Analytical solution of the bosonic three-body problem

Alexander Gogolin

Department of Mathematics
Imperial College London

Collaboration: Christophe Mora & Reinhold Egger

Plan

- Introduction [general formulation, historical remarks]

- Reduction of the regularised Skorniakov Ter-Martirosian (STM) equation to an effective 1D quantum mechanics.

- Universal problem and solution of exponential accuracy

Introduction

Briefly recall the two-body problem: two particles interacting via a spherically-symmetric ('square well') potential of the size a_0 and strength $-V_0$.

In 3D a bound state first appears when $V_0 a_0^2 > \pi^2/4$. Hence the Wigner (1933) and Bethe–Peierls (1935) approximation: take the limit $a_0 \to 0$ and $V_0 \to \infty$ but such as $V_0 a_0^2 =$ const. This is the same as a boundary condition on the wave-function:

$$\lim_{r\to 0} \ln(r\Psi) = -\frac{1}{a}$$

where a is the scattering length.

An effective range expansion [Landau-Smorodinski (1944)]

$$\frac{1}{a} \to \frac{1}{a} - \frac{1}{2}R^* k^2$$

constitutes the next-to leading approximation where the parameter $R^* > 0$ is the effective potential range.

• Thomas (1935) - a variational calculation - no lower limit on trimer bound state energy in the zero-range approximation - 'Thomas collapse'.

• Skorniakov & Ter-Martirosian (1957) derived their equation for the 'waive-function' $\psi(k)$ of bound trimer states:

$$\psi(k) + \frac{2}{\pi}\int_0^\infty dk' \ln\left(\frac{k^2 + kk' + k'^2 + \lambda^2}{k^2 - kk' + k'^2 + \lambda^2}\right)$$

$$\times \frac{\psi(k')}{a^{-1} - \sqrt{3k'^2/4 + \lambda^2}} = 0$$

and a different equation for fermions (-λ^2 is the trimer energy).

• Danilov (1961) and Minlos & Faddeev (1961) discovered the problem with the bosonic STM equation: it has an infinite number of bound states with energies extending to $-\infty$.

• Efimov (1970) solved the problem by using a real-space regularization scheme (not the effective range expansion) and found a universal hierarchy of trimer states

$$E_n = -\kappa_*^2 e^{-2\pi n/s_0}$$

where n is an integer ($n \gg 1$), $s_0 \simeq 1.00624$ and $\kappa_* R^*$ was only known numerically so far being approximately 2.5 [for a recent review see Braaten & Hammer (2007)].

• Petrov (2004) used the effective range expansion to regularize the STM equation and investigated it numerically.

Regularized STM equation

One can start directly from the Feshbach resonance model [Lona-Lasinio, Pricoupenko and Castin (2007)]

$$H = \sum_{\mathbf{k}} \epsilon_k a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{K}} (E_0 + \epsilon_K/2) b^\dagger_{\mathbf{K}} b_{\mathbf{K}}$$

$$+\Lambda \sum_{\mathbf{k},\mathbf{K}} \left(b^\dagger_{\mathbf{K}} a_{\mathbf{k}+\mathbf{K}/2} a_{-\mathbf{k}+\mathbf{K}/2} + \text{h.c.} \right).$$

The three-body problem can be solved using the ansatz

$$\sum_{\mathbf{K}} \left(\beta_{\mathbf{K}} b^\dagger_{\mathbf{K}} a^\dagger_{-\mathbf{K}} + \sum_{\mathbf{k}} A_{\mathbf{K},\mathbf{k}} a^\dagger_{\mathbf{k}+\mathbf{K}/2} a^\dagger_{-\mathbf{k}+\mathbf{K}/2} a^\dagger_{-\mathbf{K}} \right) |0\rangle,$$

leading to the equation

$$\left(\sqrt{\lambda^2 + 3K^2/4} - a^{-1} + (\lambda^2 + 3K^2/4) R^* \right) \beta_{\mathbf{K}}$$

$$= \frac{1}{\pi^2} \int d^3K' \frac{\beta_{\mathbf{K}'}}{K'^2 + K^2 + \mathbf{K}' \cdot \mathbf{K} + \lambda^2},$$

where the $R^* = 2\pi/\Lambda^2$ is the effective range. With

$$\psi = k(a^{-1} - R^*(\frac{3}{4}k'^2 + \lambda^2) - \sqrt{3k'^2/4 + \lambda^2})\beta_k$$

and integrating over the angles, one finds

$$\psi(k) + \frac{2}{\pi}\int_0^\infty dk' \ln\left(\frac{k^2 + kk' + k'^2 + \lambda^2}{k^2 - kk' + k'^2 + \lambda^2}\right)$$

$$\times \frac{\psi(k')}{a^{-1} - R^*(\frac{3}{4}k'^2 + \lambda^2) - \sqrt{3k'^2/4 + \lambda^2}} = 0$$

Quantum mechanics

In order to make progress we take several steps

• Since the integrand is odd under $k' \to -k'$, we extend k to include negative values but require that wave-functions are odd, $\psi(-k) = -\psi(k)$. The integral above is then taken over all k', with the replacement $2/\pi \to 1/\pi$.

• A useful substitution is

$$k = \frac{2\lambda}{\sqrt{3}} \sinh \xi, \quad \xi \in \mathrm{R},$$

under which two things happen: (i) the root in the integrand rationalizes, and (ii) the logarithmic kernel becomes *homogeneous* and hence is reduced (after much algebra) to a *difference kernel*

$$T(\xi) = \frac{4\pi}{3\sqrt{3}}\delta(\xi) - \frac{4}{\pi\sqrt{3}} \ln\left(\frac{e^{2\xi} + e^{\xi} + 1}{e^{2\xi} - e^{\xi} + 1}\right),$$

with Fourier transform

$$\hat{T}(s) = \int_{-\infty}^{\infty} d\xi e^{is\xi} T(\xi) = \frac{4\pi}{3\sqrt{3}} - \frac{8}{\sqrt{3}} \frac{\sinh(\pi s/6)}{s\cosh(\pi s/2)}.$$

• Any difference kernel acts on a test function $g(\xi)$ as a differential operator,

$$\int_{-\infty}^{\infty} d\xi' T(\xi - \xi') g(\xi') = \hat{T}(-id/d\xi) g(\xi).$$

The function $\hat{T}$ thus plays the role of a *kinetic energy operator*. For the standard Schrödinger equation, $\hat{T}(s) = s^2/2m$. Here the dispersion relation starts as $\hat{T}(s) \sim s^2$ at small momentum and levels off to $4\pi/(3\sqrt{3})$ as $s \to \infty$. It is thus bounded from below and from above, similar to what happens for a typical band structure of a solid.

• The regularized STM equation thus assumes the final form

$$\left[\hat{T}\left(-i\frac{d}{d\xi}\right) + U(\xi) - \mathcal{E}\right] \psi(\xi) = 0$$

[after rescaling $\psi(\xi) \to [1+U(\xi)]\psi(\xi)$], where the 'energy' is $\mathcal{E} = 4\pi/(3\sqrt{3}) - 1 \simeq 1.41899$ and the potential is:

$$U(\xi) = -\frac{1}{a\lambda}\frac{1}{\cosh\xi} + R^*\lambda\cosh\xi.$$

This quantum-mechanical equation for the antisymmetric wave-function $\psi(\xi) = -\psi(-\xi)$ formally describes the 1D motion of a fictitious particle with non-standard dispersion relation in the potential $U(\xi)$, at energy $\mathcal{E}$.

• What is the mechanism for regularization at $R^* > 0$? It is quite simple within our picture: The potential $U(\xi)$ approaches $+\infty$ at $\xi \to \pm\infty$, and hence all eigenstates must be quantized bound state solutions, similar to what happens for a simple quantum-mechanical harmonic oscillator.

• What is the spectrum is the resonant limit ($a = \infty$)? In our case, the 'energy' $\mathcal{E}$ is always fixed but the true spectral parameter is

λ – only those values of λ are allowed (possibly a finite set or countable infinity), where a bound state with energy $\mathcal{E}$ exists. These discrete values λ_n (indexed by $n \in \mathrm{Z}$) then determine the Efimov trimer bound state energies $E_n = -\lambda_n^2$. As $R^*\lambda \ll 1$, one sees that $n \gg 1$, zero energy therefore represents a spectral accumulation point.

Taking $\xi > 0$, the potential $U(\xi)$ can be neglected to exponential accuracy against $\mathcal{E}$ in the region $\xi \ll \xi_*$, where $\xi_* = \ln[2/(R^*\lambda)] \gg 1$. In this region, with $\hat{T}(s_0) = \mathcal{E}$, the (antisymmetric) solution must therefore be $\psi_1(\xi) = c_1 \sin(s_0\xi)$ with some amplitude c_1.

On the other hand, for all $\xi \gg 1$ (including the region $\xi \approx \xi_*$), the potential takes the form $U(\xi) = e^{\xi - \xi_*}$, again to exponential accuracy. Shifting ξ by ξ_*, the vicinity of the turning point is thus described by the *universal* (parameter-free) equation

$$\left[\hat{T}\left(-i\frac{d}{d\xi}\right) + e^{\xi} - \mathcal{E}\right]\psi(\xi) = 0.$$

For $\xi \to -\infty$, we have $e^{\xi} \to 0$, and thus the asymptotic behavior $\psi(\xi) \sim \sin(s_0\xi + \pi\gamma)$ with a non-trivial phase shift γ is expected. Coming back to the original ξ, we find that the solution for $1 \ll \xi \ll \xi_*$ is of the form $\psi_2(\xi) = c_2 \sin[s_0(\xi - \xi_*) + \pi\gamma]$, where c_2 is another amplitude, and should match ψ_1. With $n \in \mathcal{Z}$, this implies the *quantization condition*

$$\xi_*(\lambda_n) = \ln[2/(R^*\lambda_n)] = \frac{\pi(n+\gamma)}{s_0},$$

yielding the on-resonance *Efimov trimer energies*

$$E_n = -\frac{\hbar^2\kappa_*^2}{m} e^{-2\pi n/s_0},$$

with the famous universal ratio $E_{n+1}/E_n = e^{-2\pi/s_0} \simeq 1/515.03$ between subsequent levels. The *three-body parameter* κ_* is $\kappa_* R^* = 2e^{-\pi\gamma/s_0}$. To determine κ_* we need to calculate γ from the universal problem.

Universal problem

Remarkably, this problem can be solved exactly in terms of a Barnes-type integral

$$\psi(\xi) = \int\limits_{-i\infty+0^+}^{i\infty+0^+} \frac{d\nu}{2\pi i} e^{-\nu\xi} C(\nu),$$

which implies the recurrence relation

$$[\hat{T}(i\nu) - \mathcal{E}]C(\nu) = -C(\nu+1)$$

the solution to which also solves the differential equation provided that $C(\nu)$ has no poles in the strip $0 < \mathrm{Re}\nu < 1$.

To construct the solution to the recurrence relation, we use the Weierstrass theorem to express the function in the recurrence relation as a convergent infinite product

$$\hat{T}(i\nu) - \mathcal{E} = \prod_{p=0}^{\infty} \frac{\nu^2 - u_p^2}{\nu^2 - b_p^2}$$

in terms of poles $\pm b_p$, $b_p = 2p + 1$, and zeros $\pm u_p$: two zeros are on imaginary axes $u_0 =$

is_0, the other are real $u_1 = 4$, $u_2 = 4, 6...$ The solution with correct analytic properties is

$$C(\nu) = \frac{\pi}{\sin(\pi(\nu - is_0))} C_+(\nu),$$

with

$$C_+(\nu) = \prod_{p=0}^{\infty} \frac{\Gamma(\nu + u_p)\Gamma(1 - \nu + b_p)}{\Gamma(\nu + b_p)\Gamma(1 - \nu + u_p)} \, .$$

The poles of $C(\nu)$ nearest to the strip are $\nu = 2$ and $\nu = \pm s_0$ implying $\psi(\xi) \sim e^{2\xi}$ as $\xi \to \infty$ and $\psi(\xi) \sim \sin(s_0\xi + \gamma)$ as $\xi \to -\infty$. The **exact phase factor** follows from the ration of the residues at two poles $\nu = \pm is_0$:

$$\gamma = \frac{1}{2} - \frac{1}{\pi}\mathrm{Arg} C_+(is_0) \simeq -0.090518155 \, .$$

The three-body parameter is thus determines as

$$\kappa_* R^* = 2e^{-\pi\gamma/s_0} \simeq 2.6531.$$

This exact result roughly agrees with the available numerical estimate of 2.5.