

# Numerical calculation of the quark energy spectrum in a mesonic background field

$\pi$ -Meson: Chiral Hedgehog field

W. Kern      P. Kratochwill      M. Mandl  
B. Riederer      M. Schröfl

Project in: "Foundations of Particle Physics"

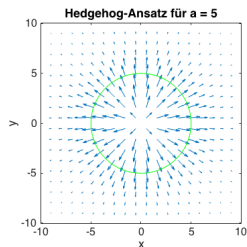
June 2018

- 1 Calculation of the total energy  $E_{tot}$  as a function of the parameter  $a$  of the hedgehog field  $\Theta(\mathbf{x}) = \hat{\mathbf{r}} \Theta(r)$

$$\Theta(r) = -\pi \begin{cases} 1 - \frac{2r}{3a} & r \leq a \\ \frac{a^2}{3r^2} & r \geq a \end{cases} \quad (1)$$

- 2 Diagonalization of the one-particle dirac hamiltonian  $h$

$$h = \mathbf{a} \cdot \mathbf{p} + \beta m (\cos \Theta(r) + i \gamma_5 \boldsymbol{\tau} \cdot \hat{\mathbf{r}} \sin \Theta(r)) \quad (2)$$

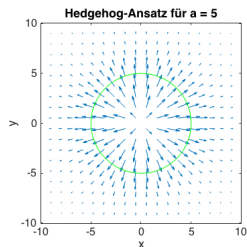


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## 2 Eigenstates: Grand-Spin operator $\mathbf{G} = \mathbf{J} + \frac{\boldsymbol{\tau}}{2} = \mathbf{I} + \frac{\boldsymbol{\sigma}}{2} + \frac{\boldsymbol{\tau}}{2}$

$$J = \begin{cases} G + 1/2, & I = \begin{cases} G + 1 \\ G \end{cases} \\ G - 1/2, & I = \begin{cases} G \\ G - 1 \end{cases} \end{cases} \quad |i, n, J, M\rangle \sim j_l(k_n r) |IJGM\rangle \quad (4)$$

## 3 Problems to solve:

- Numerical integration (matrix elements:  $\int dr r^2 f(\Theta) j_l(k_n r) j_{l'}(k_m r)$ )
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$$\text{e.g. } |1, n, J = G + 1/2, M\rangle \sim \begin{pmatrix} j_G(k_n r) |GG + 1/2GM\rangle \\ j_{G+1}(k_n r) |G + 1G + 1/2GM\rangle \end{pmatrix} \quad (4)$$

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Solving order

## Recursion relation

$$\frac{2\mu + 1}{x} j_\mu(x) = j_{\mu-1}(x) + j_{\mu+1}(x) \quad (5)$$

### Upward recurrence

$$j_\mu(x) = \frac{2\mu - 1}{x} j_{\mu-1}(x) - j_{\mu-2}(x) \quad (5a)$$

Starting values:

$$j_0(x) = \frac{\sin x}{x}$$
$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

### Downward recurrence

$$j_{\mu-1}(x) = \frac{2\mu + 1}{x} j_\mu(x) - j_{\mu+1}(x) \quad (5b)$$

Starting values ( $\nu \gg \mu$ ):

Arbitrary

$$j_\nu(x) = 0$$
$$j_{\nu+1}(x) = 1$$

## Recursion relation

$$\frac{2\mu + 1}{x} j_\mu(x) = j_{\mu-1}(x) + j_{\mu+1}(x) \quad (5)$$

**Upward recurrence** ( $x > \mu$ )

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$$j_0(x) = \frac{\sin x}{x}$$

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**Downward recurrence** ( $x \leq \mu$ )

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Starting values ( $\nu \gg \mu$ ):

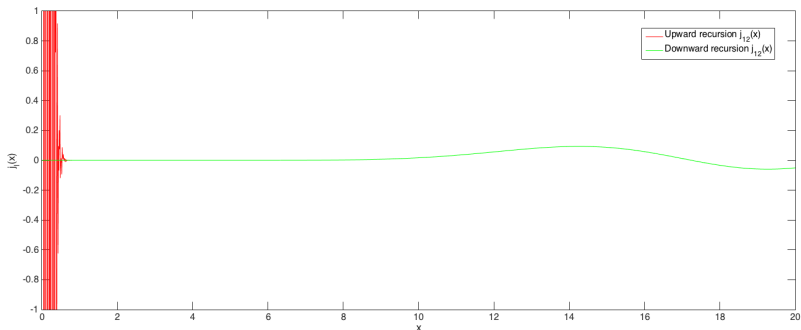
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$$j_\nu(x) = 0$$

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# Finding roots

## Bisection method

### Pseudocode:

```
function root = bisec(f,a,b,eps)
if f(a) * f(b) > 0, error('Too few or
too many roots in [a,b]')
elseif f(a) == 0, root = a
elseif f(b) == 0, root = b
else
while eps <= abs(a-b)/4 % error
c = (a + b) / 2;
root = c;
if f(a) * f(c) < 0, b = c;
elseif f(c) * f(b) < 0, a = c;
else, break
end
end
end
```

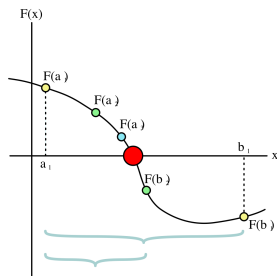


Figure: Bisection method <sup>1</sup>

Error estimation:

$$\epsilon_{Bisec}^{(n)} = \frac{a^{(n)} - b^{(n)}}{4} \quad (6)$$

<sup>1</sup>Source: [https://commons.wikimedia.org/wiki/File:Bisection\\_method.svg](https://commons.wikimedia.org/wiki/File:Bisection_method.svg)

# Numerical integration

## Simpson's rule

- Problem: Solve  $S = \int_a^b f(x) dx$
- Idea: approximate integrand  $f(x)$  by an integrable quadratic function  $P(x)$ .  $P(x)$  is the interpolant through the points  $a, b$  and  $(a + b)/2$ .
- Improvement: Divide interval  $[a, b]$  into  $N$  subintervals for good approximation.

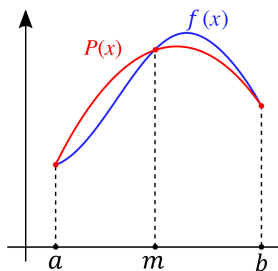


Figure: Simpson's rule <sup>1</sup>

$$S^{(n)} = \frac{h}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n-1} f(a + 2kh) + 4 \sum_{k=1}^n f(a + (2k - 1)h) \right), \quad h = \frac{b - a}{2n} \quad (7)$$

<sup>1</sup>Source: [https://commons.wikimedia.org/wiki/File:Simpsons\\_method\\_illustration.svg](https://commons.wikimedia.org/wiki/File:Simpsons_method_illustration.svg)



# Diagonalization

## Jacobi rotation

- Wanted:  $D = U^\dagger A U$  with  $D = \text{diag}(\lambda_1, \dots, \lambda_n)$  and  $A$  symmetric
- Set iteratively matrix elements to zero by applying orthogonal rotation matrices  $S^{(n)}$ :  $U = S^{(k)} \cdot \dots \cdot S^{(0)}$
- Two different versions:
  - 1 Cyclic: Sets each element of the strict upper triangle to zero
  - 2 Classic: Sets the element with the largest absolute value to zero

- Momentum values  $k_n$  are restricted by two conditions:
  - 1 Momentum Cutoff (UV-Cutoff):  $k_{max} = \Lambda \hat{=} \mathcal{O}(10^2) - \mathcal{O}(10^3) \text{ MeV}$
  - 2 Box size  $D$  (Infrared-Cutoff):  $j_l(k_n D) \stackrel{!}{=} 0$

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# Hamiltonian-matrix I

## Momentum eigenstates and matrix dimension

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- Dimension  $4N(G) \times 4N(G)$  for  $G > 0$  and  $2N(G) \times 2N(G)$  for  $G = 0$

## Hamilton matrix

$$h_{nm}^{int} = N_{G+1n} N_{G+1m} \begin{pmatrix} a_{nm}^G - b_{mn}^{G-1} + \frac{1}{2G+1} (c_{nm}^{GG-1} + c_{mn}^{GG-1}) & \frac{2\sqrt{G(G+1)}}{2G+1} (c_{nm}^{GG-1} - c_{mn}^{GG+1}) \\ \frac{2\sqrt{G(G+1)}}{2G+1} (c_{nm}^{GG-1} - c_{mn}^{GG+1}) & a_{nm}^G - b_{mn}^{G+1} + \frac{1}{2G+1} (c_{nm}^{GG+1} + c_{mn}^{GG+1}) \end{pmatrix} \quad (8)$$

$$a_{nm}^l \sim b_{nm}^l \sim \int_0^D dr r^2 (\cos \Theta(r) - 1) j_l(k_n r) j_l(k_m r) \quad (9)$$

$$c_{nm}^{ll'} \sim \int_0^D dr r^2 \sin \Theta(r) j_l(k_n r) j_{l'}(k_m r) \quad (10)$$

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# Hamiltonian-matrix II

## Putting parts together and diagonalization

- Define mass of the Valence Quark  $m_{Vq} = 400 \text{ MeV}$
- Varying parameter  $am_{Vq}$  in  $[0, 20]$
- Boxsize  $D \gg a \Rightarrow D = 5 \max(a) \hat{=} 0.25 \text{ MeV}^{-1}$
- For each  $a$ :
  - 1 Calculate  $k_n$  in  $[0, \Lambda]$  using  $j_G(k_n D) \stackrel{!}{=} 0$  (Bisec method) and corresponding energies
  - 2 Calculate  $a'_{nm}$ ,  $b'_{nm}$  and  $c''_{nm}$  (Simpson's rule)
  - 3 Calculate matrix  $h_{nm} = h_{nm}^D + h_{nm}^{int}$
  - 4 Calculate eigenvalues  $\epsilon_\mu$  (Jacobi rotations)

$E_{tot}$ 

$$E_{tot} = \underbrace{E_{vac} - E_{vac}(\Theta = 0)}_1 + \underbrace{E_{val}}_2 + \underbrace{E_m}_3 \quad (11)$$

- 1 Describes the energy variation of the vacuum from the trivial vacuum

$$E_{vac} = \frac{N_C}{2} \sum_{\mu} \left\{ \frac{\Lambda}{\sqrt{\pi}} \exp(-(\epsilon_{\mu}/\Lambda)^2) - |\epsilon_{\mu}| \operatorname{erfc}(|\epsilon_m u/\Lambda|) \right\} \quad (12)$$

- 2 Describes the energy of the Valence quark (Here:  $\Theta(x)$  stepfunction)

$$E_{val} = N_C |\epsilon_{\mu}| \Theta(\epsilon_{\mu}) \quad (13)$$

- 3 Describes the energy of the mesonic part for the hedgehog ansatz

$$E_m = 4\pi m_{\pi}^2 f_{\pi}^2 \int dr r^2 (1 - \cos(\Theta(r))) \quad (14)$$

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- [2] R. Rajaraman. *Solitons and Instantons*. Elsevier, 1989.
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- [4] R. Alkofer, H. Weigel. *Self-consistent solution to a fermion determinant with space dependent fields*, Computer Physics Communications 82 (30-41), 1994.
- [5] H. Weigel, R. Alkofer. *The Bethe-Salpeter equation for mesons as quark-anti-quark bound states in a soliton background*, Computer Physics Communications 82 (57-73), 1994.
- [6] R. Alkofer, H. Reinhardt, H. Weigel *Baryons as Chiral Solitons in the Nambu-Jona-Lasinio Model*, [arXiv:hep-ph/9501213], 1994





# Numerische Berechnung eines Quarkspektrums in einem mesonischen Hintergrundfeld

## $\pi$ -Meson: Chiraler Hedgehog-Ansatz

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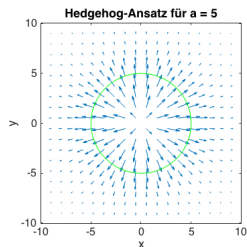
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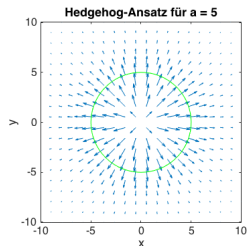


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## 2 Eigenzustände: Grand-Spin Operator $\mathbf{G} = \mathbf{J} + \frac{\boldsymbol{\tau}}{2} = \mathbf{L} + \frac{\boldsymbol{\sigma}}{2} + \frac{\boldsymbol{\tau}}{2}$

$$J = \begin{cases} G + 1/2, & l = \begin{cases} G + 1 \\ G \end{cases} \\ G - 1/2, & l = \begin{cases} G \\ G - 1 \end{cases} \end{cases} \quad |i, n, J, M\rangle \sim j_l(k_n r) |l J M\rangle \quad (4)$$

## 3 Problemstellungen:

- Numerische Integration (Matrixelement:  $\int dr r^2 f(\Theta) j_l(k_n r) j_{l'}(k_m r)$ )
- Nullstellensuche (Boxgröße und Impulseigenzustände:  $j_l(k_n D) \stackrel{!}{=} 0$ )
- Sphärische Besselfunktion (Eigenzustände:  $\sim j_l(x)$ )

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$$h = h_D + \beta m (\cos \Theta(r) - 1 + i\gamma_5 \boldsymbol{\tau} \cdot \hat{\mathbf{r}} \sin \Theta(r)) \quad (3)$$

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$$\text{e.g. } |1, n, J = G + 1/2, M\rangle \sim \begin{pmatrix} j_G(k_n r) |GG + 1/2GM\rangle \\ j_{G+1}(k_n r) |G + 1G + 1/2GM\rangle \end{pmatrix} \quad (4)$$

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Arbeitsreihenfolge

## Rekursionsrelation

$$\frac{2\mu + 1}{x} j_\mu(x) = j_{\mu-1}(x) + j_{\mu+1}(x) \quad (5)$$

### Vorwärts-Rekursion

$$j_\mu(x) = \frac{2\mu - 1}{x} j_{\mu-1}(x) - j_{\mu-2}(x) \quad (5a)$$

Startwerte:

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

### Rückwärts-Rekursion

$$j_{\mu-1}(x) = \frac{2\mu + 1}{x} j_\mu(x) - j_{\mu+1}(x) \quad (5b)$$

Startwerte ( $\nu \gg \mu$ ):

Willkürlich

$$j_\nu(x) = 0$$

$$j_{\nu+1}(x) = 1$$

## Rekursionsrelation

$$\frac{2\mu + 1}{x} j_\mu(x) = j_{\mu-1}(x) + j_{\mu+1}(x) \quad (5)$$

**Vorwärts-Rekursion** ( $x > \mu$ )

$$j_\mu(x) = \frac{2\mu - 1}{x} j_{\mu-1}(x) - j_{\mu-2}(x) \quad (5a)$$

Startwerte:

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

**Rückwärts-Rekursion** ( $x \leq \mu$ )

$$j_{\mu-1}(x) = \frac{2\mu + 1}{x} j_\mu(x) - j_{\mu+1}(x) \quad (5b)$$

Startwerte ( $\nu \gg \mu$ ):

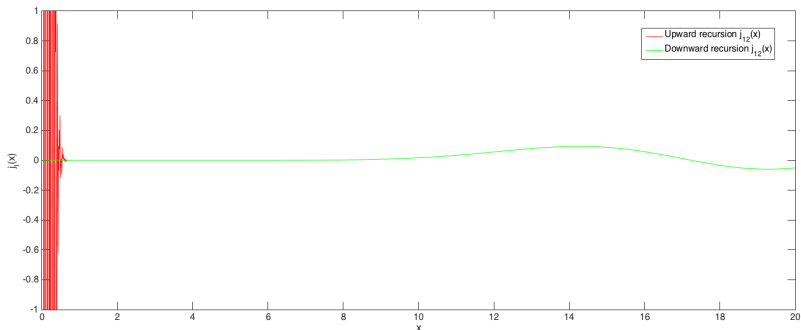
Willkürlich

$$j_\nu(x) = 0$$

$$j_{\nu+1}(x) = 1$$

## Rekursionsrelation

$$\frac{2\mu + 1}{x} j_\mu(x) = j_{\mu-1}(x) + j_{\mu+1}(x) \quad (5)$$



### Pseudocode:

```
function root = bisec(f,a,b,eps)
if f(a) * f(b) > 0, error('Too few or
too many roots in [a,b]')
elseif f(a) == 0, root = a
elseif f(b) == 0, root = b
else
while eps <= abs(a-b)/4 % error
c = (a + b) / 2;
root = c;
if f(a) * f(c) < 0, b = c;
elseif f(c) * f(b) < 0, a = c;
else, break
end
end
end
```

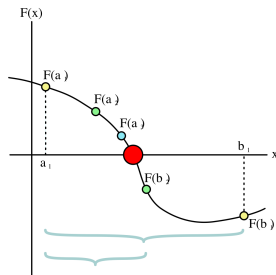


Abbildung: Bisektion-Methode <sup>1</sup>

Fehlerabschätzung:

$$\epsilon_{Bisec}^{(n)} = \frac{a^{(n)} - b^{(n)}}{4} \quad (6)$$

<sup>1</sup>Source: [https://commons.wikimedia.org/wiki/File:Bisection\\_method.svg](https://commons.wikimedia.org/wiki/File:Bisection_method.svg)



- Problem: Löse  $S = \int_a^b f(x) dx$
- Idee: ersetze zu integrierende Funktion  $f(x)$  durch integrierbare Parabel  $P(x)$ .  $P(x)$  ist hierbei ein Interpolationspolynom durch die Funktionswerte  $a$ ,  $b$  und  $(a + b)/2$ .
- Verbesserung: Teile das Intervall  $[a, b]$  in  $N$  Teilintervalle für möglichst gute Näherung.

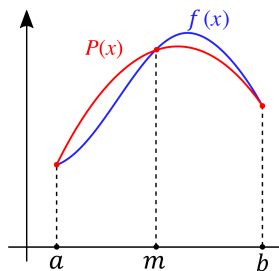


Abbildung: Simpson Regel <sup>1</sup>

$$S^{(n)} = \frac{h}{3} \left( f(a) + f(b) + 2 \sum_{k=1}^{n-1} f(a + 2kh) + 4 \sum_{k=1}^n f(a + (2k - 1)h) \right), \quad h = \frac{b - a}{2n} \quad (7)$$

<sup>1</sup>Source: [https://commons.wikimedia.org/wiki/File:Simpsons\\_method\\_illustration.svg](https://commons.wikimedia.org/wiki/File:Simpsons_method_illustration.svg)

- Gesucht:  $D = U^\dagger AU$  mit  $D = \text{diag}(\lambda_1, \dots, \lambda_n)$  und  $A$  symmetrisch
- Setze iterativ Matrixelemente auf 0 durch Multiplikation mit Rotationsmatrizen  $S^{(n)}$ :  $U = S^{(n)} \cdot \dots \cdot S^{(0)}$
- Zwei Varianten:
  - 1 Zyklisch: Setzt jedes Element der strikten oberen Dreiecksmatrix auf 0
  - 2 Klassisch: Setzt immer das Element mit dem größten Absolutwert auf 0

- Impulszustände  $k_n$  sind durch zwei Bedingungen eingeschränkt:
  - 1 Impuls Cutoff (UV-Cutoff):  $k_{max} = \Lambda \hat{=} \mathcal{O}(10^2) - \mathcal{O}(10^3) \text{ MeV}$
  - 2 Boxgröße  $D$  (Infrarot-Cutoff):  $j_l(k_n D) \stackrel{!}{=} 0$

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  - 2 Boxgröße  $D$  (Infrarot-Cutoff):  $j_l(k_n D) \stackrel{!}{=} 0 \Rightarrow$  verwende Bisektion und sphärische Besselfunktionen

# Hamiltonmatrix I

## Impulseigenzustände und Matrixdimension

- Impulszustände  $k_n$  sind durch zwei Bedingungen eingeschränkt:
  - ① Impuls Cutoff (UV-Cutoff):  $k_{max} = \Lambda \hat{=} \mathcal{O}(10^2) - \mathcal{O}(10^3) \text{ MeV}$
  - ② Boxgröße  $D$  (Infrarot-Cutoff):  $j_l(k_n D) \stackrel{!}{=} 0$
- Dimension:  $4N(G) \times 4N(G)$  für  $G > 0$  und  $2N(G) \times 2N(G)$  für  $G = 0$

## Hamilton matrix

$$h_{nm}^{int} = N_{G+1n} N_{G+1m} \begin{pmatrix} a_{nm}^G - b_{mn}^{G-1} + \frac{1}{2G+1} (c_{nm}^{GG-1} + c_{mn}^{GG-1}) & \frac{2\sqrt{G(G+1)}}{2G+1} (c_{nm}^{GG-1} - c_{mn}^{GG+1}) \\ \frac{2\sqrt{G(G+1)}}{2G+1} (c_{nm}^{GG-1} - c_{mn}^{GG+1}) & a_{nm}^G - b_{mn}^{G+1} + \frac{1}{2G+1} (c_{nm}^{GG+1} + c_{mn}^{GG+1}) \end{pmatrix} \quad (8)$$

$$a'_{nm} \sim b'_{nm} \sim \int_0^D dr r^2 (\cos \Theta(r) - 1) j_l(k_n r) j_l(k_m r) \quad (9)$$

$$c_{nm}^{ll'} \sim \int_0^D dr r^2 \sin \Theta(r) j_l(k_n r) j_{l'}(k_m r) \quad (10)$$

# Hamiltonmatrix I

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$$a_{nm}^l \sim b_{nm}^l \sim \int_0^D dr r^2 (\cos \Theta(r) - 1) j_l(k_n r) j_l(k_m r) \quad (9)$$

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- Definiere Masse des Valenz-Quarks  $m_{Vq} = 400 \text{ MeV}$
- Variiere Parameter  $am_{Vq}$  in  $[0, 20]$
- Boxgröße  $D \gg a \Rightarrow D = 5 \max(a) \hat{=} 0.25 \text{ MeV}^{-1}$
- Für jedes  $a$ :
  - 1 Berechne  $k_n$  in  $[0, \Lambda]$  mittels  $j_G(k_n D) \stackrel{!}{=} 0$  (Bisektion) und die zugehörigen Energien
  - 2 Berechne  $a'_{nm}$ ,  $b'_{nm}$  und  $c''_{nm}$  (Simpson Regel)
  - 3 Berechne Matrix  $h_{nm} = h_{nm}^D + h_{nm}^{int}$
  - 4 Berechne Eigenwerte  $\epsilon_\mu$  (Jacobi-Verfahren)

$E_{tot}$

$$E_{tot} = \underbrace{E_{vac} - E_{vac}(\Theta = 0)}_1 + \underbrace{E_{val}}_2 + \underbrace{E_m}_3 \quad (11)$$

- 1 Änderung der Vakuumsenergie im Vergleich zum trivialen Vakuum

$$E_{vac} = \frac{N_C}{2} \sum_{\mu} \left\{ \frac{\Lambda}{\sqrt{\pi}} \exp(-(\epsilon_{\mu}/\Lambda)^2) - |\epsilon_{\mu}| \operatorname{erfc}(|\epsilon_m u/\Lambda|) \right\} \quad (12)$$

- 2 Energie des Valenz-Quarks (Here:  $\Theta(x)$  Stepfunction)

$$E_{val} = N_C |\epsilon_{\mu}| \Theta(\epsilon_{\mu}) \quad (13)$$

- 3 Energie des mesonischen Parts für den Hedgehog-Ansatz

$$E_m = 4\pi m_{\pi}^2 f_{\pi}^2 \int dr r^2 (1 - \cos(\Theta(r))) \quad (14)$$



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