Energy levels of finite–volume two–particle scattering states with Bloch's boundary conditions

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outline

- Bloch's boundary conditions & external fields (twisted boundary conditions)
  - the "gauge crystal"
  - continuous physical momenta on a finite volume
- two–particle scattering states
- Lellouch–Lüscher formula
- two–particle scattering states with Bloch's b.c.
- isospin breaking
- two state non–relativistic model

external fields & Bloch's boundary conditions

Bloch's boundary conditions (b.b.c.) are defined as

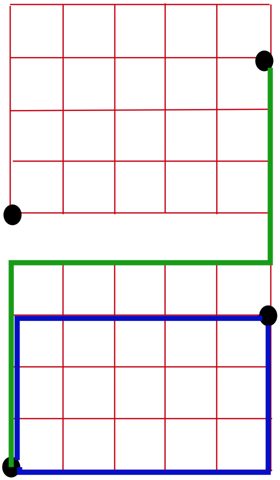
$$\psi(x + \mathbf{e}_i L) = e^{i\theta_i}\psi(x), \qquad 0 \leq \theta_i < 2\pi \qquad \theta_0 = 0$$

in a gauge theory this is equivalent to "change" the gauge field

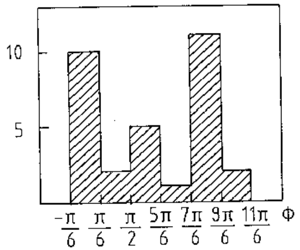
to the interaction it has been added an external filed

$$\nabla_\mu(\theta)\psi(x) = \frac{1}{a}\left[\lambda_\mu\, U_\mu(x)\psi(x + a\,\hat{\mu}) - \psi(x)\right] \qquad \lambda_\mu = e^{\frac{ia\theta_\mu}{L}}$$

In order to reduce finite volume effects in early days lattice simulations, Martinelli, Parisi, Petronzio, Rapuano (1983) first considered a “gauge crystal”



- very very small lattices ($5^3 \times 10$)
- strong fluctuations in the meson masses
- freezing of the gauge configurations in some metastable states



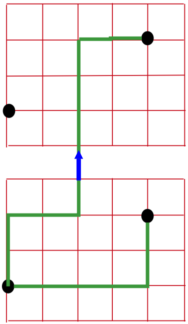
$\hat{P}_i = \langle \sum_x \mathrm{Tr} \prod_{n=0}^{N_i-1} U(x + n\mathbf{e}_i, i) \rangle$

the gauge crystal (ii)

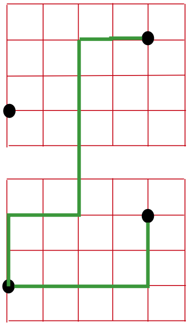
each gauge configuration is used 3×3 times by transforming the boundary gauge links

$$U(N_i - 1, i) \longmapsto \left\{ U(N_i - 1, i),\ e^{\frac{2\pi i}{3}} U(N_i - 1, i),\ e^{-\frac{2\pi i}{3}} U(N_i - 1, i) \right\}$$

$\sum$



$$= \left(1 + e^{\frac{2\pi i}{3}} + e^{-\frac{2\pi i}{3}}\right)$$



$$= 0$$

$$\int_0^{3L} dx\, \overline{\psi}(x)\hat{D}(x)\psi(x) \overset{D(x+L)=D(x)}{\longmapsto} \int_0^{L} dx \left[\overline{\psi}(x)\hat{D}(x)\psi(x) + \overline{\psi}(x)\hat{D}(x)\psi(x) + \overline{\psi}(x)\hat{D}(x)\psi(x)\right]$$

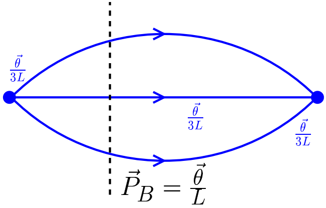
Bloch's boundary conditions, a brief history

- in the large N limit: [Gross & Kitazawa Nucl. Phys. B206 (1982)] [Kiskis, Narayanan & Neuberger hep-lat/0203005] [Kiskis, Narayanan & Neuberger hep-lat/0308033]

- at finite temperature: [Roberge & Weiss Nucl. Phys. B275 (1986)] [many others]

- in the Schrödinger Functional: [Jansen & al. hep-lat/9512009] [many others] [Bucarelli & al. hep-lat/9808005] [Guagnelli & al. hep-lat/0303012]

- Aharonov–Bohm effect (χ–PT, suggesting lattice) [Bedaque nucl-th/0402051]



flavoured mesons with continuous momenta

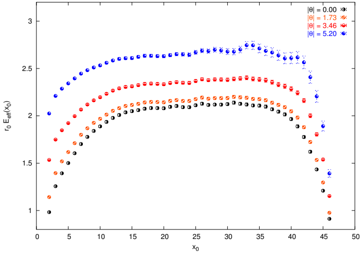
In [hep-lat/0405002] we coupled the external field to the flavour

spatial momenta are quantized according to

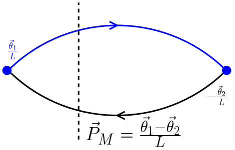
$$\int d\mathbf{p}\; e^{i\mathbf{p}\cdot(\mathbf{x}+\mathbf{e}_i L)}\psi(t;\mathbf{p}) = \int d\mathbf{p}\; e^{i(\mathbf{p}\cdot\mathbf{x}+\theta_i)}\psi(t;\mathbf{p})$$

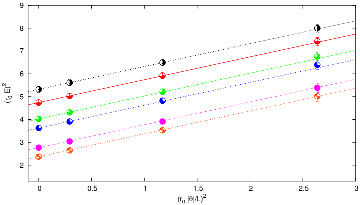
$$e^{ip_i L} = e^{i\theta_i}$$

$$p_i = \frac{\theta_i}{L} + \frac{2\pi n}{L}, \quad n \in Z^3$$



a physical momentum transfer





two–particle scattering states

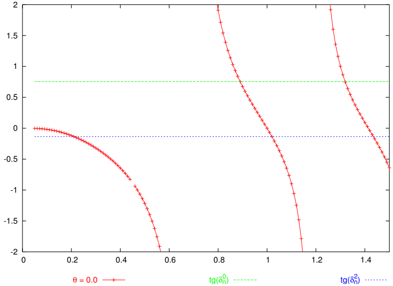
- for p.b.c. Lüscher has derived the quantization condition

Commun. Math. Phys. 104 (1986) 177
Commun. Math. Phys. 105 (1986) 153
Nucl. Phys. B354 (1991) 531
Nucl. Phys. B364 (1991) 237

$$\tan\delta_0(k) = -\tan\phi(q),$$

$$q = \frac{kL}{2\pi}, \qquad \tan\phi(q) = -\frac{q\pi^{3/2}}{\mathcal{Z}_{00}(1,q^2)},$$

$$\mathcal{Z}_{00}(s,q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\mathbf{n}\in Z^3} \frac{1}{(\mathbf{n}^2 - q^2)^s}, \qquad \Re(s) > \frac{3}{2}$$

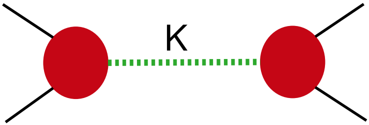


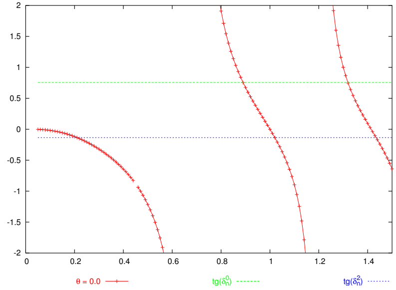
- scattering phases can be calculated “like” hadron masses
- an integral representation of the $\mathcal{Z}_{00}(1,q^2)$ is obtained by ζ–function regularization

$$\mathcal{Z}_{lm}(1,q^2) = \frac{1}{\sqrt{4\pi}} \sum_{|\mathbf{n}|<\Lambda} \frac{\mathcal{Y}_{lm}(\mathbf{n})}{\mathbf{n}^2 - q^2} + (2\pi)^3 \int_0^\infty dt \left[e^{tq^2} \mathcal{K}^{\Lambda}_{lm}(t,\mathbf{0}) - \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2 t^{3/2}} \right]$$

lellouch–lüscher formula

- let us introduce into our theory another boson: the "kaon"
- let us switch off the interaction hamiltonian $H_W = \int_{x_0=0} d^3x\ \mathcal{L}_W(x)$





- when the energy of the scattering state is equal to the kaon mass ($L \simeq 5.5fm$) one gets

$$\left\|A(\bar{k})\right\|^2 = 8\pi \left\{ q\frac{\partial\phi(q)}{\partial q} + k\frac{\partial\delta_0(k)}{\partial k} \right\}_{k=\bar{k}} \left(\frac{m_K}{\bar{k}}\right)^3 \left\|A_L(\bar{k})\right\|^2$$

- there have been many attempts to cope with such a large volume

Lin & al. hep-lat/0104006
Christ & Kim hep-lat/0210003
Kim, Sachrajda & Sharpe hep-lat/0507006
Christ, Kim & Yamazaki hep-lat/0507009

lüscher equivalence theorem (i)

Let us consider two spinless bosons of equal mass such that

- the dynamics can be described by a scalar $\lambda\phi^4$ theory
- reflection symmetry ($\phi \mapsto -\phi$) is unbroken
- one particle states are odd under this symmetry

it holds an effective Schrödinger equation

$$-\frac{1}{2\mu}\triangle\psi(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}'\; U_E(\mathbf{r},\mathbf{r}')\,\psi(\mathbf{r}') = E\psi(\mathbf{r})$$

where

$\psi(\mathbf{r})$ is the Bethe–Salpeter wavefunction

the true energy is $\mathcal{E} = 2\sqrt{m^2 + mE}$

$U_E(\mathbf{r},\mathbf{r}')$ is exponentially vanishing with $\mathbf{r}$,$\mathbf{r}'$

lüscher equivalence theorem (ii)

the system is equivalent to a non–relativistic quantum mechanical one up to corrections exponentially vanishing with the volume

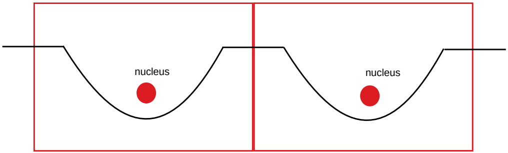
- the hamiltonian is $\hat{H} = -\triangle + V(r)$
- the potential is of finite range $V(r > R) = 0$
- the potential is periodic $V(\|\mathbf{r} + \mathbf{n}L\|) = V(r)$

$$\left(\triangle + k^2\right)\psi_\theta(\mathbf{r}) = V(\mathbf{r})\psi_\theta(\mathbf{r}), \qquad \psi_\theta(\mathbf{r} + \mathbf{n}L) = e^{i\theta\cdot\mathbf{n}}\psi_\theta(\mathbf{r})$$

note:

Schrödinger equation with a muffin thin potential:

Korringa–Kohn–Rostoker theory



the green function method

let us consider the infinite volume green function

$$\left(\triangle + k^2\right) g(\mathbf{r} - \mathbf{r}_0; k^2) = \delta(\mathbf{r} - \mathbf{r}_0)$$

the formal solution is given by

$$\begin{aligned}
\psi_\theta(\mathbf{r}) &= \int_{-\infty}^{\infty} d\mathbf{r}_0 \; g(\mathbf{r} - \mathbf{r}_0; k^2) V(\mathbf{r}_0) \psi_\theta(\mathbf{r}_0) \\
&= \int_0^L d\mathbf{r}_0 \; g_\theta(\mathbf{r} - \mathbf{r}_0; k^2) V(\mathbf{r}_0) \psi_\theta(\mathbf{r}_0) \\
&= \int_0^R d\mathbf{r}_0 \; g_\theta(\mathbf{r} - \mathbf{r}_0; k^2) V(\mathbf{r}_0) \psi_\theta(\mathbf{r}_0)
\end{aligned}$$

the greenian is given by

$$\begin{aligned}
g_\theta(\mathbf{r}; k^2) &= \sum_{\mathbf{n} \in Z^3} e^{i\theta \cdot \mathbf{n}} g(\mathbf{r} - \mathbf{n}L; k^2) \\
&= -\frac{1}{L^3} \sum_{\mathbf{n} \in Z^3} \frac{e^{i\mathbf{k}_n \cdot \mathbf{r}}}{k_n^2 - k^2} \\
\mathbf{k}_n &= \frac{2\pi \mathbf{n}}{L} + \frac{\theta}{L}
\end{aligned}$$

in the end we get

$$\psi_\theta(\mathbf{r}) = \int_0^R d\mathbf{r}_0 \; g_\theta(\mathbf{r} - \mathbf{r}_0; k^2)(\triangle_{\mathbf{r}_0} + k^2)\psi_\theta(\mathbf{r}_0)$$

quantization condition (i)

from $$\psi_\theta(\mathbf{r}) = \int_0^R d\mathbf{r}_0 \, g_\theta(\mathbf{r}-\mathbf{r}_0; k^2)(\triangle_{\mathbf{r}_0} + k^2)\psi_\theta(\mathbf{r}_0)$$

by using the simple identity $$g\triangle\psi = \psi\triangle g + \nabla\cdot(g\nabla\psi - \psi\nabla g)$$

one gets the energy quantization condition

$$\int_{\partial S_R} dS_0 \left[g_\theta(\mathbf{r}-\mathbf{r}_0; k^2)\frac{\partial\psi_\theta(\mathbf{r}_0)}{\partial r_0} - \psi_\theta(\mathbf{r}_0)\frac{\partial g_\theta(\mathbf{r}-\mathbf{r}_0; k^2)}{\partial r_0}\right]_{r_0=R} = 0$$

This condition can be rewritten by expanding in spherical harmonics the wavefunction

$$\psi_\theta(\mathbf{r}) = \sum_{lm} \alpha_{lm}(\theta,k) R_l(r;k) Y_{lm}(\hat{r}_0) \qquad R_l(r,k) = \cos\delta_l(k)\, j_l(kr) - \sin\delta_l(k)\, n_l(kr) \qquad r \geq R$$

and the greenian

$$\begin{aligned} g_\theta(\mathbf{r}-\mathbf{r}_0; k^2) &= k\sum_{lm} j_l(kr)\; Y_{lm}(\hat{r}) n_l(kr_0)\; Y^*_{lm}(\hat{r}_0) \\ &+ \sum_{lml'm'} j_l(kr)\; Y_{lm}(\hat{r})\; \mathcal{M}_{lm,l'm'}(\theta,k^2)\; j_{l'}(kr_0)\; Y_{l'm'}(\hat{r}_0) \end{aligned}$$

quantization condition (ii)

after substitution one gets an homogeneous linear system

$$q \cos \delta_l(k)\ \alpha_{lm} + \sum_{l' m'} \mathcal{M}_{lm,l'm'}\ \sin \delta_{l'}(k) \alpha_{l'm'} = 0$$

that has non trivial solutions if and only if

$$\det \left[\mathcal{M}_{lm,l'm'}(\theta, k) + k \delta_{ll'} \delta_{mm'}\ \cot \delta_l(k) \right] = 0$$

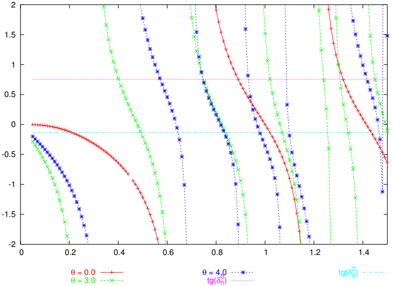
Making the assumption that all the scattering phases vanish except the S–wave, one gets:

$$\tan \delta_0(k) = -\tan \phi(\theta, q),$$

$$q = \frac{kL}{2\pi}, \qquad \tan \phi(\theta, q) = -\frac{q \pi^{3/2}}{\mathcal{Z}_{00}(1; \theta; q^2)},$$

$$\mathcal{Z}_{00}(s; \theta; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\mathbf{n} \in Z^3} \frac{1}{\left[\left(\mathbf{n} + \frac{\theta}{2\pi} \right)^2 - q^2 \right]^s}$$

$$\Re(s) > \frac{3}{2}$$



what about the real world. . . (i)

- in hep-lat/0409154 we claimed that the results discussed so far where useful for $K \longrightarrow \pi\pi$ decays
- in hep-lat/0411033 Sachrajda & Villadoro pointed out that we where wrong

we are breaking isospin (not I_3)

$$S = \int d^4x\, \bar{u}(x) \left[\not{D} - i\frac{\not{\theta}_u}{L} + m \right] u(x) + \int d^4x\, \bar{d}(x) \left[\not{D} - i\frac{\not{\theta}_d}{L} + m \right] d(x)$$

for one particle states

$$\frac{\triangle m^2_{\pi^\pm}}{m^2_{\pi^\pm}} \mapsto \frac{3m_\pi^2 e^{-m_\pi L}}{(2\pi f_\pi^2 m_\pi L)^{3/2}}$$

$$\frac{\triangle m^2_{\pi^0}}{m^2_{\pi^0}} \mapsto \frac{3m_\pi^2 e^{-m_\pi L}}{(2\pi f_\pi^2 m_\pi L)^{3/2}} \left(\frac{2}{3} \sum_{i=0}^{3} \cos\theta_i - 1 \right)$$

- partially twisting (see [Flynn & al. hep-lat/0506016] for a numerical study)

$$\frac{\Delta f_{K^\pm}}{f_{K^\pm}} \longmapsto \begin{array}{l} -\dfrac{m_\pi^2 e^{-m_\pi L}}{f_\pi^2 (2\pi m_\pi L)^{3/2}} \left(\frac{9}{4}\right) \\ -\dfrac{m_\pi^2 e^{-m_\pi L}}{f_\pi^2 (2\pi m_\pi L)^{3/2}} \left(\frac{1}{2}\sum_{i=1}^{3} \cos(\theta_i) + \frac{3}{4}\right) \\ -\dfrac{m_\pi^2 e^{-m_\pi L}}{f_\pi^2 (2\pi m_\pi L)^{3/2}} \left(\sum_{i=1}^{3} \cos(\theta_i) - \frac{3}{4}\right) \end{array}$$

what about the real world. . . (ii)

- in the case of two particle states we have mixing
- in the neutral two–pion sector we get a mixing $\| \pi\pi \rangle_{I=2} \longleftrightarrow \| \pi\pi \rangle_{I=0}$
- Sachrajda & Villadoro argument goes as follows:

$$\begin{aligned} \langle 0 \| \, \pi^0(t) \pi^0(t) \, \sigma(0) \, \| 0 \rangle &= A_{00} \, e^{-tE_0} + B_{00} \, e^{-tE_1} + \ldots \\ \langle 0 \| \, \pi^+(t) \pi^-(t) \, \sigma(0) \, \| 0 \rangle &= A_{+-} \, e^{-tE_0} + B_{+-} \, e^{-tE_1} + \ldots \end{aligned}$$

- by measuring (in principle) the "red" coefficients one can build the interpolation operators that have no overlap with the energy eigenstates ($\| E_0 \rangle$ and $\| E_1 \rangle$)
- but then there is no way to use this informations . . .

two states model (i)

- since I_3 is unbroken so we can stay within the neutral two–pion subspace

$$\begin{pmatrix} \|\pi^+\pi^-\rangle \\ \|\pi^0\pi^0\rangle \end{pmatrix} = \underbrace{\begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} \\ -\sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix}}_{\hat{R}} \begin{pmatrix} \|I=2\rangle \\ \|I=0\rangle \end{pmatrix}$$

- in the center-of-mass reference frame one can in principle have a two–pion neutral state that is a superposition of the two possible pion combinations

$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_{+-}(\mathbf{r}) \\ \psi_{00}(\mathbf{r}) \end{pmatrix} = \hat{R} \begin{pmatrix} \psi_{I=2}(\mathbf{r}) \\ \psi_{I=0}(\mathbf{r}) \end{pmatrix} = \hat{R}\psi_I(\mathbf{r})$$

- the boundary conditions for the doublet field can be written as

$$\psi(\mathbf{x}+e_i L) = \underbrace{\begin{pmatrix} e^{i\theta_i} & 0 \\ 0 & 1 \end{pmatrix}}_{\hat{B}(\theta_i)} \psi(\mathbf{x})$$

$$\psi_I(\mathbf{x}+e_i L) = \hat{R}^{-1}\hat{B}(\theta_i)\hat{R}\ \psi(\mathbf{x}) = \hat{B}_I(\theta_i)\ \psi(\mathbf{x})$$

two states model (ii)

- the Schrödinger equation for this system is

$$\left[\begin{pmatrix} \triangle + k^2 & 0 \\ 0 & \triangle + k^2 \end{pmatrix} - \begin{pmatrix} V_{+-,+-}(r) & V_{+-,00}(r) \\ V_{00,+-}(r) & V_{00,00}(r) \end{pmatrix}\right] \psi(\mathbf{r}, t) = 0$$

or, in compact notation

$$[\underbrace{\left(\triangle + k^2\right)}_{\hat{K}} - \hat{V}\,]\psi = 0$$

- the Schrödinger equation can be written also in the isospin basis, i.e.

$$\left[\hat{K} - \hat{V}_I\right] \psi_I = 0 \qquad \hat{V}_I = \hat{R}^{-1}\hat{V}\hat{R} = \begin{pmatrix} V_{I=2}(r) & 0 \\ 0 & V_{I=0}(r) \end{pmatrix}$$

- the greenian is given by

$$\hat{g}_{B_I}(\mathbf{x} - \mathbf{y}) = \sum_{\mathbf{n}} \hat{B}_I(\theta\mathbf{n})\hat{g}(\mathbf{x} - \mathbf{y} - \mathbf{n}L) = \begin{pmatrix} \frac{g_\theta + 2g_{\mathbf{0}}}{3} & \sqrt{2}\frac{g_\theta - g_{\mathbf{0}}}{3} \\ \sqrt{2}\frac{g_\theta - g_{\mathbf{0}}}{3} & \frac{2g_\theta + g_{\mathbf{0}}}{3} \end{pmatrix}$$

- the quantization condition can be derived as before and is given by

$$\frac{\partial \hat{g}_{B_l}(\mathbf{x}-\mathbf{y})}{\partial y}\psi_l(\mathbf{y}) - \hat{g}_{B_l}(\mathbf{x}-\mathbf{y})\frac{\partial \psi_l(\mathbf{y})}{\partial y} = 0$$

- the S–wave wavefunction can be written as

$$\psi(\mathbf{y}) = j_0(ky)\begin{pmatrix} c_2 \\ c_0 \end{pmatrix} - n_0(ky)\begin{pmatrix} c_2 \tan\delta_2(k) \\ c_0 \tan\delta_0(k) \end{pmatrix}$$

- the greenian can be written as

$$\hat{g}_{B_l}(\mathbf{x}-\mathbf{y}) = \frac{kj_0(kx)}{4\pi}\left[n_0(ky) - \frac{j_0(ky)}{2\pi^{3/2}kL}\begin{pmatrix} \frac{\mathcal{Z}_{00}(\theta)+2\mathcal{Z}_{00}(0)}{3} & \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3} \\ \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3} & \frac{2\mathcal{Z}_{00}(\theta)+\mathcal{Z}_{00}(0)}{3} \end{pmatrix}\right]$$

- we get again a linear system

$$\begin{pmatrix} q\ \text{ctg}\delta_2 - \frac{\mathcal{Z}_{00}(\theta)+2\mathcal{Z}_{00}(0)}{3\pi^{3/2}} & \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3\pi^{3/2}} \\ \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3\pi^{3/2}} & q\ \text{ctg}\delta_0 - \frac{2\mathcal{Z}_{00}(\theta)+\mathcal{Z}_{00}(0)}{3\pi^{3/2}} \end{pmatrix} \begin{pmatrix} c_2 \tan\delta_2 \\ c_0 \tan\delta_0 \end{pmatrix} = 0$$

- that can have a solution different from the trivial one only if

$$\left[q\text{ctg}\delta_2 - \frac{\mathcal{Z}_{00}(\theta)+2\mathcal{Z}_{00}(0)}{3\pi^{3/2}}\right]\left[q\text{ctg}\delta_0 - \frac{2\mathcal{Z}_{00}(\theta)+\mathcal{Z}_{00}(0)}{3\pi^{3/2}}\right] = 2\left[\frac{\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)}{3\pi^{3/2}}\right]^2$$

- similar formulas have been obtained in

[He, Feng & Liu hep-lat/0504019]
[Detmold & Savage hep-lat/0403005]

two states model (v)

- a somehow deeper insight in the previous formula can be gained by diagonalizing the symmetric matrix

$$\begin{pmatrix} A & M \\ M & B \end{pmatrix} = \begin{pmatrix} q\,\mathrm{ctg}\delta_2 - \frac{\mathcal{Z}_{00}(\theta)+2\mathcal{Z}_{00}(0)}{3\pi^{3/2}} & \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3\pi^{3/2}} \\ \frac{\sqrt{2}[\mathcal{Z}_{00}(\theta)-\mathcal{Z}_{00}(0)]}{3\pi^{3/2}} & q\,\mathrm{ctg}\delta_0 - \frac{2\mathcal{Z}_{00}(\theta)+\mathcal{Z}_{00}(0)}{3\pi^{3/2}} \end{pmatrix}$$

$$= \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} A + M\tan\phi & 0 \\ 0 & B - M\tan\phi \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}$$

where

$$\tan\phi = \frac{-(A-B) + \sqrt{(A-B)^2 + 4M^2}}{2M}$$

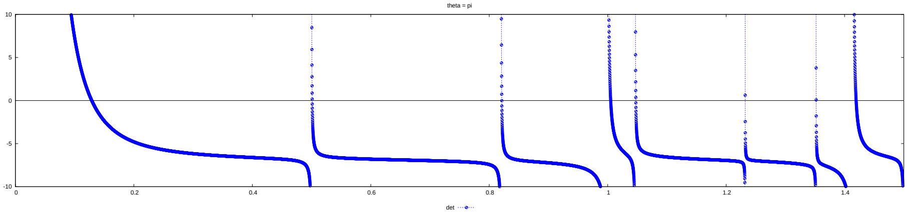
the two eigenvalues are given by

$$\frac{(A+B) + \sqrt{(A-B)^2 + 4M^2}}{2}$$

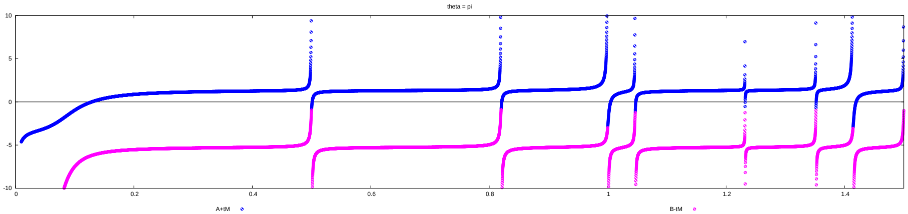
$$\frac{(A+B) - \sqrt{(A-B)^2 + 4M^2}}{2}$$

two state model (vi)

- the determinant quantization condition for $\theta = \pi$



- the two eigenvalues for $\theta = \pi$



two state model. . . conclusions

By assuming negligible finite volume corrections one can

- choose two values of θ such that the energy of the scattering state is fixed (. . . different volumes!)
- solve together the two corresponding quantization conditions
- extract the $I = 2$ and $I = 0$ scattering phases.

- the mixing can be calculated ($\tan\phi$). . . further generalization of LL formula?