Three fermions in a box at the unitary limit: universality in a lattice model

2007 J. Phys. A: Math. Theor. 40 12863

(http://iopscience.iop.org/1751-8121/40/43/003)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 12863–12872 doi:10.1088/1751-8113/40/43/003

Three fermions in a box at the unitary limit: universality in a lattice model

L Pricoupenko[1] **and Y Castin**[2]

[1] Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie, Case courier 121, 4 Place Jussieu, 75252 Paris Cedex 05, France
[2] Laboratoire Kastler Brossel, Ecole normale supérieure, UPMC, CNRS, 24 rue Lhomond, 75231 Paris Cedex 05, France

Received 10 May 2007, in final form 11 September 2007
Published 9 October 2007
Online at stacks.iop.org/JPhysA/40/12863

Abstract

We consider three fermions with two spin components interacting on a lattice model with an infinite scattering length. Low-lying eigenenergies in a cubic box with periodic boundary conditions, and for a zero total momentum, are calculated numerically for decreasing values of the lattice period. The results are compared to the predictions of the zero-range Bethe–Peierls model in continuous space, where the interaction is replaced by contact conditions. The numerical computation, combined with analytical arguments, shows the absence of negative energy solution, and a rapid convergence of the lattice model towards the Bethe–Peierls model for a vanishing lattice period. This establishes for this system the universality of the zero-interaction range limit.

PACS numbers: 03.75.Ss, 05.30.Fk, 21.45.+v

Recent experimental progress has allowed to prepare a two-component Fermi atomic gas in the BEC–BCS crossover regime and to study in the lab many of its physical properties, such as the equation of state of the gas and other thermodynamic properties, the fraction of condensed particles, the gap in the excitation spectrum corresponding to the breaking of a pair, the superfluid properties and the formation of a vortex lattice, the effect of a population imbalance in the two spin components and the corresponding possible quantum phases, ... [1–16].

The key to this impressive sequence of experimental results is the use of Feshbach resonances [17]: an external magnetic field (B) permits to tune the two-body s-wave scattering length a almost at will, to positive or negative values, so that one can, e.g. adiabatically transform a weakly attractive Fermi gas into a Bose condensate of molecules. Interestingly, close to the resonance, the scattering length diverges as $a \propto -1/(B - B_0)$ so that the infinite scattering length regime ($|a| = \infty$) can be achieved. When the typical relative momentum k

of the particles further satisfies $kb \ll 1$, $k|r_e| \ll 1$, where b is the range and r_e the effective range of the interaction potential, the s-wave scattering amplitude between two particles takes the maximal modulus value $f_k = -1/(\mathrm{i}k)$: this is the so-called unitary regime, where the gas is strongly, and presumably maximally, interacting.

The unitary regime is achieved in present experiments for broad Feshbach resonances, that is for resonances where the effective range r_e is of the order of the Van der Waals range of the interatomic forces [18, 19]. Examples of s-wave broad resonances are given for ^{6}Li atoms by the one at $B_0 \simeq 830$ G [1, 4, 5, 7] or also for ^{40}K atoms at $B_0 \simeq 200$ G [3]. On a more theoretical point of view, the unitary regime has the striking property of being universal: e.g., the zero-temperature equation of state involves only $\hbar$, the atomic mass m, the atomic density and a numerical constant independent of the atomic species; this was checked experimentally, this also appears in fixed node Monte Carlo simulations [20, 21] and more recently in exact quantum Monte Carlo calculations [22–24].

In [22, 24], exact quantum Monte Carlo simulations at the unitary regime are performed using a Hubbard model. From the condensed matter physics point of view, this modelling of the system is a clever way to avoid the fermionic sign problem. But it is more than a theoretical trick in the case of ultra-cold atoms, since it can be achieved experimentally by trapping atoms at the nodes of an optical lattice in the tight-binding regime [25]. The Bethe–Peierls zero-range model is another commonly used way of modelling the unitary regime: pairwise interactions are replaced by contact conditions imposed on the many-body wavefunction [26–33]. This model is very well adapted to analytical calculations in few-body problems [27, 32] but can also be useful to predict many-body properties like time-dependent scaling solution [34], the link between short-range scaling properties and the energy of the trapped gas [31], and hidden symmetry properties [35] of the trapped gas.

However, there is to our knowledge no general rigorous result concerning the equivalence between the discrete (Hubbard model) and the continuous (Bethe–Peierls) models for the unitary gas. As a crucial example, one may wonder if there is any few- or many-body bound state in a discrete model at the infinite scattering length limit. This is a non-trivial question, since the infinite scattering length corresponds to an attractive on-site interaction in the discrete model.

In this paper, we address this question for two and three fermions in a cubic box with periodic boundary conditions, when the interaction range tends to zero for a fixed infinite value of the scattering length. Our results for the equivalence of the lattice model and the Bethe–Peierls approach are analytical for two fermions but still rely on a numerical step for three fermions. In this few-body problem, the grid spacing can however be made very small in comparison to the grids currently used in quantum Monte Carlo many-body calculations, thus allowing a more precise study of the zero lattice step limit and a test of the linear scaling of thermodynamic quantities with the grid spacing used in [22]. Our computations also exemplify the remarkable property that short-range physics of the binary interaction does not play any significant role in the unitary two-component Fermi gas, and the fact that the Bethe–Peierls model is well behaved for three equal mass fermions.

Our model is the lattice model used in the quantum Monte Carlo simulations of [24]. It has already been described in details in [36, 37] so that we recall here only its main features. The positions $\mathbf{r}_i$ of each particle i are discretized on a cubic lattice of period b. The Hamiltonian contains the kinetic term of each particle, $\mathbf{p}^2/2m$, such that the plane wave of wave vector $\mathbf{k}$ has an energy

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \tag{1}$$

Here, the wave vector is restricted to the first Brillouin zone of the lattice:

$$\mathbf{k} \in \mathcal{D} \equiv [-\pi/b, \pi/b[^3. \tag{2}$$

We enclose the system in a cubic box of size L with periodic boundary conditions, so that the components $\{k_\alpha\}_{\alpha\in\{x,y,z\}}$ of $\mathbf{k}$ are integer multiples of $2\pi/L$. In what follows we shall, for convenience, restrict our computations to the case where the ratio $L/b = 2N + 1$ is an odd integer, so that $k_\alpha = 2\pi n_\alpha/L$ with $n_\alpha \in \{-N, -N + 1, \ldots, N\}$. The Hamiltonian also contains the interaction potential between opposite spin fermions i and j, which is a discrete delta on the lattice:

$$V(\mathbf{r}_i, \mathbf{r}_j) = \frac{g_0}{b^3}\delta_{\mathbf{r}_i,\mathbf{r}_j}. \tag{3}$$

In [37], the matrix elements of the two-body T-matrix $\langle\mathbf{k}|T(E+\mathrm{i}0^+)|\mathbf{k}'\rangle$ for an infinite box size are shown to depend only on the energy E, not on the plane wave momenta, which would imply in a continuous space a pure s-wave scattering. The bare coupling constant g_0 is then adjusted in order to reproduce in the zero energy limit the desired value of the s-wave scattering length a between two opposite spin particles [36, 37, 33]:

$$\frac{1}{g_0} - \frac{1}{g} = -\int_{\mathcal{D}} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2\epsilon_{\mathbf{k}}} = -\frac{mK}{4\pi\hbar^2 b}, \tag{4}$$

where

$$K = \frac{12}{\pi}\int_0^{\pi/4} \mathrm{d}\theta \, \ln(1 + 1/\cos^2\theta) = 2.442\,749\ldots \tag{5}$$

may be expressed in terms of the dilog function, and $g = 4\pi\hbar^2 a/m$ is the usual effective s-wave coupling constant. From the calculated energy dependence of the T-matrix, one may also extract the effective range r_e of the interaction in the lattice model; r_e is found to be proportional to the lattice period, $r_e \simeq 0.337b$ [33], and the limit $b \to 0$ is equivalent to the limit of both zero range and zero effective range for the interaction[3]. As mentioned in the introduction, this is the desired situation to reach the unitary limit when $|a| = \infty$.

We first solve the problem for two opposite spin fermions in the box, in the singlet spin state $|s\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, by looking for eigenstates of eigenenergy E with a ket of the form $|s\rangle \otimes |\phi\rangle$. We restrict to the case of a zero total momentum[4], so that the orbital part $|\phi\rangle$ may be expanded on $|\mathbf{k}, -\mathbf{k}\rangle = |1 : \mathbf{k}\rangle \otimes |2 : -\mathbf{k}\rangle$, where $|1 : \mathbf{k}\rangle$ is the normalized ket representing particle 1 with wave vector $\mathbf{k}$. The corresponding wavefunction is $\langle\mathbf{r}|\mathbf{k}\rangle = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}/L^{3/2}$. Schrödinger's equation then reduces to

$$(2\epsilon_{\mathbf{k}} - E)\langle\mathbf{k}, -\mathbf{k}|\phi\rangle + \frac{g_0}{L^{3/2}}\langle\mathbf{r}, \mathbf{r}|\phi\rangle = 0, \tag{6}$$

where the last term does not depend on a common position $\mathbf{r}$ of the two particles. A first type of eigenstates corresponds to $\langle\mathbf{r}, \mathbf{r}|\phi\rangle = 0$: these eigenstates have a zero probability to have two particles at the same point, and are also eigenstates of the non-interacting case. An example of such a state with the correct exchange symmetry is given by the wavefunction

$$\phi(\mathbf{r}_1, \mathbf{r}_2) \propto \cos\left[\frac{2\pi}{L}(x_1 - x_2)\right] - \cos\left[\frac{2\pi}{L}(y_1 - y_2)\right]. \tag{7}$$

We are interested here in the states of the second type, what we call 'interacting' states, such that $\langle\mathbf{r}, \mathbf{r}|\phi\rangle \neq 0$. Treating the interacting term in equation (6) as a source term, one

[3] In contrast, in a two-channel model for a Feshbach resonance, one finds that the effective range has a finite (and negative) limit in the zero-potential range limit (the so-called narrow Feshbach resonance limit) [33].

[4] One thus cannot conclude that the corresponding minimal eigenenergy is the absolute ground state energy.

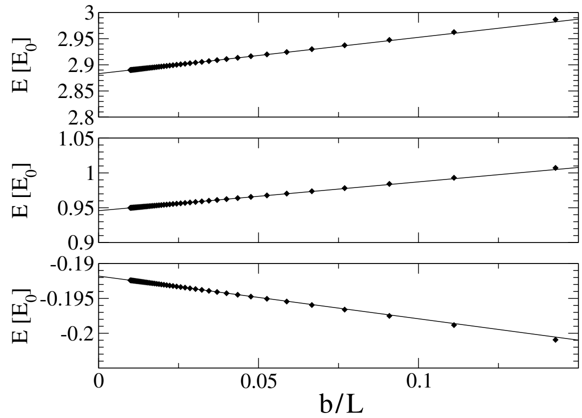

Figure 1. First three eigenenergies for the interacting states of two fermions in a box of size L for an infinite scattering length in the lattice model, as functions of the lattice period b. The total momentum of the eigenstates is fixed to zero. The computed eigenenergies are given by the plotting symbols, in units of $E_0 = (2\pi\hbar)^2/2mL^2$; the straight lines are linear fits performed on the data with $b/L < 2\times 10^{-2}$.

expresses $|\phi\rangle$ in terms of $\langle\mathbf{r},\mathbf{r}|\phi\rangle$ and a sum over $\mathbf{k}$. Projecting the resulting expression onto $|\mathbf{r},\mathbf{r}\rangle$ leads to a closed equation (now $E \neq 2\epsilon_{\mathbf{k}}$)

$$\frac{1}{g_0} + \frac{1}{L^3}\sum_{\mathbf{k}\in\mathcal{D}} \frac{1}{2\epsilon_{\mathbf{k}} - E} = 0. \tag{8}$$

The resulting implicit equation for E, of the form $u(E) = 0$, where $u(E)$ is the left-hand side of equation (8), is then readily solved numerically; to this end, one notes that $u(E)$ has poles in each $E = 2\epsilon_{\mathbf{k}}$, and that it varies monotonically from $-\infty$ to $+\infty$ between two poles, so that $u(E)$ vanishes once and only once between two successive values of $2\epsilon_{\mathbf{k}}$. In figure 1, we show for $|a| = \infty$ the first low-lying eigenenergies as functions of the lattice spacing; one observes a convergence to finite values in the $b/L \to 0$ limit, with a first correction scaling as b/L. A rewriting of the implicit equation for E that will reveal convenient in the $b = 0$ limit is

$$\frac{\pi L}{a} = \frac{(2\pi\hbar)^2}{mL^2}\left[\frac{1}{E} + \sum_{\mathbf{k}\in\mathcal{D}-\mathbf{0}}\left(\frac{1}{E - 2\epsilon_k} + \frac{1}{2\epsilon_k}\right)\right] + C(b), \tag{9}$$

where the function $C(b)$ is defined by

$$C(b) = \frac{(2\pi\hbar)^2 L}{2m}\left(\int_{\mathcal{D}} \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{\epsilon_{\mathbf{k}}} - \frac{1}{L^3}\sum_{\mathbf{k}\in\mathcal{D}-\mathbf{0}}\frac{1}{\epsilon_{\mathbf{k}}}\right), \tag{10}$$

and has a finite limit for $b \to 0$ which is given by $C(0) \simeq 8.913\,64$.

We now briefly check that the $b = 0$ limit in equation (9) coincides with the prediction of the Bethe–Peierls model, which is a continuous space model where one replaces the interaction potential by the following contact conditions on the wavefunction [26–33]: there exists a function $S(\mathbf{R})$ such that

$$\phi(\mathbf{r}_1,\mathbf{r}_2) = S(\mathbf{R})\left(\frac{1}{r} - \frac{1}{a}\right) + O(r), \tag{11}$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2| \to 0$ is the distance between the two particles and the centre of mass position $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ is fixed. At positions $\mathbf{r}_1 \neq \mathbf{r}_2$, the wavefunction solves the free

Schrödinger equation. Using this model we arrive at an implicit equation for the energy of an interacting state exactly of the form obtained by taking the $b = 0$ limit in equation (9), except that the constant $C(0)$ in the right-hand side is replaced by[5]

$$C_{\mathrm{BP}} = \lim_{\sigma\to 0}\left(\int \mathrm{d}^3\mathbf{u}\,\frac{\mathrm{e}^{-u^2\sigma^2}}{u^2} - \sum_{\mathbf{n}\in\mathbb{Z}^{3*}}\frac{\mathrm{e}^{-n^2\sigma^2}}{n^2}\right). \tag{12}$$

We expect the identity $C_{\mathrm{BP}} = C(0)$ from the general result that the Bethe–Peierls model for the two-body problem reproduces the zero range limit of a true interaction potential [28, 38]. It is however instructive to check this property explicitly for the lattice model. One can show that

$$C_{\mathrm{BP}} - C(0) = \lim_{\sigma\to 0}\sum_{\mathbf{n}\in\mathbb{Z}^{3*}}\int_{\mathcal{I}}\mathrm{d}^3\mathbf{u}[h_\sigma(\mathbf{n}+\mathbf{u}) - h_\sigma(\mathbf{n})], \tag{13}$$

where $h_\sigma(\mathbf{q}) = [\exp(-q^2\sigma^2) - 1]/q^2$ and the integration domain is $\mathcal{I} = [-1/2, 1/2]^3$. The desired identity $C(0) = C_{\mathrm{BP}}$ results from the fact that one can exchange the $\sigma = 0$ limit and the summation over $\mathbf{n}$ in the above equation [39][6].

In the lattice model, it is possible to show analytically that the spectrum of the two-body problem for an infinite scattering length is bounded from below in the $b \to 0$ limit. Since $g_0 < 0$ for $|a| = \infty$, there exists at least one non-positive energy solution, by a variational argument. One then notes that the right-hand side in equation (9) is a strictly decreasing function of E over $]-\infty, 0[$ that tends to $-\infty$ in $E = 0^-$, so that at most one negative energy solution may exist. Furthermore, one can show that the $b \to 0$ limit of the right-hand side tends to $+\infty$ when $E \to -\infty$[7], whence this negative energy solution is finite[8].

We now turn to the problem of three interacting fermions in the box. Schrödinger's equation is obtained without loss of generality by considering the particular spin component $(1{:}\uparrow; 2{:}\uparrow; 3{:}\downarrow)$, so that the interaction takes place only among the pairs $(1, 3)$ and $(2, 3)$, and in the lattice model one obtains

$$\left[\sum_{i=1}^{3}\frac{\mathbf{p}_i^2}{2m} + \frac{g_0}{b^3}\left(\delta_{\mathbf{r}_1,\mathbf{r}_3} + \delta_{\mathbf{r}_2,\mathbf{r}_3}\right) - E\right]\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0. \tag{14}$$

[5] Usually, one expresses the Green function of the Laplacian in a cubic box in terms of plane waves. This leads to $C_{\mathrm{BP}} = \lim_{x\to 0} v(\mathbf{x})$, with $v(\mathbf{x}) = \int \mathrm{d}^3\mathbf{u}\exp(\mathrm{i}\mathbf{u}\cdot\mathbf{x})/u^2 - \sum_{\mathbf{n}\in\mathbb{Z}^{3*}}\exp(\mathrm{i}\mathbf{n}\cdot\mathbf{x})/n^2$. This definition of $v(\mathbf{x})$ should be understood within the frame of the theory of distributions. We define the $x = 0$ limit of $v(\mathbf{x})$ as the limit for $\sigma \to 0$ of $\int \mathrm{d}^3\mathbf{x} v(\mathbf{x})\phi(\mathbf{x}/\sigma)/\sigma^3$, where ϕ is a C^∞ rapidly decreasing function with $\int \mathrm{d}^3\mathbf{x}\phi(\mathbf{x}) = 1$. In equation (12) we have taken for simplicity ϕ to be a Gaussian, but we have shown that C_{BP} is independent of this choice.

[6] One uses the rewriting $h_\sigma(\mathbf{n}+\mathbf{u}) - h_\sigma(\mathbf{n}) = T_1 + T_2$, with $T_1 = [\hat\phi[\sigma(\mathbf{n}+\mathbf{u})] - \hat\phi(\sigma\mathbf{n})]/(\mathbf{n}+\mathbf{u})^2$, $T_2 = [\hat\phi(\sigma\mathbf{n}) - 1][1/(\mathbf{n}+\mathbf{u})^2 - 1/n^2]$ and $\hat\phi(\mathbf{x}) = \exp(-x^2)$. Using a large n expansion, one finds that the integral of T_2 over the symmetric integration domain $\mathcal{I}$ is $O(1/n^4)$, so that the theorem of dominated convergence applies. For T_1, one uses the Taylor–Lagrange formula up to second order for the numerator: for a given $\mathbf{u}$, there exists a vector $\mathbf{x_u}$ on the line connecting $\sigma\mathbf{n}$ and $\sigma(\mathbf{n}+\mathbf{u})$ such that $\hat\phi[\sigma(\mathbf{n}+\mathbf{u})] - \hat\phi(\sigma\mathbf{n}) = \sum_i \sigma u_i\partial_i\hat\phi(\sigma\mathbf{n}) + \frac{1}{2}\sum_{i,j}\sigma^2 u_i u_j\partial_i\partial_j\hat\phi(\mathbf{x_u})$. The term involving the first-order derivatives of $\hat\phi$ vanishes after integration over $\mathbf{u}$. Since the second-order derivatives of $\hat\phi(\mathbf{x})$ are rapidly decreasing functions, they are in particular $\leqslant A/x^2$ at large x for some number A, so that the integral of T_1 over $\mathcal{I}$ is bounded by A/n^4 and the theorem of dominated converge applies again.

[7] One uses the fact that for $n \in \mathbb{N}^*$, $\epsilon/[n^2(n^2+\epsilon)]$ is positive when $\epsilon > 0$, and tends to $1/n^2$ for $\epsilon \to +\infty$. The fact that $\sum_{\mathbf{n}\in\mathbb{Z}^{3*}} 1/n^2 = +\infty$ gives the result.

[8] In the limit $b \to 0$, there exists a negative energy solution $E < 0$ for all a. Its energy can be calculated accurately directly from the Bethe–Peierls model from a more convenient representation of the function $v(\mathbf{x})$ in footnote 5, using Poisson's summation formula applied to the function $\mathbf{u} \to \mathrm{e}^{\mathrm{i}\mathbf{u}\cdot\mathbf{x}}/(u^2+\lambda^2)$ where $\lambda > 0$ is arbitrary. One obtains $C_{\mathrm{BP}} = \lambda^{-2} + 2\pi^2\lambda - \sum_{\mathbf{n}\in\mathbb{Z}^{3*}}[\lambda^2 n^{-2}(\lambda^2+n^2)^{-1} + \pi\exp(-2\pi\lambda n)/n]$, an expression whose value does not depend on λ. Specializing to the unitary limit, and taking $\lambda = \alpha/(2\pi)$, where $\alpha = 1.945\,766\ldots$ solves $\alpha = \sum_{\mathbf{n}\in\mathbb{Z}^{3*}}\exp(-\alpha n)/n$, one finds a minimal eigenenergy $E = -\alpha^2\hbar^2/mL^2$.

We restrict to a zero total momentum modulo $2\pi/b$ along each direction (see footnote 4); using the fermionic antisymmetry condition for the transposition of particles 1 and 2, we express the part of equation (14) involving the interaction in terms of a function of the position of a single particle:

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1) = f(\mathbf{r}_2 - \mathbf{r}_1) \tag{15}$$

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_2) = -f(\mathbf{r}_1 - \mathbf{r}_2). \tag{16}$$

We then project equation (14) on the plane waves in the box, which leads to

$$\langle \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3|\psi\rangle = \frac{g_0 \delta^{\mathrm{mod}}_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3,\mathbf{0}}}{E - \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_3}} \left(f_{\mathbf{k}_2} - f_{\mathbf{k}_1}\right), \tag{17}$$

where δ^{mod} is a discrete delta modulo $2\pi/b$ along each direction, and where the Fourier transform of $f(\mathbf{r})$ is defined as

$$f_{\mathbf{k}} = \langle \mathbf{k}|f\rangle = \frac{b^3}{L^{3/2}} \sum_{\mathbf{r}\in[0,L[^3} \exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}) f(\mathbf{r}). \tag{18}$$

Replacing $f(\mathbf{r})$ in the right-hand side of this equation by its expression in terms of $\langle \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3|\psi\rangle$ deduced from equation (15), we obtain a closed equation for $f_{\mathbf{k}}$:

$$\frac{L^3}{g_0} f_{\mathbf{k}} = f_{\mathbf{k}} \sum_{\mathbf{q}\in\mathcal{D}} a_{\mathbf{k},\mathbf{q}} - \sum_{\mathbf{q}\in\mathcal{D}} a_{\mathbf{k},\mathbf{q}} f_{\mathbf{q}}, \tag{19}$$

where we have introduced the matrix

$$a_{\mathbf{k},\mathbf{q}} = \frac{1}{E - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}} - \epsilon_{[\mathbf{k}+\mathbf{q}]_{\mathrm{FBZ}}}}, \tag{20}$$

and for an arbitrary wave vector $\mathbf{u}$, $[\mathbf{u}]_{\mathrm{FBZ}}$ denotes the vector in the first Brillouin zone that differs from $\mathbf{u}$ by integer multiples of $2\pi/b$ along each direction. The eigenvalues E of the three-body problem are such that the linear system (19) admits a non-identically vanishing solution $f_{\mathbf{k}}$, that is the determinant of this linear system is zero. Note that from equation (19), one has $f(\mathbf{0}) \propto \sum_{\mathbf{q}\in D} f_{\mathbf{k}} = 0$, a consequence of the Pauli exclusion principle.

For $|a| = \infty$, we have computed numerically the first eigenenergies of the system, by calculating the determinant as a function of E. In figure 2, we give these eigenenergies as functions of the ratio b/L. A rapid convergence in the zero-b limit is observed, with a linear dependence in b/L.

This rapid convergence illustrates the fact that equal mass fermions easily exhibit universal properties, as revealed by experiments; here b plays the role of the finite Van der Waals range of the true potential (given by $(mC_6/\hbar^2)^{1/4}$, where C_6 is the Van der Waals coefficient), and L is of the order of the mean interparticle distance in a real gas. As an example, for ^{6}Li atoms $b \sim 3$ nm and in experiments for the broad Feshbach resonance in the s-wave channel at $\sim$830 G the atomic density is of the order of 10^{13} cm^{-3}, so that the ratio b/L is of the order of 10^{-2} which is well within the zero-b limit.

The absence of negative three-body eigenenergies in the unitary limit can be obtained numerically very efficiently through a formal analogy between equation (19) and a set of rate equations on fictitious occupation numbers of the single particle modes in the box. Assuming $E \leqslant 0$, we note $\Pi_{\mathbf{k}}$ the fictitious occupation number in the mode $\mathbf{k}$ and $\Gamma_{\mathbf{k}\to\mathbf{q}} = g_0 a_{\mathbf{q},\mathbf{k}}/L^3$ the transition rate from the mode $\mathbf{k}$ to the mode $\mathbf{q}$. From equation (20), one obtains the property $\Gamma_{\mathbf{k}\to\mathbf{q}} = \Gamma_{\mathbf{q}\to\mathbf{k}}$, and the rate equation can be written as

$$\frac{\mathrm{d}\Pi_{\mathbf{k}}}{\mathrm{d}t} = -\left(\sum_{\mathbf{q}\neq\mathbf{k}} \Gamma_{\mathbf{k}\to\mathbf{q}}\right) \Pi_{\mathbf{k}} + \sum_{\mathbf{q}\neq\mathbf{k}} \Gamma_{\mathbf{q}\to\mathbf{k}} \Pi_{\mathbf{q}}. \tag{21}$$

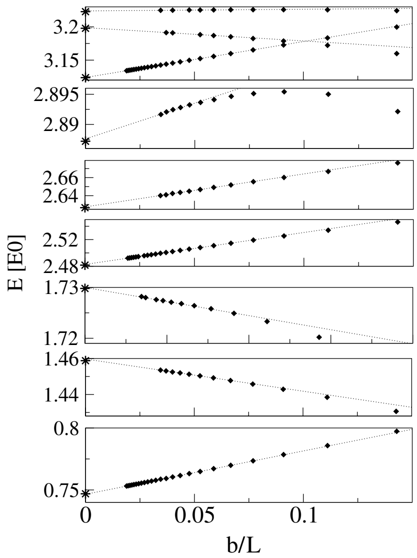

Figure 2. First eigenenergies of three fermions in a box of size L for an infinite scattering length in the lattice model, for a zero total momentum. The computed eigenenergies (diamonds) are given in units of $E_0 = (2\pi\hbar)^2/2mL^2$ for different values of the lattice period b. For functions $f(\mathbf{r})$ invariant by reflection along x, y, z and by arbitrary permutation of x, y, z we have computed the eigenenergies down to smaller values of b/L. The straight lines are a linear fit performed on the data over the range $b/L \leqslant 1/15$, except for the energy branch $E \simeq 2.89E_0$ which becomes more slowly linear than the other branches. The eigenenergies predicted by the Bethe–Peierls model are given by stars in $b = 0$.

The symmetric matrix $M(E)$, which defines the first-order linear system in equation (21), $\mathrm{d}\mathbf{\Pi}/\mathrm{d}t = M(E)\mathbf{\Pi}$, has the following properties: (i) its eigenvalues are non-positive, since it is a set of rate equations; (ii) its eigenvalues are decreasing function of the energy E, which can be deduced from the fact that $\mathrm{d}M(E)/\mathrm{d}E$ is a matrix of rate equations and obeys property (1), and from the Hellman–Feynman theorem; and (iii) eigenmodes of equation (21) with an eigenvalue equal to -1 correspond to solutions $f_{\mathbf{k}}$ of equation (19) with $\Pi_{\mathbf{k}} = f_{\mathbf{k}} \exp(-t)$. Therefore, in order to check that there is no nonzero solution of equation (19) for $E < 0$, it is sufficient to check that all eigenvalues of $M(E = 0)$ are strictly larger than -1.

We have computed the lowest eigenvalue m_0 of the matrix $M(E = 0)$ as a function of the ratio b/L. A fit of m_0 as a function of b/L suggests $\lim_{b\to 0} m_0 \simeq -1$. To better see what happens in the zero-(b/L) limit, we note that having $m_0 > -1$ is equivalent to having $(m_0 + 1)/g_0 < 0$, or more simply $(m_0 + 1)/(b/L) > 0$. We have thus plotted in figure 3 the ratio $(m_0 + 1)/(b/L)$, which is seen to tend to a positive value for $b \to 0$, $\simeq 1.085$, with a negative slope; this excludes the existence of negative eigenenergies for the three fermions at infinite scattering length even in the small b limit[9].

[9] One may fear at this stage that an eigenvalue m_x of $M(E = 0)$, although not being the lowest one for the values of b/L considered in the figure, may be such that $(m_x + 1)/(b/L)$ varies rapidly with b/L, e.g. with a large and *positive* slope, so as to converge for $b/L \to 0$ to a lower value than 1.08. To test this possibility, we have considered the lowest twenty eigenvalues of $M(E = 0)$ in each symmetry sector with respect to reflections along x, y, z. All these eigenvalues m_i are found to lead to $(m_i + 1)/(b/L)$ having a *negative* slope as functions of b/L and converging for $b/L \to 0$ to values $\simeq 2.13, 2.27, 2.51, \ldots$, larger than 1.08.

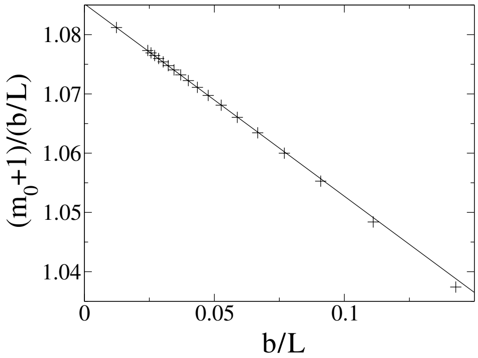

Figure 3. Quantity $(m_0 + 1)/(b/L)$ as a function of the lattice period b. Here m_0 is the lowest eigenvalue of the matrix $M(E)$ defining the linear system equation (21), for $E = 0$ and for an infinite scattering length. The fact that $m_0 + 1 > 0$ shows that there is no negative eigenenergy for the three fermions (see the text). The symbols are obtained from a numerical calculation of m_0. The solid line is a linear fit over the range $b/L \leqslant 1/29$, not including the point with $b/L = 1/81$: for this point, the matrix M has more than half a million lines so that m_0 was obtained by a computer memory-saving iterative method rather than by a direct diagonalization.

In a last step, we compare the results of the lattice model to the predictions of the Bethe–Peierls approach for three fermions in a continuous space, which was shown to be a successful model in free space [29, 30] and in a harmonic trap at the unitary limit [32]. For this purpose, we introduce the function $F_{\mathbf{k}}$ which is the Fourier transform of the regular part of the wavefunction as $|\mathbf{r}_1 - \mathbf{r}_3| \to 0$,

$$F(\mathbf{R}) = \lim_{r\to 0}\left[r\psi\left(\mathbf{R} + \frac{\mathbf{r}}{2}, \mathbf{0}, \mathbf{R} - \frac{\mathbf{r}}{2}\right)\right], \tag{22}$$

where we have used the translational invariance. By reproducing a calculation procedure analogous to what we have done for the lattice model, we obtain the following infinite-dimension linear system:

$$\frac{L^3}{g}F_{\mathbf{k}} = F_{\mathbf{k}}\left[A_{\mathbf{k},\mathbf{0}} + \sum_{\mathbf{q}\neq\mathbf{0}}\left(A_{\mathbf{k},\mathbf{q}} + \frac{1}{2\epsilon_{\mathbf{q}}}\right) + \frac{mL^2C_{\mathrm{BP}}}{(2\pi\hbar)^2}\right] - \sum_{\mathbf{q}} A_{\mathbf{k},\mathbf{q}}F_{\mathbf{q}}, \tag{23}$$

where the wave vectors $\mathbf{k}$ and $\mathbf{q}$ now run over the whole space $(2\pi/L)\mathbb{Z}^3$, and

$$A_{\mathbf{k},\mathbf{q}} = \frac{1}{E - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}} - \epsilon_{\mathbf{k}+\mathbf{q}}}. \tag{24}$$

The similarity between the structure of (19) and (23) is apparent. Numerically, at $|a| = \infty$, we have verified the convergence between the two models as $b \to 0$ in equation (19) (see figure 2). Analytically, one can even formally check the equivalence between the two sets of equations (19) and (23): first, we eliminate the integral of $1/\epsilon_{\mathbf{k}}$ between (4) and (10), to express $1/g_0$ in terms of $1/g$ and $C(b)$. Second, we replace $1/g_0$ by the resulting expression in equation (19). Third, we take the limit $b \to 0$: we exactly recover the system (23). Hence, if the eigenenergy E and the corresponding function f in the lattice model have a well-defined limit for $b = 0$, this shows that the limit is given by the Bethe–Peierls model. Of course, the real mathematical difficulty is to show the existence of the limit, in particular for all eigenenergies. This property is not granted: for example, the present lattice model generalized to the case of a $\downarrow$ particle of a mass m_3 different from the mass m of the two

↑ particles leads, for a large enough mass ratio m/m_3, to a three-body energy spectrum not bounded from below in the $b = 0$ limit, even though the Pauli exclusion principle prevents from having the three particles on the same lattice site[10].

In conclusion, we have computed numerically the low-lying eigenenergies of three spin-1/2 fermions in a box, interacting with an infinite scattering length in a lattice model, for a zero total momentum and for decreasing values of the lattice period. Our results show numerically the equivalence between this model and the Bethe–Peierls approach in the limit of zero lattice period. This is related to the fact that the eigenenergies E are bounded from below in the zero lattice period limit $b \to 0$, more precisely $E > 0$. Such a convergence of the eigenstates of fermions in a lattice model towards universal states when $b \to 0$ is a key property used in Monte Carlo simulations at the N-body level [22–24].

Acknowledgments

We thank F Werner for interesting discussions on the subject. Laboratoire de Physique Théorique de la Matière Condensée is the Unité Mixte de Recherche 7600 of Centre National de la Recherche Scientifique (CNRS). The cold atom group at LKB is a member of IFRAF.

References

[1] O'Hara K M, Hemmer S L, Gehm M E, Granade S R and Thomas J E 2002 *Science* **298** 2179
[2] Gehm M E, Hemmer S L, Granade S R, O'Hara K M and Thomas J E 2003 *Phys. Rev.* A **68** 011401
[3] Regal C, Ticknor C, Bohn J and Jin D 2003 *Nature* **424** 47
[4] Bourdel T, Cubizolles J, Khaykovich L, Magalhães K M F, Kokkelmans S J J M F, Shlyapnikov G and Salomon C 2003 *Phys. Rev. Lett.* **91** 020402
[5] Jochim S, Bartenstein M, Altmeyer A, Hendl G, Riedl S, Chin C, Hecker Denschlag J and Grimm R 2003 *Science* **302** 2101
[6] Greiner M, Regal C A and Jin D S 2003 *Nature* **426** 537
[7] Zwierlein M W, Stan C A, Schunck C H, Raupach S M F, Gupta S, Hadzibabic Z and Ketterle W 2003 *Phys. Rev. Lett.* **91** 250401
[8] Bourdel T, Khaykovich L, Cubizolles J, Zhang J, Chevy F, Teichmann M, Tarruell L, Kokkelmans S J J M F and Salomon C 2004 *Phys. Rev. Lett.* **93** 050401
[9] Bartenstein M, Altmeyer A, Riedl S, Jochim S, Chin C, Hecker Denschlag J and Grimm R 2004 *Phys. Rev. Lett.* **92** 120401
[10] Chin C, Bartenstein M, Altmeyer A, Riedl S, Jochim S, Hecker Denschlag J and Grimm R 2004 *Science* **305** 1128
[11] Zwierlein M W, Abo-Shaeer J R, Schirotzek A, Schunck C H and Ketterle W 2005 *Nature* **435** 1047

[10] For an arbitrary mass ratio, the coupling constant g_0 for an infinite scattering length is $g_0 = -2\pi\hbar^2 b/(\mu K)$ where $1/\mu = 1/m + 1/m_3$ is the inverse of the reduced mass. One may take as a simple variational ansatz the ground state of the three-body problem for $m = \infty$, of the form $|\psi_\infty\rangle = [|\mathbf{r}_1\rangle|\mathbf{r}_2\rangle - |\mathbf{r}_2\rangle|\mathbf{r}_1\rangle]|\chi\rangle$, with $\mathbf{r}_1 - \mathbf{r}_2 = b\mathbf{e}_x$ and $\mathbf{e}_x$ the unit vector along x; $|\chi\rangle$ has a simple expression in momentum space and one finds $\chi(\mathbf{r}_1) = \chi(\mathbf{r}_2)$. For a finite value of m the expectation value of H in $|\psi_\infty\rangle$ gives an upper bound E_v on the ground state three-body energy

$$E_v = \frac{\hbar^2\pi^2}{2m_3 b^2}\left(A + B\frac{m_3}{m}\right),$$

where A is the smallest root of $F(A) = 1 + \int_{[-1,1]^3} d^3q[1 + \cos(\pi\mathbf{q}\cdot\mathbf{e}_x)]/[2\pi K(A - q^2)]$ and $B = 2 + 1/F'(A)$. One finds $A \simeq -0.042\,088$ and $B \simeq 1.757\,62$. Then $E_v \to -\infty$ when $b \to 0$ for a mass ratio m/m_3 above the critical value $\simeq 41.8$. Actually the exact critical mass ratio is expected to be below $13.6069\ldots$ since the Efimov phenomenon takes place for $m/m_3 > 13.6069\ldots$. (From [29] we find that the minimal mass ratio m/m_3 leading to the Efimov phenomenon solves $-\frac{\pi}{2}\sin^2(2\theta) + \cot 2\theta + 2\theta = 0$, excluding the trivial root $\theta = \pi/4$, with $\theta = \arctan[(1 + 2m/m_3)^{1/2}]$.) Note: in the bosonic case, for the lattice model at $|a| = \infty$ with N_B bosons of mass m in the same spin state, one may take as a variational ansatz the state vector where all the N_B bosons are on the same lattice site; one then finds an upper bound on the ground state energy $E_v^B = g_0 N_B[N_B - (1 + \pi K/4)]/(2b^3)$, with $1 + \pi K/4 \simeq 2.9185$, so that the ground state energy tends to $-\infty$ for $b \to 0$ if $N_B \geqslant 3$.

[12] Partridge G B, Li W, Kamar R I, Liao Y A and Hulet R G 2006 *Science* **311** 503
[13] Shin Y, Zwierlein M W, Schunck C H, Schirotzek A and Ketterle W 2006 *Phys. Rev. Lett.* **97** 030401
[14] Stewart J T, Gaebler J P, Regal C A and Jin D S 2006 *Phys. Rev. Lett.* **97** 220406
[15] Altmeyer A, Riedl S, Kohstall C, Wright M, Geursen R, Bartenstein M, Chin C, Hecker Denschlag J and Grimm R 2007 *Phys. Rev. Lett.* **98** 040401
[16] Luo L, Clancy B, Joseph J, Kinast J and Thomas J E 2007 *Phys. Rev. Lett.* **98** 080402
[17] Feshbach H 1962 *Ann. Phys., NY* **19** 287
[18] Moerdijk A J, Verhaar B J and Axelsson A 1995 *Phys. Rev.* A **51** 4852
[19] Vogels J M, Tsai C C, Freeland R S, Kokkelmans S J J M F, Verhaar B J and Heinzen D J 1997 *Phys. Rev.* A **56** R1067
[20] Chang S-Y, Pandharipande V R and Schmidt K E 2003 *Phys. Rev. Lett.* **91** 050401
[21] Astrakharchik G E, Boronat J, Casulleras J and Giorgini S 2004 *Phys. Rev. Lett.* **93** 200404
[22] Burovski E, Prokof'ev N, Svistunov B and Troyer M 2006 *Phys. Rev. Lett.* **96** 160402
Burovski E, Prokof'ev N, Svistunov B and Troyer M 2006 *New J. Phys.* **8** 153
[23] Bulgac A, Drut J E and Magierski P 2006 *Phys. Rev. Lett.* **96** 090404
[24] Juillet O 2007 *New J. Phys.* **9** 163
[25] Greiner M, Mandel O, Esslinger T, Hänsch T W and Bloch I 2002 *Nature* **415** 39
[26] Bethe H and Peierls R 1935 *Proc. R. Soc. Lond.* A **148** 146
[27] Efimov V 1971 *Sov. J. Nucl. Phys.* **12** 589
Efimov V 1973 *Nucl. Phys.* A **210** 157
[28] Albeverio S, Gesztesy F, Høegh-Krohn R and Holden H 1988 *Solvable Models in Quantum Mechanics* (New York: Springer)
[29] Petrov D S 2003 *Phys. Rev.* A **67** 010703
[30] Petrov D, Salomon C and Shlyapnikov G 2004 *Phys. Rev. Lett.* **93** 090404
Petrov D, Salomon C and Shlyapnikov G 2005 *Phys. Rev.* A **71** 012708
[31] Tan Shina 2004 *Preprint* cond-mat/0412764
[32] Werner F and Castin Y 2006 *Phys. Rev. Lett.* **97** 150401
[33] Castin Y 2007 *Proc. the Enrico Fermi Varenna School on Fermi gases (June 2006)* ed M Inguscio, W Ketterle and C Salomon (Bologna: SIF)
[34] Castin Y 2004 *C. R. Phys.* **5** 407
[35] Werner F and Castin Y 2006 *Phys. Rev.* A **74** 053604
[36] Mora C and Castin Y 2003 *Phys. Rev.* A **67** 053615
[37] Castin Y 2004 *Proc. the School 'Quantum Gases in Low Dimensions' (J. Phys. IV (France)* vol 116*)* p 89
[38] Olshanii M and Pricoupenko L 2002 *Phys. Rev. Lett.* **88** 010402
[39] The value of C_{BP} disagrees with the one ($7.44 \simeq \pi \times 2.37\ldots$) given in equation (53) of Huang K and Yang C N 1957 *Phys. Rev.* **105** 767