Low energy scattering parameters from the solutions of the non-relativistic Yukawa model on a 3-dimensional lattice

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October 3, 2017

Abstract

The numerical solutions of the non-relativistic Yukawa model on a 3-dimensional size lattice with periodic boundary conditions are obtained. The possibility to extract the corresponding – infinite space – low energy parameters and bound state binding energies from eigensates computed at finite lattice size is discussed.

1 Introduction

The description of deconfined hadronic states from a low energy confining theory is an exciting theoretical problem and a challenging numerical task. With the increasing power of computers devoted to Lattice QCD and the progress made by algorithms, it is nowadays possible to study low energy hadron-hadron systems from first QCD principles.

Contrarily to hadron masses and form factors, scattering properties can not be computed from infinite volume euclidean simulations [1]. The link between a field theory formulated in an euclidean space and the scattering observables is however made possible by studying the volume dependence of the bound state spectra in a finite box with periodic boundary conditions. The underlying formalism was developed by M. Luscher and collaborators in a series of papers [2] [3] [4] [5] [6] [7] and has been recently updated in view of applications to nuclear and hadronic physics [8] [9] [10] [11].

This formalism was formerly applied to extract the hadron-hadron scattering lengths in the quenched approximation [12], and more recently to obtain the low energy scattering parameters in $\pi\pi$ [13] [14] [15] [17] [18], $K\pi$ [18] and even nucleon-nucleon [16] systems from fully dynamical lattice QCD calculations. These calculations are crucial in providing some insight on the fundamental parameters of the hadron-hadron interaction, as well as low energy observables which are poorly known since hardly accessible experimentally.

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The aim of our work is to test the applicability of Luscher relations in a model which, on one hand, would contain the main physical ingredients of hadron-hadron interaction and, on another hand, would be simple enough to be independently controlled. This is provided by the Yukawa model, in which a massive scalar particle is exchanged between two fermions. When generalized to pseudoscalar and vector exchanges, it constitutes the keystone of baryon-baryon interaction models [19].

In the present paper we have considered the non relativistic reduction of the Yukawa model that we have solved in a 3-dimensional $L^3$ lattice with periodic boundary conditions. The solutions have been obtained using finite difference schemes in close analogy with the methods used in lattice field theory simulations. The $L$-dependence of the eigenenergies have been used to extract the infinite volume low energy parameters, namely the scattering length and the effective range. Contrary to the quantum field lattice calculation, these quantities can be besides accurately computed by solving the corresponding one-dimensional Schrödinger radial equation in an independent way.

Despite its simplicity, the non relativistic Yukawa model considered here contains an essential ingredient of a realistic interaction – its finite range – which plays a relevant role in view of extracting the low energy parameters from the finite volume spectra. It offers a wieldy and physically sound tool to test the validity of the different approaches discussed in the literature, in particular the large and small $L$-expansion. The full quantum field contents of this model have also been considered in a lattice calculation. Preliminary results can be found in [24].

A similar study was undertaken in [9] in the framework of an effective field theory without pions EFT($\pi$) and from a slightly different point of view. These authors fix the values of the low energy parameters and obtain the energy levels assuming they satisfy Luscher equations [2, 3, 5] while in our case all these quantities are independently generated by solving a dynamical model and used to find their applicability conditions.

The properties of the non relativistic Yukawa model in the continuum are briefly introduced in Section 2. Section 3 is devoted to explain the numerical methods used for its solution on a 3-d torus. Results concerning scattering and bound states are displayed in Section 4 and some final remarks are given in the conclusions.

## 2 The model

We consider a system of two non relativistic particles interacting by a Yukawa potential of strength $g$ and range parameter $\mu$

$$U(r) = -\frac{g^2}{4\pi} \frac{e^{-\mu r}}{r}$$

This potential is obtained by Fourier transforming the Born amplitude $T_B$

$$T_B(k_1, k_2, k'_1, k'_2) = \bar{u}(\vec{k}')u(\vec{k}) \frac{g^2}{(k - k')^2 - \mu^2} \bar{u}(-\vec{k}')u(-\vec{k})$$

of the meson-fermion interaction lagrangian (See figure 1):

$$\mathcal{L}(x) = g\bar{\Psi}(x) \Phi(x) \Psi(x)$$
where $\Psi$ is a Dirac field with mass $M$, $\Phi$ a scalar field with mass $\mu$ and in which the non relativistic reduction $-u = 1\ g^2 = -\bar{q}^2$ has been applied [20, 21]. The same potential results from a model with purely scalar fields.

The reduced S-wave radial Schrodinger equation (in $\hbar = c = 1$ units) reads

$$u_0''(r) + M \left[ E + \frac{g^2}{4\pi} e^{-\mu r} \right] u_0(r) = 0 \tag{3}$$

and the corresponding tridimensional wavefunction is

$$\Psi(\vec{r}) = \frac{1}{\sqrt{4\pi}} \frac{u_0(r)}{r} \tag{4}$$

The solutions of (4) depend a priori on the three parameters $(M, \mu, g)$ but written in terms of the dimensionless variable $x = \mu r$, this equation is equivalent to

$$u''(x) + \left[ \epsilon \frac{G}{x} e^{-x} \right] u(x) = 0 \tag{5}$$

which depends on a unique dimensionless strength parameter

$$G(M, \mu, g) = \frac{g^2}{4\pi} \frac{M}{\mu}$$

In particular, the bound state energy $(E)$ and scattering length $(a_0)$ of the two-body system (3) are given by the scaling relations

$$\frac{E}{M} = \left( \frac{\mu}{M} \right)^2 \epsilon(G) \tag{6}$$

$$a_0 \mu = A_0(G) \tag{7}$$

where $\epsilon(G)$ and $A_0(G)$ are respectively the binding energy and scattering length of the dimensionless problem (5).

We will focus hereafter on finding the solutions of a unit mass particle in the potential

$$V(x) = -G \frac{e^{-x}}{x} \tag{8}$$

what we will call the dimensionless Yukawa model. All length parameters involved must be therefore understood in units of the inverse exchanged mass $\mu^{-1}$. The lagrangian [2] gives
rise to an attractive potential, but disregarding its relation with the underlying field theory, the repulsive case $G < 0$ can be considered as well.

The asymptotic norm $N_s$ of a bound state with energy $\epsilon_0$ is defined as

$$N_s = \lim_{x \to \infty} u_0(x)e^{+k_0x} \quad k_0 = \sqrt{-\epsilon_0}$$  \hspace{1cm} (9)

with $u_0$ normalized by

$$\int_0^\infty u_0^2(x)dx = 1$$

The convention used for the scattering length is such that the regular zero-energy solution of (5) is asymptotically given by

$$u_0(x) \sim x + A_0$$  \hspace{1cm} (10)

or equivalently the low-energy (S-wave) phase-shifts given by

$$\delta_0(k) = -A_0k + o(k^2) \quad k^2 = \epsilon$$

It can be shown that, in the limit of weak coupling constant, one has

$$A_0(G) = -G + o(G^2)$$  \hspace{1cm} (11)

which correspond to the Born approximation of the Schrodinger equation with the Yukawa model (see Appendix A).

![Figure 2: Bound state binding energies for the ground ($\epsilon_0$) and first excited ($\epsilon_1$) S-wave state as a function of the coupling constant $G$ in the dimensionless Yukawa model.](image)

The "universal" functions $\epsilon(G)$ and $A_0(G)$ are displayed in figures and . The system has a first bound state ($\epsilon_0$) for coupling constant $G$ above some critical value $G_0 \approx 1.680$ at which $A_0(G)$ has a pole. An infinity of similar branches – and corresponding $A_0(G)$ poles – appear for the excited states: $\epsilon_1$ at $G_1 = 6.44$, $\epsilon_2$ at $G_2 = 14.34 \ldots$
Figure 3: Scattering length $A_0$ in the dimensionless Yukawa potential as a function of the coupling constant $G$. Dashed line correspond to the repulsive case ($G < 0$). The tangents at the origin indicates the corresponding Born approximation $A_0^{(B)}(G) = \pm G$ and the vertical asymptote the two first bound state singularities at $G_0 = 1.68$ and $G_1 = 6.44$.

It will be of further interest to consider also the effective range parameter $R_0$ which appears in the low energy expansion

$$k \cot \delta_0(k) = -\frac{1}{A_0} + \frac{1}{2} R_0 k^2 + o(k^4)$$  \hspace{1cm} (12)

It is worth noticing that the solutions obtained by inserting potential in the Schrodinger equation correspond to summing up the iterations of the diagram displayed in figure i.e. the so called "ladder" approximation. This represents a small – though infinite – part of the diagrams included in the interaction lagrangian. Attempts to include all the interaction terms of this lagrangian in two-body bound and scattering states have been presented in in the framework of lattice quantum field calculation.

Though the solutions of (5) can be easily obtained with great accuracy, we are interested on the results provided by the same numerical schemes than the ones used on lattice calculations. Thus, by using finite difference methods on an equidistant grid with stepsize $a$, i.e.

$$a^2 u''(x) = u(x + a) - 2u(x) + u(x - a)$$

one obtains the ground state binding energies $\epsilon_0$ and low-energy scattering parameters given respectively in Tables 1 and 2.

One can remark the different sensibility of the bound and scattering results with respect to the stepsize. While low energy parameters vary only of few percent for $a \in [0.1, 0.5]$, except near the resonant value $G = 1.5$, the binding energy varies by a more than a factor 2 in the same interval.
Table 1: Binding energy $\epsilon$ and radius $\rho = \sqrt{<x^2>}$ for the ground state of the Yukawa model using finite difference methods with stepsize $a$.

| $G$  | $a=0.50$ | $a=0.20$ | $a=0.10$ | Exact |
|------|----------|----------|----------|-------|
| $\epsilon_0$ | $\epsilon_0$ | $\epsilon_0$ | $\epsilon_0$ |       |
| 2.0  | -0.0076  | -0.0177  | -0.0198  | -0.0206 | 5.63  |
| 2.5  | -0.0791  | -0.1270  | -0.1364  | -0.1397 | 2.50  |
| 3.0  | -0.2210  | -0.3386  | -0.3625  | -0.3710 | 1.69  |
| 4.0  | -0.6831  | -1.0665  | -1.1531  | -1.1849 | 1.07  |

Table 2: S-wave low energy scattering parameters (scattering length $A_0$ and effective range $R_0$ for different lattice step values $a$.

| $G$  | $a=0.50$ | $a=0.20$ | $a=0.10$ | Exact |
|------|----------|----------|----------|-------|
| $A_0$ | $R_0$    | $A_0$    | $R_0$    |       |
| 0.10 | -0.1029  | 40.25    | -0.1049  | 40.16  | -0.1052 | 40.15 |
| 0.20 | -0.2170  | 20.24    | -0.2227  | 20.14  | -0.2224 | 20.13 |
| 0.40 | -0.4881  | 10.20    | -0.5015  | 10.10  | -0.5035 | 10.09 |
| 0.50 | -0.6518  | 8.180    | -0.6721  | 8.078  | -0.6751 | 8.063 |
| 1.00 | -2.034   | 4.076    | -2.177   | 3.958  | -2.199  | 3.940 |
| 1.50 | -8.039   | 2.628    | -10.81   | 2.488  | -11.40  | 2.467 |

3 Solutions on a torus

Let us consider now the solutions of the dimensionless Yukawa model \(^{(8)}\) on a the 3-d torus, i.e. the solutions of

$$[-\Delta_{\vec{x}} + V_L(\vec{x})] \Phi(\vec{x}) = \epsilon(L) \Phi(\vec{x})$$ (13)

satisfying periodic boundary conditions

$$\Phi(\vec{x} + \vec{n}aL) = \Phi(\vec{x}) \quad \forall \vec{n} \in \mathbb{Z}^3$$

where $a > 0$ is the lattice step and $L \in \mathbb{N}$ is the number of lattice points on each spatial dimension.

The "lattice" potential $V_L$ is defined as

$$V_L(\vec{x}) = \sum_{\vec{n} \in \mathbb{Z}^3} V(\vec{x} + \vec{n}aL)$$ (14)

where $V$ is the infinite volume interaction given in \(^{(8)}\). $V_L$ incorporates the same periodicity than the solutions and contains the interaction with the "surrounding world".

For large values of $aL$, $V_L$ is well approximated by $V$ but below $aL \sim 10$ the "mirror" contributions are sizeable and dramatically modify the low-$L$ behaviour of the observables. We display in figure \(^{(14)}\) the comparison between $V_L$ – converged with respect to the sum over mirror images \(^{(14)}\) – and $V$ obtained with $a = 0.2$ and different values of $aL$.

In order to obtain the numerical solutions of (13), we introduce in the 3-d cubic lattice the coordinates

$$x_\mu(i_\mu) = a \left(i_\mu - \frac{L}{2}\right) \quad \mu = 1, 2, 3 \quad i_\mu = 0, 1, \ldots, L - 1$$
Using the finite difference scheme on gets the following expression for the 3-d laplacian

\[
\Delta \Phi_i = -\frac{6}{a^2} \left\{ \Phi_i - \frac{1}{6} \sum_{\mu=1,3} \Phi_{i+\mu} + \Phi_{i-\mu} \right\}
\]  

where \( i \) labels the set of coordinate indices \( i \equiv \{i_1, i_2, i_3\} \) and \( i+\mu \) denotes the nearest neighbour of \( i \) in the direction \( \mu \).

The stationary states can be obtained by solving directly the eigenvalue equation (13) together with (15). However, in order to follow as close as possible the lattice methods we alternatively use an euclidean time-dependent approach. To this aim we consider the evolution operator between \( t \) and \( t + \Delta \)

\[
U(t, t + \Delta) = e^{-iH\Delta}
\]

The time-dependent wave function propagates in this interval according to

\[
\Psi(x, t + \Delta) = U(t, t + \Delta)\Psi(x, t) = e^{-iH\hat{\Delta}}e^{-iH\hat{\Delta}}\Psi(x, t)
\]

which can be written in the form

\[
e^{+i\hat{\Delta}H}\Psi(x, t + \Delta) = e^{-i\hat{\Delta}H}\Psi(x, t)
\]

For short \( \Delta \) values, we approximate \( U \) by its Taylor expansion up to \( \Delta^2 \) terms, and get the following relation between the wave functions at two consecutive time steps \( t \) and \( t + 1 \)

\[
\Psi_{j+1}^t = \frac{1 - \frac{i\Delta}{2}H}{1 + \frac{i\Delta}{2}H} \Psi_j^t
\]

where we use the notation \( \Psi_j^t \equiv \Psi(x_{\mu}(j), t\Delta) \).

This approximate numerical scheme has the advantage of preserving the unitarity. Using relation (17) would however imply the inversion of \( 1 + iH \) which is an unpleasant task. This can be avoided by noting that (17) is actually equivalent to the system of equations

\[
\left(1 + \frac{i\Delta}{2}H\right)\chi_j^t = 2\Psi_j^t
\]
\[ \Psi_j^{t+1} = -\Psi_j^t + \chi_j^t \]

The unknown \( \chi_j^t \) is a solution of an inhomogeneous Schrödinger-like equation which can be solved using the same discretization schemes described above for the stationary states.

The binding energies can be then obtained by propagating an arbitrary initial solution \( \eta_j \) in the euclidean time \( \tau = it \). Indeed, by expanding the initial state in terms of stationary eigenfunctions \( \Phi^{(n)} \)

\[ \eta = \sum_n c_n \Phi^{(n)}_j \]

it follows that

\[ \Psi^\tau_j = \sum_n c_n \Phi^{(n)}_j e^{-\epsilon_n \tau \Delta} \approx \epsilon_0 \Phi_0^{(0)} e^{-\epsilon_0 \tau \Delta} \]

where \( \epsilon_0 \) is the ground state energy and \( \Phi_0^{(0)} \) the corresponding eigenfunction. The stationary wavefunction will be normalized according to

\[ (aL)^3 \sum_i \Phi_i^2 = 1 \quad (18) \]

Figure 5: Convergence of the ground state effective energy \( \epsilon_0(\tau) \) defined in (19) as a function of the euclidean time \( \tau \) for two different spatial lattice sizes \( aL \). The values are normalized to \( \epsilon_0(\infty) \). The ground state energy is well separated from excited states at \( \tau \Delta \approx aL \). Results correspond to \( G = 0.4 \) and \( \Delta = 0.1 \).

One can get rid of the spatial degrees of freedom by defining at each time-step \( \tau \)

\[ C(\tau) = \frac{1}{(aL)^3} \sum_j \Psi_j^\tau \sim e^{-\epsilon_0 \tau \Delta} \]

This procedure is very similar to the time-slice approach in lattice calculations and can be used to disentangle the ground state from the first excitation energies. To this aim it is interesting
to define the effective energy of the state

$$\epsilon_0(\tau) = \frac{1}{\Delta} \log \frac{C(\tau)}{C(\tau + 1)}$$

(19)

and study the convergence $\epsilon_0(\tau) \to \epsilon_0$. The density of states increases with the size of the box, making their separation increasingly difficult. However until moderate lattice sizes $aL \sim 10$ – values we will be further interested in – the energy levels are well isolated, what makes easy the convergence of the euclidean-time propagation of the ground state. This is illustrated in Figure 5 showing the $\tau$-dependence of the ground state effective energy (19) – normalized to $\epsilon_0(\infty)$ – for two different $aL$ values obtained with $G = 0.4$, $a = 0.2$ and $\Delta = 0.1$. In these cases the results are converged for $\tau \Delta \approx aL$.

4 Results

![Figure 6: L-dependence of the first free two-body energy states](image)

Before presenting the results of the Yukawa model for bound and scattering states we will summarize the free case. The non relativistic energies of two – unit mass – particle states in a lattice with periodic boundary conditions are given by

$$\epsilon_n^{(0)}(L) = \frac{2}{a^2} \sum_{\mu=1}^{3} \left\{ 1 - \cos \frac{2\pi}{L} n_{\mu} \right\} = 4 \frac{3}{a^2} \sum_{\mu=1}^{3} \sin^2 \left\{ \frac{\pi}{L} n_{\mu} \right\}$$

(20)

with $n_{\mu} = 0, 1, 2 \ldots, L - 1$. The continuum limit of an energy state $\{n_{\mu}\}$ is reached – independently of $a$ – for $L \gg \pi \text{Max}\{n_{\mu}\}$ with

$$\epsilon_n^{(0)}(L) \approx \vec{p}^2 \quad \vec{p} = \frac{2\pi}{aL} \vec{n}$$

The ground state energy ($n_{\mu} = 0$) is zero for any value of $L$ and the corresponding wavefunction is a constant, which normalized according to (18), equals

$$\Phi_i^{(0)} = \frac{1}{\sqrt{(aL)^3}}$$

(21)
All excited state energies depend on the lattice size and decreases asymptotically like $1/(aL)^2$, a regime already reached with a number of lattice points $L \sim 10$ for the first excitation. The lowest part of the free spectrum is displayed in figure 6. One can remark the high degeneracy of the states.

Figure 7: Evolution of the first free $\epsilon_n(L)$ trajectories (solid lines) with the interaction strength in the Yukawa model. Results correspond to $G = 0.4$ (dotted) and $G = 1.5$ (dashed), both below the bound state threshold and $G = 2.5$ (dotted-dashed) where the two-body systems has a bound state with $\epsilon_0 = -0.12$.

The generic evolution of the free trajectories when increasing the interaction is displayed in Figure 7. The ground $\epsilon_0(L)$ and first excited $\epsilon_1(L)$ state energies are plotted as a function of the lattice size $L$ for different values of coupling constant $G$.

In the attractive case we are considering, the ground state energy $\epsilon_0$ becomes negative and $L$-dependent. For $G < G_0$, i.e. before the appearance of the first bound state, the excited states remain with positive energy and all trajectories tend to zero in the limit $(aL) \to \infty$. This behaviour is illustrated for $G = 0.4$ (dotted line) and $G = 1.5$ (dashed line) in figure 7. In this range all states tend to the free solutions $\epsilon_n(L) \to \epsilon_n^{(0)}(L)$ for large enough values of the lattice size.

When $G_0 < G < G_1$ the ground state trajectory $\epsilon_0(L)$ tends to a non zero negative value corresponding to the infinite volume binding energy $\epsilon_0$ while the first excited state $\epsilon_1(L)$ tends to zero as for the $G < G_0$ case. Results corresponding to $G = 2.5$ are displayed in figure 7 in dot-dashed line. The sign of the $\epsilon_1(L)$ will in fact depend on the value of $G$. For $G$ close to
the first bound state pole \( G_0 \) (see figure 3), \( \epsilon_1(L) \) is always positive while for larger values of \( G \), close to the second bound state singularity \( G_1 \), \( \epsilon_1(L) \) is negative. The change of sign depends actually on \( L \) but for large enough lattice sizes it corresponds to the zero of \( A_0(G) \).

It is interesting to remark that despite the singular behaviour of \( A_0(G) \) displayed in figure 3, the \( G \)-dependence of \( \epsilon_n(L) \) at a fixed lattice size remains smooth even when crossing the bound state singularities. This is illustrated in figure 8 where the \( \epsilon_n(G) \) dependence is shown for two different values of \( aL \). Notice the change of sign of \( \epsilon_1(L) \) at \( G \approx 4.5 \) for which \( A_0(G) \approx 0 \).

A striking difference between the free and the interacting case – not clearly manifested in figure 7 – is the \( \epsilon_n(L) \) dependence in the limit of small lattice sizes. We will see in the next section that for interacting systems, this dependence is \( \sim \frac{G}{(aL)^3} \) while for the free case they behave like \( \sim \frac{n^2}{(aL)^3} \).

The behaviour described above is qualitatively the same in all the intervals \( G_n < G < G_{n+1} \) of the coupling constant for the corresponding \( \epsilon_n(L) \) state.

![Figure 8: Dependence of \( \epsilon_n(L) \) on the coupling constant at fixed lattice size. Results correspond to \( aL = 4 \) (solid line) and \( aL = 6 \) (dashed) with \( a = 0.1 \).](image)

Whatever the value of the interaction strength, the two-body spectrum in a finite box is always discrete. The main achievement of Luscher and collaborators is to take profit of the \( L \)-dependence of \( \epsilon_n \) – or more precisely of the differences \( \epsilon_n - \epsilon_n^{(0)} \) – to extract the infinite volume low energy parameters and bound state energies. Such a possibility will be discussed in the next subsections.
4.1 Low energy scattering parameters

For a coupling constant $G < G_0 = 1.68$, the two-body system in the infinite volume has only
scattering states while in a finite box the spectrum is constituted by a series of discrete values.

In his first work devoted to this subject [3], Luscher established a relation between
the two-body binding energy $\epsilon_n(L)$ on a 3-dimensional spacial lattice with periodic boundary
conditions and the corresponding scattering length. For the $S$-wave ground state energy $\epsilon_0(L)$
it reads [22]

$$\epsilon_0(L) = \frac{4\pi A_0}{(aL)^3} \left\{ 1 + c_1 \left( \frac{A_0}{aL} \right) + c_2 \left( \frac{A_0}{aL} \right)^2 + \ldots \right\}$$  \hspace{1cm} (22)

where $A_0$ is the infinite volume scattering length and $c_1 = 2.837297$ and $c_2 = 6.375183$ are
universal constants, independent of the details of the particular dynamics. This relation was
proved to be valid in non relativistic quantum mechanics as well as in quantum field theory and
must be considered as an asymptotic series on powers of $A_0/(aL)$. For attractive potentials,
and with our convention for the scattering length, one has $A_0(G < G_0) < 0$ and consequently
$\epsilon_0(L) < 0$.

Equation (22) is the most popular of the Luscher relations and has been widely used
in lattice calculations to extract the value of $A_0$ from a fit to the computed $\epsilon_0(L)$. We adopt a
slightly different point of view by constructing from the $\epsilon_0(L)$ values, quantities tending to $A_0$
– the quantity we are interested in – for large values of $aL$. This merely consists in inverting
(22).

To this aim it is interesting to consider slowly varying functions and to use – rather
than $\epsilon_0(L)$ – the combination

$$A_0^{(0)}(L) \equiv \frac{1}{4\pi} (aL)^3 \epsilon_0(L)$$ \hspace{1cm} (23)

It tends asymptotically ($aL \to \infty$) to the infinite volume scattering length $A_0$ and constitutes
the zero-th order approximation of Luscher expansion which can be written as

$$A_0^{(0)}(L) = A_0 \left\{ 1 + c_1 \left( \frac{A_0}{aL} \right) + c_2 \left( \frac{A_0}{aL} \right)^2 + \ldots \right\}$$ \hspace{1cm} (24)

It is possible to get a series $A_0^{(n)}(L)$ of improved values converging towards $A_0$ by solving
equation (24) truncated at the order $n$ for a fixed value of $L$. One thus obtains, for instance

$$A_0^{(2)}(L) = aL \ z^{(2)}$$ \hspace{1cm} (25)

where $z^{(2)}$ is a solution of the cubic equation

$$z(c_2z^2 + c_1z + 1) = \frac{A_0^{(0)}(L)}{aL}$$

This expansion is however of small practical interest for it requires lattice sizes one or
two order of magnitude larger than the scattering length, as it was already noticed in reference [9].

Figure 9 represents the $A_0^{(0)}(L)$ results for the ground state obtained with $G = 0.40$
and $a = 0.20$. Dashed lines correspond to the solutions with the infinite volume interaction.
$V$ alone and continuous line with the full interaction $V_L$ in (14). In both cases, $A_0^{(0)}$ tends indeed asymptotically towards the physical value $A_0 = 0.501$ (horizontal dotted line) in very good agreement with the results given in Table 2 with the same value of $a$, but the convergence is very slow. Even for computing such a scattering length value, small with respect to the lattice sizes, a consequent number of grid points would be required. With $aL = 10$ only a 20% accuracy is reached. One can also remark the sizeable effects of the ”interactions with the surrounding world” below $aL \approx 10$; these contributions – which are absent in the pionless EFT considered in [9] – are essential in providing the very smooth variation of $A_0^{(0)}(L)$ observed in the whole range of $aL$.

![Figure 9: Zero-th order scattering length $A_0^{(0)} = (aL)^3 \varepsilon_0/4\pi$ for $G = 0.4$ and $a = 0.2$ obtained with the infinite volume potential $V$ alone (dashed line) and (solid line) with the full lattice potential $V_L$.](image)

![Figure 10: Wavefunctions corresponding to the results of figure 9 for selected values of $L$ and normalized according to (18).](image)

Corresponding wavefunctions – normalized according to (18) – for $L = 40, 60, 100$ are displayed in Figure 10. For small values of $L$ they look similar to the bound states ones (see next subsection) but their central values depends strongly on the lattice size. Outside the interaction region the wave function behaves – according to (10) – like $\Phi(x) \sim 1 + \frac{A_0}{x}$ and would thus provide an alternative way to extract $A_0$ in case it was numerically accessible. In the infinite volume limit they spread over all the lattice with constant amplitude, like in the free case.

The behaviour illustrated in figure 9 is in fact generic and easy to understand. On one hand we have shown (see Appendix B) that, under reasonable assumptions, the $aL \to 0$ limit of $A_0^{(0)}$ is finite. For the Yukawa model it gives

$$\lim_{aL \to 0} A_0^{(0)}(L) = -G$$  \hspace{1cm} (26)

On the other hand, the large $aL$ limit is, by construction,

$$\lim_{aL \to \infty} A_0^{(0)}(L) = A_0(G)$$
with $A_0(G)$ given in figure 3. For small values of the coupling constant, the L-dependence of $A_0^{(0)}$ is almost flat due to the fact that $A_0(G) \approx -G$ but for increasing values of $G$ the presence of the bound state pole in figure 3 makes the variation range increasingly large.

The inclusion of first and second order corrections in (24) – i.e. $A_0^{(1)}$ and $A_0^{(2)}$ – does not significantly improve this situation, specially when dealing with large scattering length values. This will be illustrated below. On the other hand it is inconvenient to include higher order terms since the additional coefficients involved depend on dynamical parameters others than $A_0$ [2].

![Figure 11: Function $S(\eta)$ defined by (28)](image)

Equation (22) is in fact a large-$L$ expansion of a more general relation established in [3] between the two-body phase shifts and the corresponding energy eigenstates on a finite size box. For the ground state and using the notations of reference [9] it reads

$$k \cot \delta_0(k) = \frac{1}{\pi a L} S(\eta)$$

where

$$\eta = \frac{(aL)^2 \epsilon_0(L)}{4\pi^2} = \frac{A_0^{(0)}}{\pi a L}$$

$k^2 = \epsilon_0(L)$ and $S$ is a universal function, independent of the interaction model, defined by

$$S(\eta) = \lim_{\Lambda \to \infty} \sum_{n \in \mathbb{Z}^3} \frac{1}{n^2 - \eta} - 4\pi \Lambda$$

It is represented in figure 11. The domain of interest for the ground state is $\eta < 0$.

It is worth noticing that equation (27) is exact for lattice sizes $aL > 2R$ where $R$ is the interaction range, i.e. $V(x > R) = 0$. For interactions of physical interest this regime is reached exponentially and independently of the coupling constant and the $A_0$ value. This constitutes a remarkable advantage with respect to expansion (22).
Using the effective range expansion (12) one finds the following relation between the low energy parameters and the eigenenergies \( \epsilon_0(L) \)

\[
- \frac{1}{A_0} + \frac{1}{2} R_0 \epsilon_0(L) = \frac{1}{\pi a L} S \left( \frac{(aL)^2 \epsilon_0(L)}{4\pi^2} \right)
\]  

By setting \( R_0 = 0 \), this relation can be written in the form

\[
\epsilon_0(L) = \left( \frac{2\pi}{a L} \right)^2 S^{-1} \left( -\frac{a L}{A_0} \right)
\]

where \( S^{-1} \) denotes the reciprocal function of \( S \). The Luscher expansion (22) is recovered by developing \( S^{-1} \) for \( z \to \infty \) in power series of \( 1/z \): \( S^{-1}(z) = -\frac{1}{2} + \frac{a L}{R_0} - \frac{a L}{R_0^2} + \ldots \).

Equation (29) suggests the possibility to obtain \( A_0 \) as a function of \( \epsilon_0(L) \) … provided \( R_0 \) is known, which is in general never the case.

To check the applicability of (29) in the Yukawa model we fix the \( R_0 \) value from the infinite volume results given on table 2 and study the convergence of the scattering length thus obtained as a function of the lattice size \( aL \). We denote by \( A_0^{(s)}(L) \) the quantity extracted this way, i.e.:

\[
A_0^{(s)}(L) = \frac{\pi a L}{\frac{1}{2} \pi R_0 (aL) \epsilon_0(L) - S \left[ \frac{(aL)^2 \epsilon_0(L)}{4\pi^2} \right]}
\]

It generalizes the series of values \( A_0^{(n)}(L) \) define above.

Figure 12 shows the results for \( G = 0.40 \) and \( a = 0.20 \), the same parameters than those used in figure 9. Only results including the fully lattice potential \( V_L \) are hereafter shown. Several remarks are in order: (i) \( A_0^{(2)} \) represents an improvement with respect to \( A_0^{(0)} \) for \( aL \gtrsim 5 \), but it is significant only in this particular case due to the smallness of \( A_0/aL \) at small values of \( G \). (ii) \( A_0^{(s)} \) is practically converged at \( aL \approx 5 \), distance at which \( A_0^{(0)} \) remains almost unchanged with respect to its value at \( aL = 0 \) i.e. to the Born approximation (iii) the effective range contribution is sizeable: if \( R_0 \) is neglected – dashed curve obtained setting \( R_0 = 0 \) in (29) – the improvement with respect to \( A_0^{(2)} \) – and for \( aL \lesssim 5 \) even to \( A_0^{(0)} \) – disappears.

Similar results are displayed in figure 13 for a value of the coupling constant \( G = 1.5 \) near the bound state singularity and a lattice space \( a = 0.10 \). The infinite volume scattering length – with \( a = 0.10 \) – is \( A_0 = -11.4 \). It corresponds to \( a_0 = \frac{4\pi a}{\mu} \approx -16 \) fm if a pion exchange \( (\mu = 0.14 \text{ GeV}) \) is supposed to govern the two-body interaction. This value is close to the experimental \(^1\)S\(_0\) nucleon-nucleon scattering length. One can see from this figure that, despite the large \( A_0 \) value, the convergence of \( A_0^{(s)}(L) \) is the same as in Figure 12: a few % accuracy is already reached at \( aL \approx 5 \). The effective range contribution is here essential: by setting \( R_0 = 0 \) in (30) one would get a result wrong by a factor two (dashed curve) even at \( aL = 10 \). Note that for small lattices, \( A_0^{(0)}(L) \) is practically constant – i.e. \( \epsilon_0(L) \) displays a \( 1/L^3 \) behaviour – but this constant differs from \( A_0 \) by one order of magnitude. One can also remark the slow convergence of \( A_0^{(2)} \), which, contrary to the \( G = 0.4 \) case, provides practically the same results than \( A_0^{(0)} \): even at \( aL = 10 \) they differ from the asymptotic value \( A_0 \) by a factor 4.

The preceding results show the applicability of (29) in extracting the scattering length \( A_0 \) for all cases of physical interest, provided that the effective range \( R_0 \) is taken into account. In practice, both values could be determined by fitting the computed finite size energies \( \epsilon_0(L) \) with
The two-parameter function (29) for $aL \gtrsim 5$. This procedure is however not very comfortable for the fitting function (29) is defined implicitly. We alternatively propose to determine $A_0$ and $R_0$ by computing the energies $\epsilon_0(L)$ at two different lattice sizes near $aL = 5$ and solving the linear system resulting from (29). This gives, e.g. for the effective range

$$R_0 = \frac{2}{\pi} \frac{\frac{1}{aL_1} S \left( \frac{(aL_1)^2 \epsilon_0(L_1)}{4\pi^2} \right) - \frac{1}{aL_2} S \left( \frac{(aL_2)^2 \epsilon_0(L_2)}{4\pi^2} \right)}{\epsilon_0(L_1) - \epsilon_0(L_2)}$$

(31)

The results obtained using this procedure for $G = 1.5$ are given in table 3. The corresponding infinite volume values calculated with $a = 0.10$ are respectively $A_0 = -11.4$ and $R_0 = 2.47$. One sees from these results that a lattice size $aL \approx 6$ provides an $A_0$ value better than $3\%$ though the accuracy for $R_0$ is slightly worse. The inclusion of an additional term – $P^4$ – in the low energy expansion (12) does not improve the results.

It could have some interest to summarize the different results obtained with equation (29) depending on the way $R_0$ is taken into account. This is done in figure 14 for $G = 1.5$. Solid line corresponds to the result of table 3 with an averaged value on abscissa $aL = 0.5a(L_1 + L_2)$ – where the two parameters $A_0$ and $R_0$ are simultaneously determined. Dotted-dashed and dotted lines are the same than in figure 13 and correspond respectively to $R_0$ taken from Table 2 and $R_0 = 0$. Notice the different kind of convergence for $A_0^{(S)}$ and the key role of $R_0$. 

Figure 12: Different approximations used in calculating the scattering length from energy eigenstates: $A_0^{(0)}$ defined in (23), $A_0^{(2)}$ obtained by solving the cubic equation (25), $A_0^{(S)}$ given by (30) with $R_0 = 0$ (dashed line) and with $R_0$ taken from the infinite volume results on table 2 (dotted line).
Figure 13: The same as figure (12) for a coupling constant $G = 1.5$ near the bound state pole. $A_0^{(S)}$ is practically converged at $aL \sim 5$, a lattice size smaller than the infinite volume scattering length $A_0(G) = 11.4$ (horizontal dotted line). Note that for small lattice, $A_0^{(0)}$ is practically constant – i.e. $\epsilon_0(L)$ displays a $1/L^3$ behaviour – but this constant differs from $A_0$ by one order of magnitude.

This method applies well in all the range of coupling constants. We would like to make some final comments concerning the extraction of $A_0$. The usual way of doing so is by first fitting the $L$-dependence of the finite volume energies by a $c/(aL)^3$ curve and identifying the coefficient $c$ with $4\pi A_0$. In our notations, this is equivalent to use the $A_0^{(0)}$ value, which is the leading term of Luscher expansion (24). As we have previously shown, this approach can lead to wrong conclusions when using nowadays available lattice sizes, unless the coupling constant – and consequently the scattering length – is very small. In this case $A_0$ is already given by the Born approximation. For the Yukawa model – and for small values of the lattice size – it actually coincides with $-G$.

As one can see from figures 12 and 13, $A_0^{(0)}(L)$ varies very smoothly even for almost resonant systems. Thus, when using lattice sizes $aL \sim 2 - 3$, $\epsilon_0(L)$ will be well fitted by a $c/L^3$ dependence but, as we have shown in these examples, the coefficient $c$ can strongly differ from the infinite volume scattering length. Only the use of equation (29) at lattice sizes greater than the interaction range – $aL \gtrsim 5$ in the Yukawa model – could lead to unambiguous extraction of the low energy parameters, provided both $A_0$ and $R_0$ are taken into account.

Finally, we would like to notice that equation (26) – corresponding to a $\epsilon_0(L) \approx -\frac{G}{(aL)^3}$ behaviour of the ground state eigenenergy – depends only on general properties of the interaction as we have shown in Appendix B. This result is totally independent of the Luscher relation.
Table 3: Low energy parameters extracted from ground state energy at different lattice sizes $\epsilon_0(L)$ by mean of equations (31) and (29). They correspond to $G = 1.5$ and $a = 0.1$. Last row indicates the infinite volume results.

| $aL_1$ | $aL_2$ | $R_0$ | $A_0$ |
|--------|--------|-------|-------|
| 4.0    | 4.60   | 1.9   | -28.8 |
| 4.6    | 5.00   | 2.1   | -17.2 |
| 5.0    | 5.60   | 2.3   | -13.9 |
| 5.6    | 6.00   | 2.4   | -12.5 |
| 6.0    | 7.0    | 2.5   | -11.7 |
| 7.0    | 8.0    | 2.6   | -11.3 |
| 8.0    | 10.0   | 2.6   | -11.3 |
| 10.0   | 12.0   | 2.6   | -11.4 |
| Inf. volume | 2.47 | 11.4 |

and they have even different domains of applicability, namely $aL << 1$ and $aL >> 1$. It is striking to note that $\epsilon_0(L)$ has, in both limits, the same $L$-dependence.

The results presented above concern the S-wave ground state energy $\epsilon_0(L)$. For excited states, Luscher expansion (22) reads

$$\epsilon_n(L) = \epsilon_n^{(0)}(L) + \Delta_n(L)$$

with $\epsilon_n^{(0)}(L)$ given by (20) and $\Delta_n(L)$ having the same form with different values for the coefficients $\epsilon_i$. In practice it has the same drawbacks as those described for the ground state. Equation (29) can be used, in principle, to obtain $A_0$ from the first excited state energy $\epsilon_1(L)$, now with $\eta > 0$. At large values of $aL$, the L-dependence of excited states $\epsilon_n(L)$ is however dominated by the $1/(aL)^2$ term of free solutions $\epsilon_n^{(0)}(L)$, thus making the calculations numerically more difficult. It is worth noticing that in the limit $aL \to 0$, all the excited states tend to the same value than $\epsilon_0$ but this limit is reached at lattice sizes increasingly small (see Appendix B). This behaviour is illustrated in figure 15 for the case $G = 0.4$.

4.2 Bound states

Bound states are not affected by the "no go" theorem in the euclidean formulation [1] and can be directly computed on lattice simulations at finite volume. However, the finite size effects are often non negligible in practice and can be controlled by similar expressions than those used for scattering states. In addition, the determination of their binding energies in finite size lattice calculations is made difficult by the existence of another length scale, independent of the interaction range, given by the size of the state.

In his pioneer work [2] Luscher established the following relation between the ground state energy $\epsilon_0$ of a non relativistic two body system and its value $\epsilon(L)$ computed in a finite size box with periodic boundary conditions [20]:

$$\epsilon(L) = \epsilon_0 - 6N_s^2 e^{-\kappa_0 aL}$$

where $\kappa_0 = \sqrt{-\epsilon_0}$ is the corresponding wave vector and $N_s$ the asymptotic norm, defined in [9], and determining the large $x$ behaviour of the wavefunction [11].
Figure 14: Different results obtained with equation (29) depending on the value given to $R_0$. Solid line corresponds to the results of table 3 with an averaged value on abscissa $aL = 0.5a(L_1 + L_2)$ where the two parameters are simultaneously determined. Dotted-dashed and dotted correspond respectively to $R_0$ taken from Table 2 and $R_0 = 0$.

Figure 15: L-dependence of the ground $\epsilon_0$ and first energy $\epsilon_1$ states for $G = 0.4$ in the limit of small lattice sizes. All states converge to the same value, with different slopes depending on their quantum number.

The two-body energy in a box $\epsilon(L)$ tends exponentially towards the infinite volume bound state binding energy $\epsilon_0$. However its decreasing rate $\kappa_0$ contains already the required
information and can be consequently extracted well before the asymptotic region is reached.

We first present the results concerning a deeply bound state. They have been obtained with \( G = 4.0 \) and \( a = 0.1 \) and the \( \epsilon(L) \) dependency is displayed in Figure 16. The asymptotic value \( \epsilon_0 = -1.16 \) is in good agreement with the results of Table II with the same lattice spacing \( a = 0.10 \). Although this value is reached – at 1\% accuracy – from \( aL = 6 \), the same accuracy can be obtained by doing a two-parameter fit with function 32 in the region \( aL \in [3, 4] \), where \( \epsilon_0(L) \) is far from being converged.

![Figure 16: L-dependence of the ground state binding energy in the dimensionless Yukawa model with \( G = 4 \) and \( a = 0.1 \). Dashed line corresponds to one single term \( V \) in expansion (14) and solid line to the full interaction \( V_L \). Horizontal dotted line indicates the infinite volume result.](image)

![Figure 17: Wavefunctions corresponding to figure 16 for different values of L.](image)

Corresponding wavefunctions, normalized according to 18, are displayed in Figure 17 for different lattice sizes. The periodic boundary conditions give rise to non vanishing values at the lattice edges, which are reminiscent of the free ground state solution 21. The characteristic length of this state is \( \rho = \sqrt{\langle x^2 \rangle} = 1.07 \), smaller than the interaction range \( R \) of the potential 8. One can thus expect that, like for the scattering states, its properties would be well defined at \( aL \sim 5 \). At distances greater than the interaction range, the wavefunctions are not sensible to the boundary conditions and show the typical exponential behaviour of the bound states. On the contrary at small values of lattice sizes, they look very similar to the scattering states displayed in figure 10. The difference between bound and scattering wavefunctions can be formalised by the parameter \( s(L) = \frac{\Phi(L)}{\Phi(0)} \) which tends exponentially to 0 (bound) or like \( 1/(aL) \) to 1 (scattering) at large \( aL \) values.

In analogy with what we have done for scattering states, it is possible to extract both \( \epsilon_0 \) and \( N_a \) by writing relation 32 at two different lattice spacings. The binding energy is thus
determined by the solutions of the non linear equation

$$\frac{\epsilon_{L_1} - \epsilon_0}{\epsilon_{L_2} - \epsilon_0} = \frac{L_2}{L_1} e^{-\sqrt{-\epsilon_0} a(L_1 - L_2)}$$  \hspace{1cm} (33)$$

Corresponding results for $G = 4.0$ and $a = 0.1$ are given in Table 4:

| $aL_1$ | $aL_2$ | $\kappa_0$ | $\epsilon_0$ |
|-------|-------|-----------|-------------|
| 2.0   | 3.0   | 1.14      | -1.30       |
| 3.0   | 4.0   | 1.09      | -1.19       |
| 4.0   | 5.0   | 1.08      | -1.16       |
| 5.0   | 6.0   | 1.08      | -1.16       |
| Inf. volume | 1.07 | -1.15 |

Table 4: Ground states energy for $G = 4.0$ and $a = 0.1$ by solving equations (33) at different lattice sizes. Infinite volume results are taken from table 1 with the same value of $a$.

The binding energy and characteristic length of this example roughly correspond to the physical case of $^4$He nuclei. Indeed, by inserting the $\epsilon = -1.16$ and $\mu/M = 0.15$ in equation (6) one gets a binding energy in units of nucleon mass $E/M = -0.026$ while the experimental value for $^4$He is $E/He/M = -0.030$.

The situation is less comfortable when dealing with loosely bound states. An example, close to the deuteron, is obtained with $G = 2.5$ for which $\epsilon = -0.136$ and, according to (6), $E/M = -0.003$. Corresponding results are displayed in figures 18 and 19. The convergence of

$\epsilon(L)$ is reached in this case at $aL \geq 15$ due to the larger size of the state, for which $\rho = 2.5$. It is however possible, by using equation (33), to reach already a few percent accuracy in the range $aL \in [8, 10]$. Results obtained this way are given in Table 5.
These examples indicate that the critical lattice size is not given by the interaction range but by the size of the bound state itself. It is nevertheless possible by means of equation (33) to access the binding energies of loosely bound states like deuteron. Notice however, that in order to have a few percent accuracy on the binding energy, a consequent number of lattice points $L \sim 100$ would be in this case required.

The limit $aL \to 0$ of $\epsilon_0(L)$ obtained in Appendix B holds for bound as well as for scattering ones: in both cases the eigenenergies display the $1/L^3$ law given by equation (26). The differences in $\epsilon_0(L)$ appear clearly in the regions where the interaction plays no role, which in the Yukawa model is at $aL \approx 5$. They are manifested by calculating the quantity $(aL)^3\epsilon_0(L)/(4\pi G)$ – which corresponds to $A_0^{(0)}/G$ of the previous section – and comparing the results for bound and scattering states. This has been done in figure 20 for increasing values of $G$. For the bound state case (solid lines) one can see a cubic divergence corresponding to $\epsilon_0$ term in (32). For scattering states (dashed lines) one observe a linear dependence before reaching an horizontal asymptote $A_0(G)/G$. Both behaviours are easy to disentangle in the extreme cases of deeply bound state or small scattering length but it becomes increasingly difficult when approaching resonant scattering and/or loosely bound state, unless huge number of lattice points are used.

5 Conclusion

We have obtained the solutions of the non relativistic Yukawa model (11) in a 3-dimensional lattice with periodic boundary conditions and examined the possibility to extract infinite volume low energy parameters – scattering length $A_0$ and effective range $R_0$ – and bound state binding energies from the computed eigenstates $\epsilon_n(L)$ at finite lattice sizes $aL$. The eigenenergies $\epsilon_n(L)$, and corresponding eigenfunctions, have been calculated using finite difference schemes and propagation in the euclidean time, in close analogy with the methods used in lattice field theory simulations. The low energy parameters have been independently computed by solving the corresponding one-dimensional Schrodinger radial equation.

We have considered different approximations of the Luscher relations and shown that a lattice size of $aL \approx 5$ – in units of the meson exchanged Compton wave length $\frac{1}{\mu}$ – is enough to determine the low energy parameters at few % accuracy. The method is based in computing the energies at two different lattice sizes and solving a linear system of rank two. Such a possibility is independent of the scattering length value and applies in the resonant case as well. We have
Figure 20: Comparison of the $(aL)^3 \epsilon_0(L)/(4\pi G)$ behaviour for bound (solid lines) and scattering (dotted lines) states. At $aL \to 0$ they all tend to $-1$ as given by (26) but at large $aL$, they manifest either a cubic divergence or a slow $1/L$ convergence towards the asymptotic value $A_0(G)/G$.

found in particular that the effective range $R_0$ plays a crucial role in determining the scattering length value at moderate lattice volumes.

We have shown that in the limit of small lattice sizes, the $L$-dependence of eigenenergies is dominated by an $\epsilon_n(L) = -G/(aL)^3$ term, where $G$ is the strength parameter of the dimensionless potential. This regime is already reached at moderate sizes $aL \lesssim 2$, making ambiguous the extraction of the scattering length by means of Luscher expansion. The behaviour is the same for bound and scattering states and applies to a large class of potentials.

For loosely bound states, the critical lattice size is determined by the spatial extension $\rho$ of the state. We have shown that for the deuteron case it is however possible to get accurate values of the binding energy and asymptotic norm with $aL = 10$. The parameters of deeply bound states are well determined, like for the scattering case, with lattice volumes $aL \approx 5$.

The results have been obtained with a non relativistic model, which is justified by the small energies involved in the calculations. Despite its simplicity, the model considered contains an essential ingredient of the hadron-hadron interaction – its finite range – which plays a relevant role in view of extracting the low energy parameters from the finite volume spectra. It offers a wieldy and physically sound tool to test the validity of the different approaches discussed in the literature to study the low energy scattering of baryon-baryon or meson-baryon systems from a lattice simulations in QCD.

The results presented in this work have been essentially limited to the ground state of central attractive interactions, depending only on one parameter. The method can be easily
applied to more involved interactions, like hard core repulsive terms or non central potentials leading to coupled channel equations.

Acknowledgement

We are warmly grateful to our colleagues J.P. Leroy, Ph. Boucaud, O. Pene (L.P.Th. Orsay) and C. Roiesnel (CPhT Ecole Polytechnique) for many useful discussions during the elaboration of this work. We are indebted to S. Sint for pointing out relevant aspects of Luscher’s work during his visit to LPSC. We thank M. Mangin-Brinet for a critical reading of the manuscript.

A Born approximation

Let us consider the solution of (3) in terms of the equivalent Lipmann-Schwinger equation for the K-matrix

\[ K = U + P.V. \{UG_0K\} \]

where P.V. denotes the principal value. The lowest order in the coupling constant \((g^2)\) is given by the Born term, i.e.

\[ K = U \]

The K-matrix is related to the S-wave phaseshifts \(\delta_0\) at momentum \(k_0\) by

\[ K_0(k_0, k_0) = -\frac{1}{(2\pi)^2 m_R} \tan \delta_0(k_0) \]

where \(K_0\) denotes the on-shell \(L = 0\) term of the \(K\)-partial wave expansion and \(m_R\) the reduced mass of the system. In the limit \(k_0 \rightarrow 0\) on gets

\[ a_0 = (2\pi)^2 m_R K_0(0, 0) \]

The lowest order (Born approximation) is thus given by

\[ a_0(g) = (2\pi)^2 m_R U(0, 0) + o(g^4) \]

where \(U\) must be understood as the \(\vec{k} = \vec{k}' = 0\) matrix element of the potential in momentum space \(U(\vec{k}, \vec{k}')\). For the Yukawa model one has

\[ U(\vec{k}, \vec{k}') = -\frac{1}{(2\pi)^3} \frac{g^2}{\vec{q}^2 + \mu^2} \quad \vec{q} = \vec{k} - \vec{k}' \]

and in case of two identical particles with mass \(M = 2m_R\)

\[ a_0(g) = -\frac{g^2}{4\pi} \frac{M}{\mu^2} + o(g^4) \]

In dimensionless units it reads

\[ A_0(G) = -G + o(G^2) \]

which is our equation (11).
B Small volume limit

We would like to study here the zero volume limit of equation (13) with periodic boundary conditions and a potential of the form (14). To this aim, it is useful to develop the periodic wave function in a Fourier series:

$$\Phi(x) = \sum_{\vec{n} \in \mathbb{Z}^3} C_{\vec{n}} e^{2\pi i \vec{n} \cdot \vec{x}},$$

and similarly for the potential,

$$V_L(x) = \sum_{\vec{n} \in \mathbb{Z}^3} V_{\vec{n}} e^{2\pi i \vec{n} \cdot \vec{x}}$$

By inserting these expressions into equation (13) it results the following infinite system of coupled linear equations:

$$\left[ \left( \frac{2\pi}{aL} \right)^2 \vec{n}^2 - E \right] C_{\vec{n}} + \sum_{\vec{n} \in \mathbb{Z}^3} V_{\vec{n}-\vec{n}'} C_{\vec{n}'} = 0 . \quad (34)$$

The Fourier coefficients of the potential, $V_{\vec{n}}$, take a rather simple form due to the interactions with the "surrounding world",

$$V_{\vec{m}} = \begin{cases} \frac{-4\pi G (aL)^3}{m} & \vec{m} = (0, 0, 0) \\ \frac{-4\pi G (aL)^3}{m} \frac{m \pi}{aL} & \vec{m} \neq (0, 0, 0) \end{cases}$$

For the dimensionless Yukawa potential, $V_{\vec{0}}$, they read:

$$V_{\vec{m}} = \begin{cases} -\frac{4\pi G}{(aL)^3} & \vec{m} = (0, 0, 0) \\ -\frac{4\pi G}{(aL)^3} \frac{\frac{m \pi L}{aL}}{1 + \left( \frac{m \pi L}{aL} \right)^2} & \vec{m} \neq (0, 0, 0) \end{cases}$$

The leading term in the small volume limit is given by $V_{\vec{0}}$. Neglecting other components, the system of equations (34) decouple into

$$\left[ \left( \frac{2\pi}{aL} \right)^2 \vec{n}^2 - \epsilon \right] C_{\vec{n}} + V_{\vec{0}} C_{\vec{n}} = 0 ,$$

and the eigenenergies are given by:

$$\epsilon_{\vec{n}}(L) = V_{\vec{0}} + \left( \frac{2\pi}{aL} \right)^2 \vec{n}^2 = -\frac{4\pi G}{(aL)^3} + \left( \frac{2\pi}{aL} \right)^2 \vec{n}^2 . \quad (36)$$

They correspond to the continuum limit of the free result (20) shifted by a constant potential of depth $V_{\vec{0}}$. 

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One has for the ground state

\[ \epsilon_0(L) = -\frac{4\pi G}{(aL)^3} \]  

(37)

a result which is equivalent, and prove, equation (26). Notice that in the limit \(aL \to 0\) all the excited states \(\epsilon_n\) display also the same \(\frac{1}{(aL)^3}\) behaviour and furthermore they all tend to the same value \(\epsilon_0(L)\), independently of \(n\). The lattice size at which they become negative \(aL = \frac{G}{\pi n^2}\) are however increasingly small.

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