EFFECTIVE RANGE EXPANSION FOR THE INTERACTION DEFINED ON THE LATTICE

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The relation between the interaction parameters for fermions on the spatial lattice and the two-body $T$ matrix is discussed. The presented method allows determination of the interaction parameters through the relatively simple computational scheme which include the effect of finite lattice spacing. In particular the relation between the interaction parameters and the effective range expansion parameters is derived in the limit of large lattices.

1. Introduction

One of the most promising approaches to describe the nonrelativistic many-fermion system is to define the problem on the spatial lattice and subsequently apply the Monte Carlo technique to probe the configuration space. This approach is particularly efficient when dealing with strongly interacting and dilute systems. In the limit of low densities the interaction between particles has predominantly two-body character. Moreover it can be described by few parameters only, characterizing the low energy physics of two-body collisions. For example in the case of trapped fermionic atoms, which have been recently the subject of intensive theoretical studies (see and references therein), the scattering length is the only parameter which determines the interatomic interaction. Similarly, the physics of dilute neutron matter at densities corresponding to $k_F \lesssim 0.6 \text{ fm}^{-1}$ is captured by two parameters: scattering length and effective range in the $^1S_0$ channel.

The basic problem of the lattice formulation is the determination of the Hamiltonian parameters in order to describe properly the scattering phase shifts of two-body collisions. The prescription given by Lüscher relates the discrete energy spectrum of two-particle states in a box to the scattering phase shifts. However in order to use the Lüscher’s formula, the exact two-particle energy spectrum has to be determined first, which in general is a nontrivial task. Another prescription, given by Seki and Kolck for the case of large lattices, is more suitable for the low-energy nuclear problems. In this approach the interaction parameters are determined by
consistently applying the effective field theory power counting rules.

In this paper we present an alternative approach to determine the two-body interaction parameters. The method is especially well suited to deal with the discrete form of the interaction, commonly used in the lattice calculations. All finite lattice spacing effects are properly included in the limit of large lattice volume. The final prescription bypass the tedious Lüscher’s algebra leading to a simple expression convenient for practical applications.

2. Interaction on the lattice

To capture the low energy physics of a Fermi system let us consider the interaction which depends only on the relative coordinates of two particles:

\[ \hat{V} = \frac{1}{2} \sum_{\lambda,\lambda'=\uparrow\downarrow} \int d^3r d^3r' \hat{\psi}_{\lambda}^\dagger(r) \hat{\psi}_{\lambda'}^\dagger(r') V(r-r') \hat{\psi}_{\lambda'}(r') \hat{\psi}_{\lambda}(r), \]  

(1)

where the field operators obey the fermionic anticommutation relations \( \{\hat{\psi}_{\lambda}^\dagger(r), \hat{\psi}_{\lambda}(r')\} = \delta_{\lambda\lambda'} \delta(r-r') \) and \( \lambda \) denotes the spin degree of freedom. In order to place the system on a 3D spatial lattice with lattice spacing \( b \) and size \( L = N_s b \) the discretization of the above expression has to be performed. This leads to the replacement: \( \hat{\psi}_{\lambda}(r) \to \hat{\psi}_{\lambda}(r_i) \), where \( r_i = ib \) and \( i = (i_x, i_y, i_z) \) denotes lattice sites, and \( i_x, i_y, i_z = 1, \ldots, N_s \). Consequently one gets instead of (1):

\[ \hat{V} = \frac{1}{2} b^6 \sum_{\lambda,\lambda'=\uparrow\downarrow} \sum_{i,j} \hat{\psi}_{\lambda}^\dagger(r_i) \hat{\psi}_{\lambda'}^\dagger(r_j) V(r_i-r_j) \hat{\psi}_{\lambda'}(r_j) \hat{\psi}_{\lambda}(r_i). \]  

(2)

Note that for the problem defined on the lattice, we need only a discrete set of values of the interaction potential defined for the lattice sites \( R_{k(i,j)} = r_i - r_j \). Hence it is sufficient to introduce the interaction on the lattice which is defined only on the lattice sites. It can be written in the form:

\[ V(r-r') = \sum_{k=1}^{D} g_k \delta(r-r' - R_k). \]  

(3)

The coupling constants \( g_k \) contain the full information about the interaction between the particles. The simplest case corresponds to the on-site interaction when \( g_k \) is nonzero only when \( R_k = (D = 1) \). A more complicated case when the neighboring sites are included leads to the so called extended Hubbard model (\( D = 7 \), widely used in Monte Carlo simulations (see [7] and references therein). It requires effectively two coupling constants (due to the rotational invariance of the Hamiltonian): \( g_0 \) for \( R = (0,0,0) \) (on-site interaction) and \( g_1 \) for \( R \in \{(\pm b,0,0),(0,\pm b,0),(0,0,\pm b)\} \) (nearest-neighbor interaction). Then the interaction reads:

\[ \hat{V} = g_0 b^6 \sum_i \hat{n}_\uparrow(r_i) \hat{n}_\downarrow(r_i) + \frac{g_1}{2} b^3 \sum_{\lambda,\lambda'=\uparrow\downarrow} \sum_{<i,j>} \hat{n}_{\lambda}(r_i) \hat{n}_{\lambda'}(r_j), \]  

(4)

where \( \hat{n}_{\lambda}(r_i) = \hat{\psi}_{\lambda}^\dagger(r_i) \hat{\psi}_{\lambda}(r_i) \), and \( <i,j> \) denotes the summation over all neighboring pairs.
3. $T$ matrix for the lattice interaction

In order to link the coupling constants $g_k$ to the phase shifts one has to consider the $T$ matrix, which in the case of low energy scattering can be parametrized as:

$$-\frac{4\pi}{m}T^{-1}_{pp} \approx -\frac{1}{a} + \frac{1}{2}r_{\text{eff}}p^2 - ip + O(p^4),$$

where $a$ is the scattering length and $r_{\text{eff}}$ denotes the effective range. The $T$ matrix fulfills the Lippmann-Schwinger equation:

$$T_{pp'} = V_{pp'} + \frac{1}{L^3} \sum_k V_{pk}G_{p'k}T_{kp'},$$

where $G_{pp'} = m/(p^2 - p'^2)$ is the free particle propagator with the reduced mass $m/2$. Summation over momenta is limited to the first Brillouin zone i.e. $-\pi/b \leq p_{x,y,z} \leq \pi/b$, and each momentum component is discretized due to the box quantization conditions. As a first step, let us rewrite Eq. (6) in an iterative form, more suitable for numerical applications. Expanding the Lippmann-Schwinger equation one obtains:

$$T_{pp'} = V_{pp'} + \frac{1}{L^3} \sum_k V_{pk}G_{p'k}V_{kp'} + \frac{1}{L^6} \sum_{k,k'} V_{pk}G_{p'k'}V_{kk'}G_{p'k'}V_{k'p'} + \ldots$$

If we define the matrix $M^{(1)}$ as:

$$M^{(1)}_{pp'} = \frac{1}{L^3} \sum_k V_{pk}G_{p'k}M^{(0)}_{kp'},$$

where $M^{(0)}_{pp'} = V_{pp'}$ then Eq. (7) takes the form:

$$T_{pp'} = M^{(0)}_{pp'} + M^{(1)}_{pp'} + \frac{1}{L^3} \sum_k V_{pk}G_{p'k}M^{(1)}_{kp'} + \ldots$$

Clearly the $T$ matrix can be written as an infinite sum:

$$T_{pp'} = \sum_{n=0}^{\infty} M^{(n)}_{pp'},$$

where the $M^{(n)}$ matrices are related to each other through the recurrence relation:

$$M^{(n+1)}_{pp'} = \frac{1}{L^3} \sum_k V_{pk}G_{p'k}M^{(n)}_{kp'},$$

$$M^{(0)}_{pp'} = V_{pp'}.\tag{12}$$

The equation Eq. (10) holds in general case. However in the case when the effective range expansion Eq. (5) is valid, only the diagonal matrix elements are required. For the lattice interaction given by Eq. (3) the contribution $M^{(0)}$ takes the following form:

$$M^{(0)}_{pp} = \sum_{i=1}^{D} g_i e^{-ipR_i} e^{ipR_i} = \text{Tr} \, L^{(0)},$$

$$L^{(0)} = \sum_{i=1}^{D} g_i R_i.$$
where the square matrix $L^{(0)}$ of dimension $D \times D$ is defined as:

$$L_{ij}^{(0)} = g_i e^{-ip(R_i - R_j)}. \quad (14)$$

The contribution to $M^{(1)}$ reads:

$$M_{pp}^{(1)} = \sum_{i,j=1}^{D} g_i g_j e^{-ip(R_i - R_j)} G_p(R_j - R_i) = \sum_{i,j=1}^{D} g_j L_{ij}^{(0)} G_p(R_j - R_i) = \text{Tr} L^{(1)}, \quad (15)$$

where:

$$L_{ij}^{(1)} = \sum_{k=1}^{D} g_k L_{ik}^{(0)} G_p(R_k - R_j), \quad (16)$$

$$G_p(r) = \frac{1}{L^3} \sum_k e^{-ikr} G_p kr. \quad (17)$$

Continuing this procedure for higher order contributions it can be shown that:

$$T_{pp} = \sum_{n=0}^{\infty} \text{Tr} L^{(n)}, \quad (18)$$

where:

$$L_{ij}^{(n+1)} = \sum_{k=1}^{D} g_k L_{ik}^{(n)} G_p(R_k - R_j), \quad (19)$$

$$L_{ij}^{(0)} = g_i e^{-ip(R_i - R_j)}. \quad (20)$$

Hence the problem of computing diagonal elements of the $T$ matrix was reduced to calculation of traces of a relatively small matrices $L^{(n)}$, of dimension $D \times D$. It is important to note that the final result includes the effects related to the finite lattice spacing (incorporated by the relative coordinates of the lattice sites $R_k$).

Let us examine the large lattice limit, by letting $L \rightarrow \infty$ while keeping the lattice constant $b$ fixed. Then the momentum is continuous within the first Brillouin zone, and the summation can be replaced by the integration. To simplify the analysis, however, we place a spherically symmetric cut-off, including only momenta satisfying $p \leq p_{\text{cut}} = \pi/b$:

$$\int d^3 p \rightarrow \int_0^{2\pi} dp_\phi \int_0^\pi dp_\theta \cos p_\theta \int_0^{p_{\text{cut}}} dp \quad (21)$$

This prescription sets to zero all two-body matrix elements, if the relative momentum of two particles exceeds a given momentum cut-off. Note that the function $G_p(r)$ will depend on the momentum cut-off and consequently the scattering parameters like $a_i r_{\text{eff}}$ will also be the functions of $p_{\text{cut}}$. Performing the integration
with respect to the variables $dp_{\phi} d\rho_{\theta}$ the Eq. (17) transforms into:

$$G_{p}(r) = \frac{m}{2\pi^2 r} \int_{0}^{p_{\text{cut}}} dk \frac{\sin kr}{p^2 - k^2}. \quad (22)$$

The remaining integral can be calculated analytically by expanding $\sin kr$ and using the relation:

$$\frac{1}{x + i0^+} = \mathcal{P} \frac{1}{x} - i\pi \delta(x), \quad (23)$$

where $\mathcal{P}$ stands for the principal value. The final result has the form:

$$G_{p}(r) = -\frac{m}{4\pi^2} \sum_{j=0}^{\infty} \frac{(-1)^j r^{2j}}{(2j+1)!} F(j, p) \quad (24)$$

where:

$$F(j, p) = \sum_{l=0}^{j} \frac{2p_{\text{cut}}^{2j-2l+1} p_l^{2j-2l+1}}{2j - 2l + 1} + p^{2j+1} \ln \left| \frac{p_{\text{cut}} - p}{p_{\text{cut}} + p} \right| + i\pi p^{2j+1}. \quad (25)$$

The expression (18) together with (24) and (5) provides the most convenient prescription for numerical applications.

4. Example: on-site interaction

As an example let us consider the on-site interaction:

$$V(r - r') = g_0 \delta(r - r'). \quad (26)$$

It corresponds to the well-known Hubbard model and is presently widely used to simulate the system of dilute, cold fermionic atoms. \[9\] In this particular case, it is possible to find an analytic formula relating the coupling constant $g_0$ to the scattering length and the effective range. It is easy to realize that $L^{(n)}$ become now one-dimensional matrices i.e.:

$$L^{(n)} = g_0 (g_0 G_{p})^n, \quad (27)$$

where:

$$G_{p} = G_{p}(0) = -\frac{m}{4\pi^2} \left( 2p_{\text{cut}} - p \ln \left| \frac{p + p_{\text{cut}}}{p - p_{\text{cut}}} \right| + i\pi p \right). \quad (28)$$

The sum of the geometric series (18) reads:

$$T_{pp} = \frac{g_0}{1 - g_0 G_{p}}. \quad (29)$$

In order to find the inverse of the diagonal matrix elements of $T$ for small values of the momentum, we expand the logarithmic function:

$$\ln \left| \frac{p + p_{\text{cut}}}{p - p_{\text{cut}}} \right| \approx \frac{2}{p_{\text{cut}}} p + \frac{2}{3p_{\text{cut}}^3} p^3. \quad (30)$$
and get:

\[- \frac{4\pi}{m} T_{pp}^{-1} = - \frac{4\pi}{mg_0} - \frac{2p_{cut}}{\pi} + \frac{2}{\pi p_{cut}} p^2 - ip + O(p^4). \tag{31}\]

Comparing this equation with Eq. (5) one reproduces the well-known results:

\[ \frac{1}{a} = \frac{4\pi}{mg_0} + \frac{2p_{cut}}{\pi}, \quad r_{\text{eff}} = \frac{4}{\pi p_{cut}}. \tag{32}\]

It is worth noting that due to the finite lattice spacing the zero range potential acquires the non-zero effective range \( r_{\text{eff}} \).

5. Conclusions

In this work we have presented the method to determine the two-body effective interaction parameters from the low energy scattering data when the problem is defined on the lattice. In the limit of large lattices we have obtained expressions which are particularly convenient for numerical applications. The prescription relates the interaction coupling constants to the effective range expansion parameters and can be applied to Monte Carlo simulations of many-body systems on large lattices.

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