dT_{(l,j)}}{dr}\right)^2 + \left(W_l(r) + 2\frac{U_{(l,j)}(r)}{W_l(r)}\right)\frac{dT_{(l,j)}}{dr} = -\left(\frac{U_{(l,j)}(r)}{W_l(r)}\right)^2 - \frac{d\left(\frac{U_{(l,j)}(r)}{W_l(r)}\right)}{dr}$$

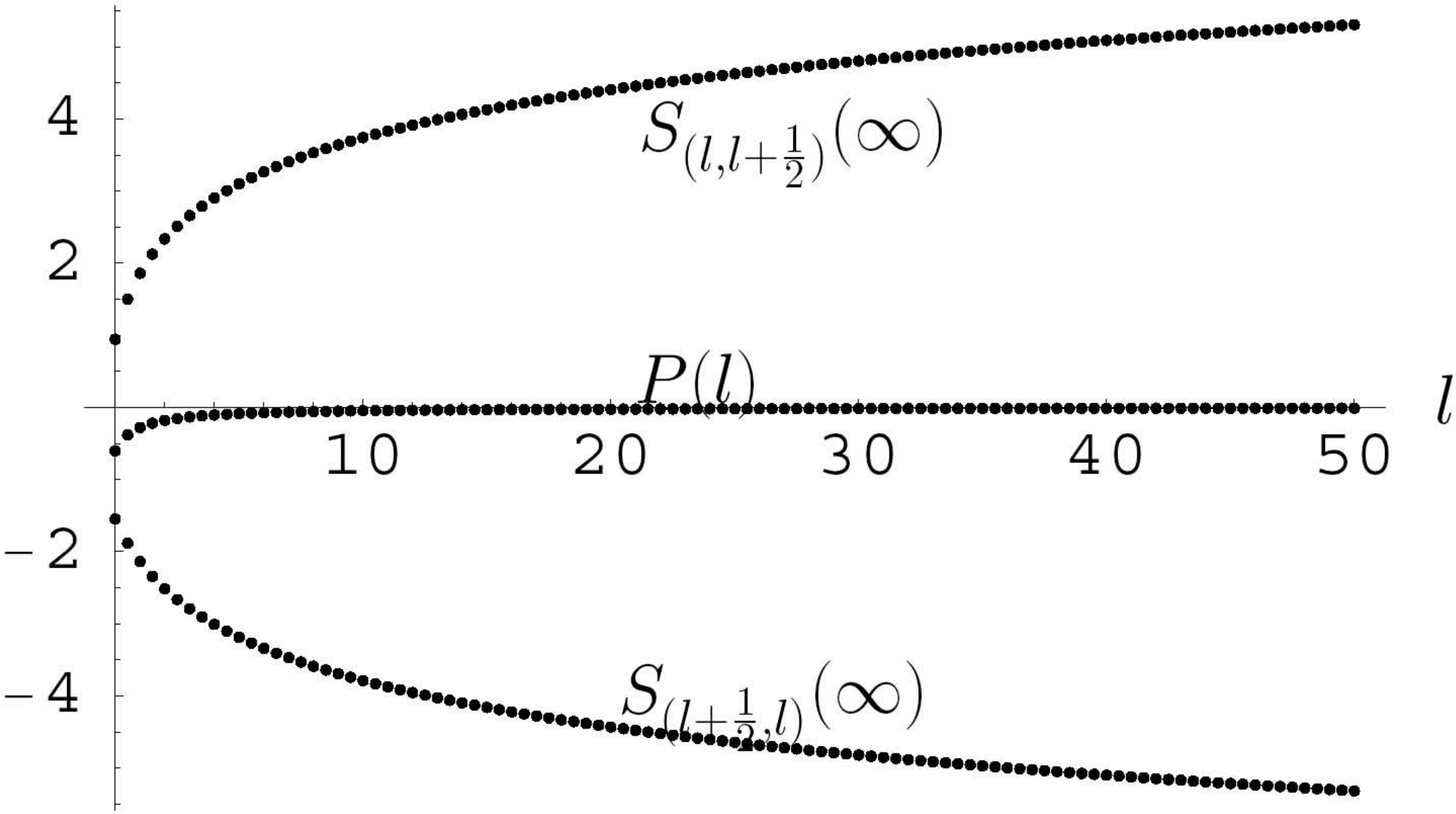
exact, but more stable numerically

Radial integration results

$$\Gamma^S(A;m) = \sum_{l=0,\frac{1}{2},\ldots} d_l \left\{ S_{(l,l+\frac{1}{2})}(r=\infty) + S_{(l+\frac{1}{2},l)}(r=\infty) \right\}$$

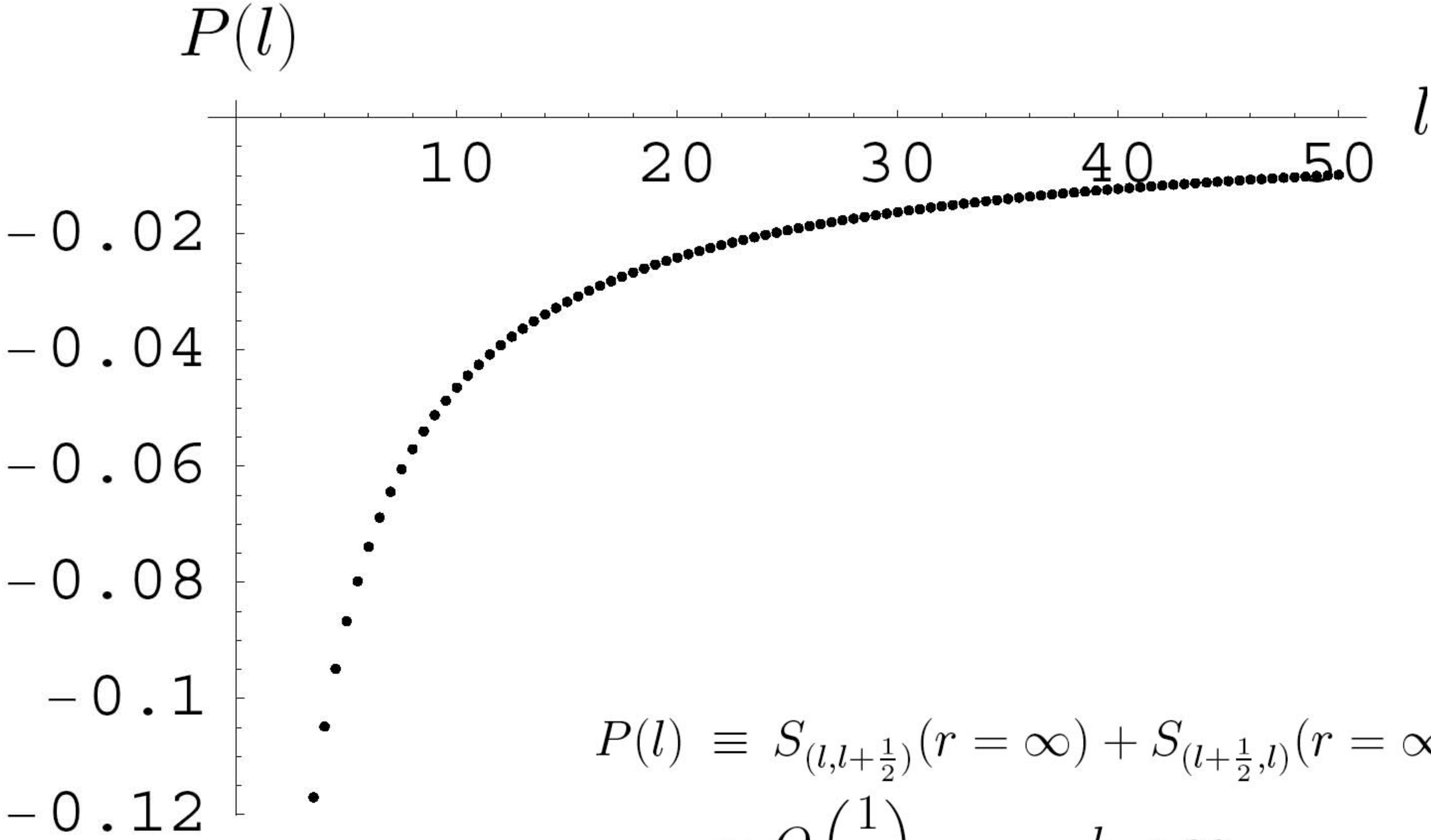


l dependence of log det



$$P(l) \equiv S_{(l,l+\frac{1}{2})}(r=\infty) + S_{(l+\frac{1}{2},l)}(r=\infty)$$

l dependence of log det



$$P(l) \equiv S_{(l,l+\frac{1}{2})}(r=\infty) + S_{(l+\frac{1}{2},l)}(r=\infty)$$

$$\sim O\left(\frac{1}{l}\right) \quad , \quad l \to \infty$$

“Bad” news !

$$\Gamma = \sum_{l=0,\frac{1}{2},1,\ldots} (2l+1)(2l+2)P(l)$$

quadratically divergent sum !!!

BUT : bare expression, without regularization or renormalization

Regularization and renormalization

Regularization : Pauli-Villars regulator mass Λ

$$\Gamma^S_\Lambda(A;m) = \ln\left[\frac{\mathrm{Det}(-D^2+m^2)}{\mathrm{Det}(-\partial^2+m^2)}\frac{\mathrm{Det}(-\partial^2+\Lambda^2)}{\mathrm{Det}(-D^2+\Lambda^2)}\right]$$

Renormalization : Minimal subtraction renormalization condition

$$\Gamma^S_{\mathrm{ren}}(A;m) = \lim_{\Lambda\to\infty}\left[\Gamma^S_\Lambda(A;m) - \frac{1}{12}\frac{1}{(4\pi)^2}\ln\left(\frac{\Lambda^2}{\mu^2}\right)\int d^4x\ \mathrm{tr}(F_{\mu\nu}F_{\mu\nu})\right]$$

$$= \lim_{\Lambda\to\infty}\left[\Gamma^S_\Lambda(A;m) - \frac{1}{6}\ln\left(\frac{\Lambda}{\mu}\right)\right]$$

Regularization and renormalization

$$\Gamma_\Lambda = \sum_{l=0,\frac{1}{2},\ldots} (2l+1)(2l+2)\left\{\ln\det\left(\frac{\mathcal{H}_{(l,l+\frac{1}{2})}+m^2}{\mathcal{H}^{\text{free}}_{(l)}+m^2}\right)+\ln\det\left(\frac{\mathcal{H}_{(l+\frac{1}{2},l)}+m^2}{\mathcal{H}^{\text{free}}_{(l+\frac{1}{2})}+m^2}\right)\right.$$

$$\left.-\ln\det\left(\frac{\mathcal{H}_{(l,l+\frac{1}{2})}+\Lambda^2}{\mathcal{H}^{\text{free}}_{(l)}+\Lambda^2}\right)-\ln\det\left(\frac{\mathcal{H}_{(l+\frac{1}{2},l)}+\Lambda^2}{\mathcal{H}^{\text{free}}_{(l+\frac{1}{2})}+\Lambda^2}\right)\right\}$$

problem : large l and large Λ limits ?

solution : split sum into 2 parts, with L large but finite

$$\Gamma^S_\Lambda(A;m) = \sum_{l=0,\frac{1}{2},\ldots}^{L} \Gamma^S_{(l)}(A;m) + \sum_{l=L+\frac{1}{2}}^{\infty} \Gamma^S_{\Lambda,(l)}(A;m)$$

evaluate **numerically**, for large L

evaluate **analytically**, for large L

Large L behavior from WKB

analytic WKB (large l) computation :

$$\sum_{l=L+\frac{1}{2}}^{\infty} \Gamma^S_{\Lambda,(l)}(A;m) \sim \frac{1}{6}\ln\Lambda + 2L^2 + 4L - \left(\frac{1}{6}+\frac{m^2}{2}\right)\ln L$$

$$+\left[\frac{127}{72} - \frac{1}{3}\ln 2 + \frac{m^2}{2} - m^2\ln 2 + \frac{m^2}{2}\ln m\right] + O\left(\frac{1}{L}\right)$$

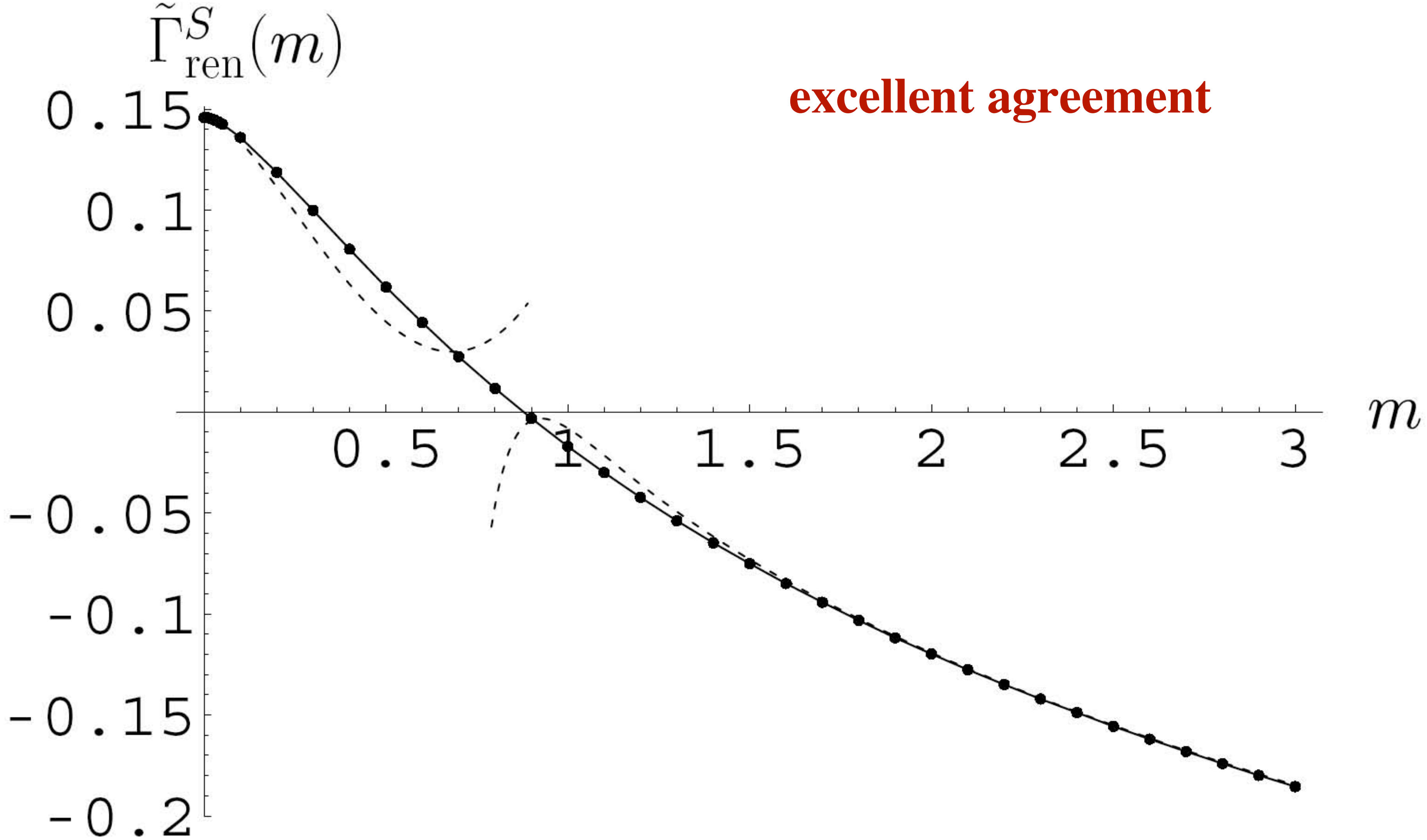
2nd order WKB (higher orders don't contribute in large L limit)

NOTE :

- $\ln\Lambda$ term exactly as required for renormalization
- quadratic, linear and log divergences, and finite part
- exactly cancel divergences from numerical sum in large L limit !!!
- note mass dependence in "subtraction" terms

Comparison with asymptotic results

excellent agreement



mid-way conclusions

- ODE determinant method extends to radial problems, and is very easy to implement numerically
- naively leads to divergent sum over angular momentum l
- **regularization** and **renormalization** solve this problem
- split sum over l into **numerical** small l part and analytic **WKB** large l piece

Continued in Part II by Hyunsoo Min …