Threshold phenomena in three-body systems

by

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Motivation: three-body recombination rates

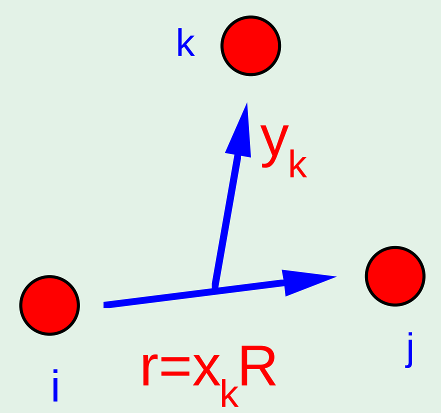
One of the main issues in Bose-Einstein condensation is the systematics of three-body recombination rates. A Bose condensate of some atoms, is not the lowest energy state but a metastable state, where the atoms are so far apart that they interact weakly. Such systems can fall into lower energy states, i.e., clusters of atoms, by recombination. Usually the main loss is due to recombination to dimers, B2. Such recombination cannot occur by simple two-body reactions. Something has to carry away the extra energy and momentum. The important process is thus

$$B + B + B \rightarrow B_2 + B$$

. We do this by approximating the two-body interaction by a zero-range potential which is defined by the scattering length a_l alone.

Zero-range potentials and three-body wave functions

Jacobi coordinates for three particles:



Other sets are obtain by cyclic permutation.

Zero-Range Potentials are included via the boundary conditions

$$\left[\frac{(2\ell+1)!!}{(2\ell-1)!!}\frac{d^{2\ell+1}(x_k^{\ell+1}\Psi)}{dx_k^{2\ell+1}} + \frac{(x_k^{\ell+1}\Psi)}{a_\ell^{2\ell+1}}\right]_{x_k\to 0} = 0, \quad k = 1,\ 2,\ 3.$$

where a_l is the scattering length associated with two-body interactions.

The Skorniakov and Ter-Martirosian integral equation

The Schrödinger equation is separable in standard independent particle coordinates $\boldsymbol{r}_k$, but the boundary conditions are not. Writing the solution as a contour integral over separable solutions in these coordinates and matching the boundary conditions gives the STM (Skorniakov and Ter-Martirosian) integral equation for $\ell = 0$ bosons. The equation was solved analytically by Danilov in the limit as $a_0 \to \infty$. For finite a_0 it is solved numerically.

ZRP in hyperspherical coordinates

The hyperspherical coordinates are given by

the hyper-radius $R^2 = x_i^2 + y_i^2$

hyper-angle $\alpha_i = \arctan(x_i/y_i)$

and the direction vector $\hat{\boldsymbol{x}}_{\boldsymbol{i}}$ and $\hat{\boldsymbol{y}}_{\boldsymbol{i}}$.

In these coordinates the Schrödinger equation has the form

$$\left[\frac{1}{R^5}\frac{\partial}{\partial R}\left(R^5\frac{\partial}{\partial R}\right)+\frac{\Lambda^2_{\hat{\boldsymbol{R}}}}{R^2}+K^2\right]\Psi=0,$$

where $K^2 = 2E$, and is separable on angular and radial equations

$$\left[\Lambda^2-\left(\nu^2-4\right)\right]S(\nu,\widehat{\mathbf{R}})=0,$$

$$\left[\frac{1}{R^5}\frac{\partial}{\partial R}\left(R^5\frac{\partial}{\partial R}\right)+\frac{\nu^2}{R^2}+K^2\right]Z_\nu\left(KR\right)=0$$

where $Z_\nu(KR)$ is a Bessel function and ν is the separation constant.

Boundary conditions in hyperspherical coordinates

In hyperspherical coordinates the boundary conditions for $\ell = 0$ and $\ell = 1$ become

$$\left[\frac{(2\ell+1)!!}{(2\ell-1)!!}\frac{\partial^{2\ell+1}(\alpha_k^{\ell+1}\Psi)}{\partial\alpha_k^{2\ell+1}} + \left(\frac{R}{a_\ell}\right)^{2\ell+1}(\alpha_k^{\ell+1}\Psi)\right]_{\alpha_k\to 0} = 0, \quad k = 1,\ 2,\ 3$$

which are clearly non-separable.

In the limit that $R \to 0$ and $a_0 \to \infty$ the Schrödinger equation and the boundary conditions are separable.

For $\ell > 1$ the boundary conditions in hyperspherical coordinates are more complicated and never separable.

Separable cases

For $R \to 0$ and $a_0 \to \infty$ the Schrödinger equation and the boundary conditions are separable and solutions have the form

$$\Psi_j(\boldsymbol{R}) = S(\nu_j, \hat{\boldsymbol{R}}) R^{-2} J_{\nu_j}(KR)$$

In the case $\ell = 0$ we have

$$S(\nu, \hat{\boldsymbol{R}}) = \sum_{k=1}^{3} \frac{\sin \nu(\pi/2 - \alpha_k)}{\sin 2\alpha_k}$$

and the separation constants ν_j are roots of the boundary equation

$$\nu \cos \nu \frac{\pi}{2} - \frac{8}{\sqrt{3}} \sin \nu \frac{\pi}{6} = 0.$$

Thomas effect

In the limit $R \to 0$ one can find the Thomas solutions $\Psi \approx R^{\nu_j - 2}$ as $R \to 0$

One of ν_j is complex with $\nu_j = it_0,\ t_0 = 1.00625$ and the solutions diverge as $R \to 0$.

The presence of the Thomas divergence means that many-body wave functions are not well defined for psuedopotentials even though the potentials are well adapted to the description of many-particle systems. This is basically a technical issue since the divergences can be easily avoided; however, it is necessary to recognize their possible presence.

Efimov states

For $a_0 \to \infty$ the Schrödinger equation and the boundary conditions are separable thus the effective hyper-radial potential $V_{\text{eff}}(R) = \frac{\nu_j^2 - 1/4}{2R^2}$ holds for all R and is given by

$$\Psi_j(\boldsymbol{R}) = S(\nu_j, \hat{\boldsymbol{R}}) R^{-2} J_\nu(KR)$$

where $J_\nu(KR)$ is a Bessel function.

Issues: The roots $\nu_0 = \pm i t_0$, $t_0 = 1.00625...$ are complex and the solutions diverge as $R \to 0$. Discard solutions? Efimov's answer: no. Separable solutions for large R hold for finite range potentials if $a_0 \to \infty$. The complex root implies an attractive effective potential

$$V_{\text{eff}}(R) = -\frac{t_0^2 + 1/4}{2R^2}.$$

There are an infinite number of three-body bound states (Efimov states) for such potentials.

Exact solution in general

We have seen that Efimov states correspond to exact separable solutions of the three-body Schrödinger equation with ZRPs, where the scattering length $a_0 \to \infty$, have the form

$$\Psi_j(\boldsymbol{R}) = S(\nu_j, \hat{\boldsymbol{R}}) R^{-2} Z_{\nu_j}(KR)$$

When the a_0 is finite (not infinite) then the boundary conditions are non-separable

$$\nu \cos \nu \frac{\pi}{2} - \frac{8}{\sqrt{3}} \sin \nu \frac{\pi}{6} = -\frac{R}{a_0} \sin \nu \frac{\pi}{2}$$

A general solution is a contour integral over the separation constant ν (a superposition of separable functions)

$$\Psi(\boldsymbol{R}) = R^{-2} \int_c A(\nu) S(\nu, \hat{\boldsymbol{R}}) Z_\nu(KR) \nu d\nu.$$

The function $\Psi(\boldsymbol{R})$ is just a sort of Kontorovich-Lebedev transform where the integration contour c is defined by initial conditions. The function $Z_\nu(KR)$ can be any of the Bessel function $J_\nu(z)$, $H_\nu^{(1,2)}(z)$ or $K_\nu(z)$, depending on total energy E.

Boundary conditions

It follows from the boundary conditions that $A(\nu)$ is given by the three-term recurrence relation

$$X(\nu+1)A(\nu+1) + X(\nu-1)A(\nu-1) = 2\nu\frac{1}{Ka}A(\nu)$$

with

$$X(\nu) = \nu - \frac{8}{\sqrt{3}}\frac{\sin\frac{\pi}{6}\nu}{\cos\frac{\pi}{2}\nu}$$

(1) The integral along a contour c must be define.

(2) $A(\nu)$ must have no singularities on the strip $0 < \mathrm{Re}\,\nu \leq 2$.

Three-term recurrence relation

General solutions of three-term recurrence relations have the form

$$A(\nu) = A_R(\nu)P_R(\nu) + A_L(\nu)P_L(\nu),$$

where $P_{R,L}(\nu)$ are arbitrary periodic functions, i.e. $P_{R,L}(\nu) = P_{R,L}(\nu+1)$. Two linearly independent solutions $A_{R,L}$ are defined by the asymptotic behavior for large ν

$$\lim_{\nu\to\infty} A_{R,L}(\nu) \to \exp[\mp\nu\alpha_K] \qquad \text{with} \qquad \sinh\alpha_K = 1/(Ka)$$

In this case the three-term recurrence relation are easily solved but there are problems to find periodic functions.

Kontorovich-Lebedev transform

The Kontorovich-Lebedev (KL) transform $f(x)$ of a function $g(x)$ is

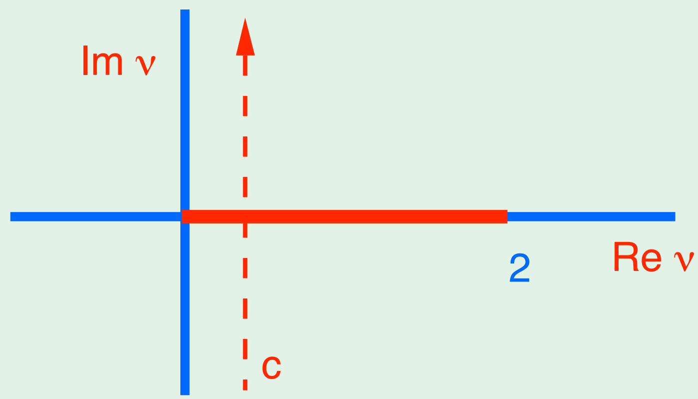
$$f(x) = i \int_0^{i\infty} g(\nu) K_\nu(x) \nu d\nu.$$

where

$$g(\nu) = -2\pi^{-2}\nu \sin(\pi \nu) \int_0^{\infty} f(t) K_\nu(t) t^{-1} dt.$$

H. Bateman and A. Erdelyi, *Table of Integral Transform*, McGraw-Hill Book Company, New York, p. 131 (1954).

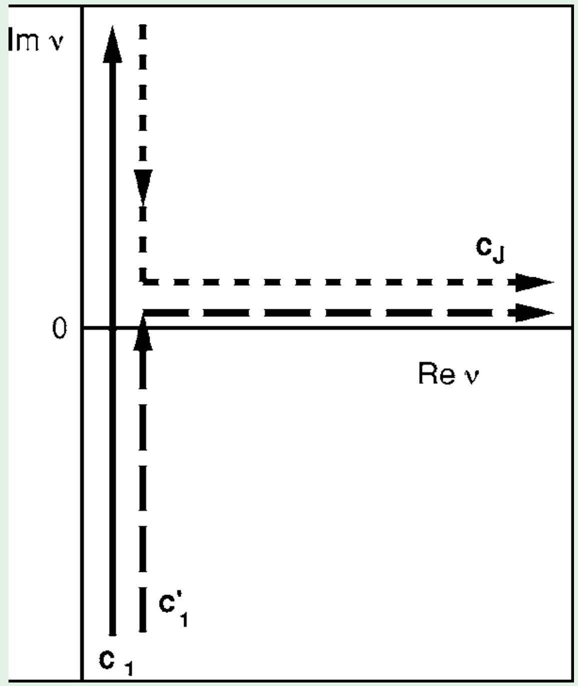
$\underline{E < 0}$



$$\Psi(\boldsymbol{R}) = R^{-2} \int_{-i\infty}^{i\infty} A(\nu) S(\nu, \hat{\boldsymbol{R}}) K_\nu(KR) \nu d\nu.$$

The proper Bessel function is K_ν, the contour of integration is a line in the complex ν plane that runs from $-i\infty$ to $i\infty$ along the imaginary axis and the integral representation is the Kontorovich-Lebedev transform with $K = \sqrt{-2E}$.

$\underline{E > 0}$



$$\Psi(\boldsymbol{R}) = R^{-2}\int_{c_1} A(\nu)S(\nu,\hat{\boldsymbol{R}})H_\nu^{(1)}(KR)\nu d\nu$$
$$+ \; 2R^{-2}\int_{c_J} A_R(\nu)P_R(\nu)S(\nu,\hat{\boldsymbol{R}})J_\nu(KR)\nu d\nu$$

More than one contour integral is needed to write the solution with the correct asymptotic behavior and then the representation becomes a generalization of the Kontorovich-Lebedev transform with $K = \sqrt{2E}$.

Exact solution for $E = 0$

At $E = 0$ one can get exact solutions since $\lim_{x\to 0} K_\nu(x) \to x^\nu$

$$\Psi(\boldsymbol{R}) = R^{-2}\int_{-i\infty}^{i\infty} C(\nu) S(\nu, \hat{\boldsymbol{R}})(R/a)^\nu d\nu.$$

In this case $C(\nu)$ satisfies the two-term recurrence relation

$$C(\nu+1) = \frac{\nu}{\nu + b(\nu)} C(\nu)$$

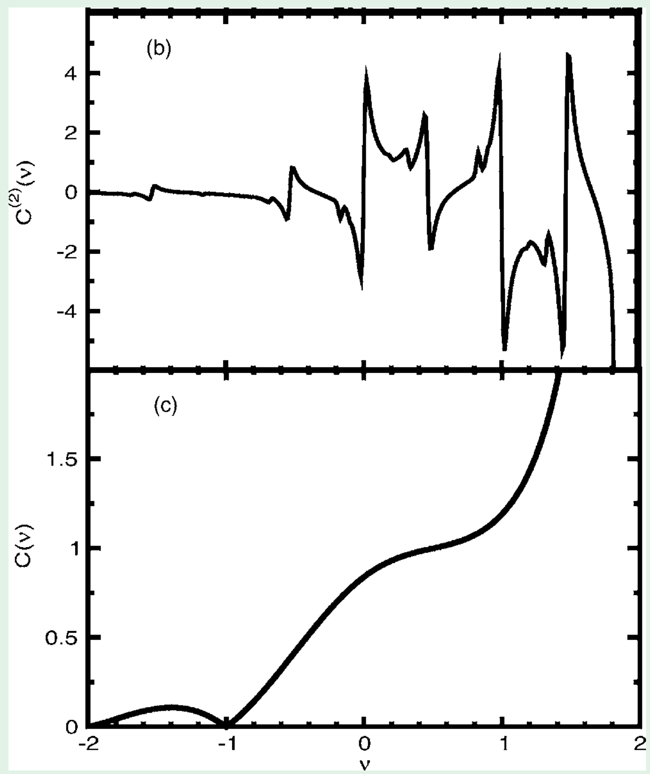
with

$$b(\nu) = -\frac{8}{\sqrt{3}} \frac{\sin\frac{\pi}{6}\nu}{\cos\frac{\pi}{2}\nu}.$$

The solution of this two-term recurrence relation can be found in the closed form

$$C(\nu) = \frac{6^\nu}{\Gamma(\nu)} \prod_{n=0}^{5} \frac{\Gamma(\frac{\nu+n+b(\nu+n)}{6})}{\Gamma(\frac{3+b(\nu+n)}{6})}$$

Coefficient $C(\nu)$



$C(\nu)$ (upper curve) has poles at ν_j. We should fine a periodic function $P(\nu)$ such that move the poles of $C(\nu)$ to the zeros so that $P(\nu)C(\nu)$ is smooth on the interval $0 \leq \nu \leq 1$

Periodic functions

$C(\nu)$ is analytic on the strip $0 < \Re\,\nu < 1$ and has on the interval $0 \le \nu \le 1$ an infinite number of poles at $\nu = \nu_j$ and the same number of zeros at $\nu = d_j$ where ν_j and d_j are roots of the equations

$$\frac{8}{\sqrt{3}}\frac{\sin\frac{\pi}{6}(\nu+n)}{\cos\frac{\pi}{2}(\nu+n)} = \nu + n + 6m \qquad \text{and} \qquad \frac{8}{\sqrt{3}}\frac{\sin\frac{\pi}{6}(\nu+n)}{\cos\frac{\pi}{2}(\nu+n)} = 3 + 6m$$

respectively, where $j = \{n, m\}$, $n = 0,\ 1,\ 2,\ 3,\ 4,\ 5$ and $m = 0,\ 1,\ ...$

The pole at ν_j can be shifted to the zero d_j by multiplying by the function

$$P_j(\nu) = \frac{\sin\pi(\nu - \nu_j)}{\sin\pi(\nu - d_j)}.$$

Therefore $C(\nu)P(\nu)$, where $P(\nu) = \prod_j P_j(\nu)$, has no poles at ν_j or d_j.

Limits as $R \to \infty$ and $R \to 0$

With the coefficient completely determined one can evaluate

$$\psi = \frac{1}{R^2} \int_{-i\infty}^{+i\infty} C(\nu) P(\nu) S(\nu, \hat{\boldsymbol{R}}) (R/a)^{-\nu} d\nu$$

in the limits as $R \to \infty$ and $R \to 0$ by conventional means:

$$\lim_{R \to \infty} \psi \longrightarrow \frac{e^{-x/a}}{xy} \left(e^{\pi t_0} e^{i(ky+\delta_\infty)} - e^{-\pi t_0} e^{-i(ky-\delta_\infty)} \right), \quad k = \frac{1}{a}$$

$$\lim_{R \to 0} \psi \longrightarrow R^{-2} e^{i\Delta(R)} S(-it_0, \hat{\boldsymbol{R}}), \qquad \Delta(R) = \delta_0 + t_0 \ln(R/a),$$

$$\delta_0 = \arg[C(-it_0) P(-it_0) \Gamma(-it_0)]$$

The function ψ has a divergent phase at the origin, consistent with the Thomas effect.

Elastic scattering phase shift

It is necessary to renormalize the function to remove this divergence. The linear combination of ψ and ψ^*

$$\Psi = e^{-i\Delta(R_0)}\psi + e^{i\Delta(R_0)}\psi^*$$

vanishes at $R = R_0$. The asymptotic form of Ψ

$$\lim_{R\to\infty} \Psi \propto \frac{e^{-x/a}}{xy}\left(e^{-iky} - S_{00}e^{+iky}\right),$$

gives the S_{00} matrix element

$$S_{00} \equiv e^{2i\delta} = e^{2i\delta_\infty}\left(\frac{e^{i\Delta(R_0)}e^{\pi t_0} + e^{-i\Delta(R_0)}e^{-\pi t_0}}{e^{i\Delta(R_0)}e^{-\pi t_0} + e^{-i\Delta(R_0)}e^{\pi t_0}}\right)$$

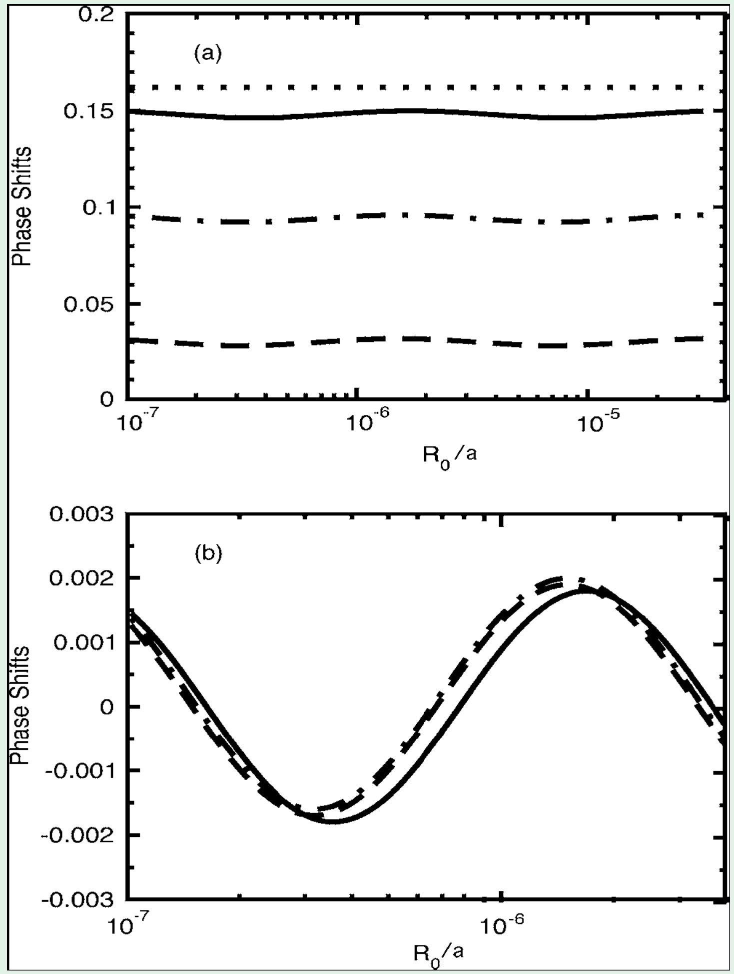
the elastic scattering phase shift at zero energy

$$\delta = \delta_\infty - \Delta(R_0) + \arctan\frac{e^{-2\pi t_0}\sin 2\Delta(R_0)}{1 + e^{-2\pi t_0}\cos\Delta(R_0)}$$

where

$$\delta_\infty = -\pi\sum_j(\nu_j - d_j), \quad \Delta(R) = \delta_0 + t_0\ln(R/a)$$

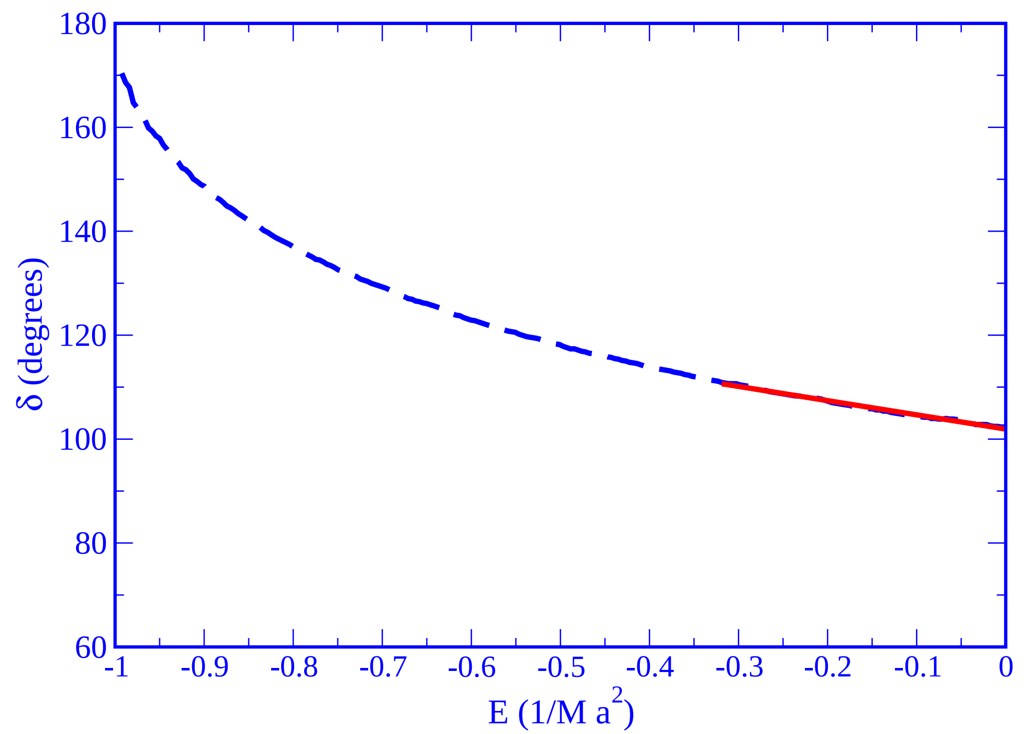
Our exact results are $\delta_\infty = 1.736$ and $\delta_0 = 1.588$ which compare well with similarly exact results of $\delta_\infty = 1.75$ from EFT (Braaten and Hammer e-print cond-mat/0410417 v1).



Plot of the phase shifts $\delta + t_0 \ln(R_0/a)$ vs R_0/a The solid curve is the exact result, the dashed curve is the one-channel close-coupling result, the dot-dashed curve is the adiabatic phase, and the dotted curve is the adiabatic phase in the WKB approximation. In (b) the curves are shown on a finer scale and moved to a common zero to compare the small oscillations.

Exact solutions $E < 0$

For $E < 0$ the three-term recurrence relation is solved numerically and used to compute the elastic scattering phase shift. Results are compared with those of Bedaque *et al*, Nuc. Phys. A 646, 444 (1999).



Exact solution $E > 0$

In this case $A(\nu)$ is defined by a three-term recurrence relation. There are two independent solutions $A_{L,R}(\nu)$ called L for left and R for right related by

$$A_L(\nu) = \frac{A_R(-\nu)}{\sin \pi\nu}$$

Periodic functions $P_{L,R}(\nu)$ and a constant A_0 are used to construct

$$A(\nu) = iA_0 A_L(\nu) P_L(\nu) + A_R(\nu) P_R(\nu)$$

such that $A(\nu)$ is free of poles on the interval $0 < \Re\,\nu \leq 2$.

As it was pointed out that in our case the three-term recurrence relation are easily solved but to find periodic functions is challenging.

Threshold phenomena in three-body systems, $E \to 0$

In the limit $E \to 0$ we used that

$$A_R(\nu) = (Ka)^\nu C(\nu),$$

where $C(\nu)$ satisfies the $E = 0$ two-term recurrence relation, and

$$P_R(\nu) = P_L(-\nu)\frac{\sin\pi(\nu + it_0)}{\sin\pi\nu}.$$

Then A_0 chosen to remove the pole at $\nu = 2$ has the form

$$A_0 = (Ka)^4 \lim_{\varepsilon\to 0}\frac{C(\epsilon+2)}{C(-\epsilon-2)}\frac{\sin^2\pi\varepsilon}{\sinh(\pi t_0)} = \frac{8(Ka)^4}{\sinh\pi t_0}\left(\frac{4\pi}{3\sqrt{3}} - 1\right)$$

The wave functions at large and small R are computed as before, except that for $E > 0$ a more complicated contour must be used.

$$\lim_{R\to\infty}\ \psi \to \frac{e^{-x/a}}{xy}\left([e^{\pi t_0} + iA_0]e^{i(ky+\delta_\infty)} - e^{-\pi t_0}e^{-i(ky-\delta_\infty)}\right), \quad k = \frac{1}{a}$$

The magnitude of the S_{00} is no longer unity since $A_0 \neq 0$.

The S-matrix elements, $E \to 0$

The matrix element S_{00} is

$$S_{00} = e^{2i\delta}\left[1 + 2iA_0\frac{e^{i\Delta(R_0)}\sin\Delta(R_0)}{1+e^{-2\pi t_0}e^{2i\Delta(R_0)}}\right] = e^{2i\delta}\left[1 + 2iPe^{i\Delta_r(R_0)}\sin\Delta_r(R_0)\right]$$

where

$$P = \frac{4(Ka)^4}{\sinh^2\pi t_0}\left(\frac{4\pi}{3\sqrt{3}} - 1\right), \qquad \delta = \delta_\infty + \Delta_r(R_0),$$

$$\Delta_r(R_0) = \Delta(R_0) + \arctan\frac{\mathrm{e}^{-2\pi\,t_0}\sin 2\Delta(R_0)}{1+\mathrm{e}^{-2\pi\,t_0}\cos 2\Delta(R_0)}$$

The matrix element S_{01} for the process

$$B + B_2 \to B + B + B$$

is

$$|S_{01}|^2 = 1 - |S_{00}|^2 = 4\,P\,(1-P)\sin^2\Delta_r(R_0)$$

Three-body recombination rate

The three-body recombination rate is

$$K_3 = 2(2\pi)^2 3^{3/2} \frac{|S_{01}|^2}{(Ka)^4} \frac{\hbar}{m} a^4 = C_3 \sin^2 \Delta_r \frac{\hbar}{m} a^4$$

with

$$C_3 = 2^7 \pi^2 (4\pi - 3\sqrt{3}) / \sinh^2 t_0 = \quad 67.1177\ldots$$

$$\Delta_r(R_0) \approx \Delta(R_0) = t_0 \ln(R_0/a) + 1.588$$

In excellent agreement with the fit $C_3 = 67.1 \pm 0.7\%$ to exact numerical computations [P.F. Bedaque, et al., Phys. Rev. Lett. **85**, 908 (2000)] and with exact solutions of the STM equation by D.S. Petrov.

The approximate hidden crossing theory [E. Nielsen and J. Macek Phys.Rev. Lett. **83**, 1566 (1999)] gets

$$K_3(HC) = 68.4 \sin^2(t_0 \ln(R_0/a) + 1.572) \frac{\hbar}{m} a^4$$

in surprisingly good agreement with the exact result.

Hidden crossing theory

Transition matrix element $|S_{01}|^2$ is

$$|S_{01}|^2 = 4P_{\mathrm{HC}}(1 - P_{\mathrm{HC}})\sin^2\Delta_{\mathrm{HC}}$$

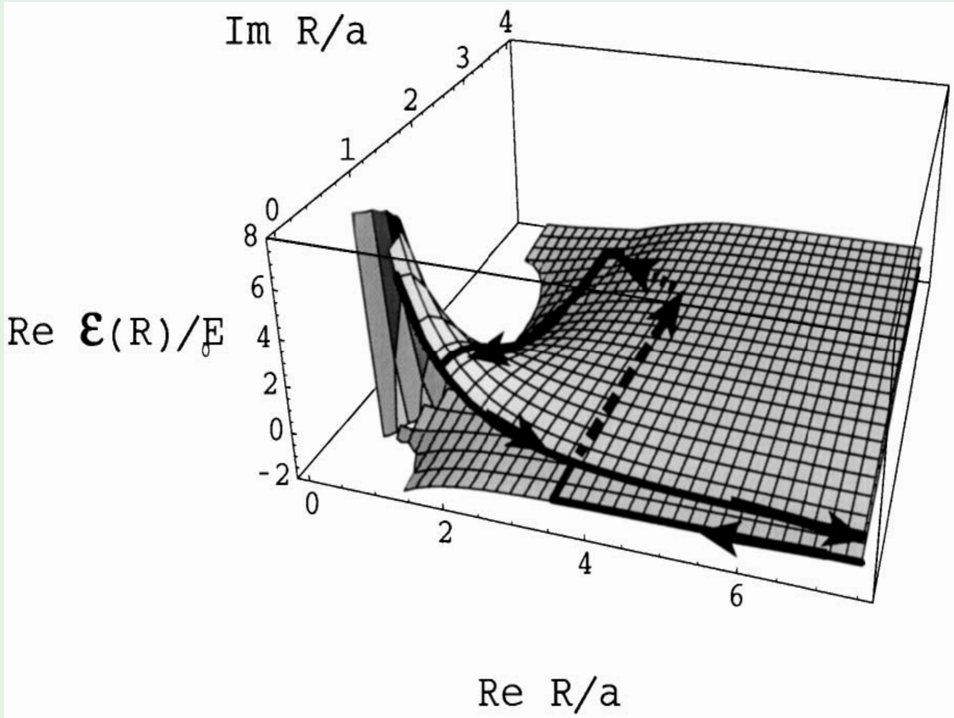
where

$$P_{\mathrm{HC}} = e^{-2\mathrm{Im}(I)} \qquad \Delta_{\mathrm{HC}} = \mathrm{Re}(I)$$

with

$$I = \int_{R_0}^{R_1} \sqrt{K^2 - 2\mathcal{E}(R) + \frac{1/4}{R^2}}dR.$$

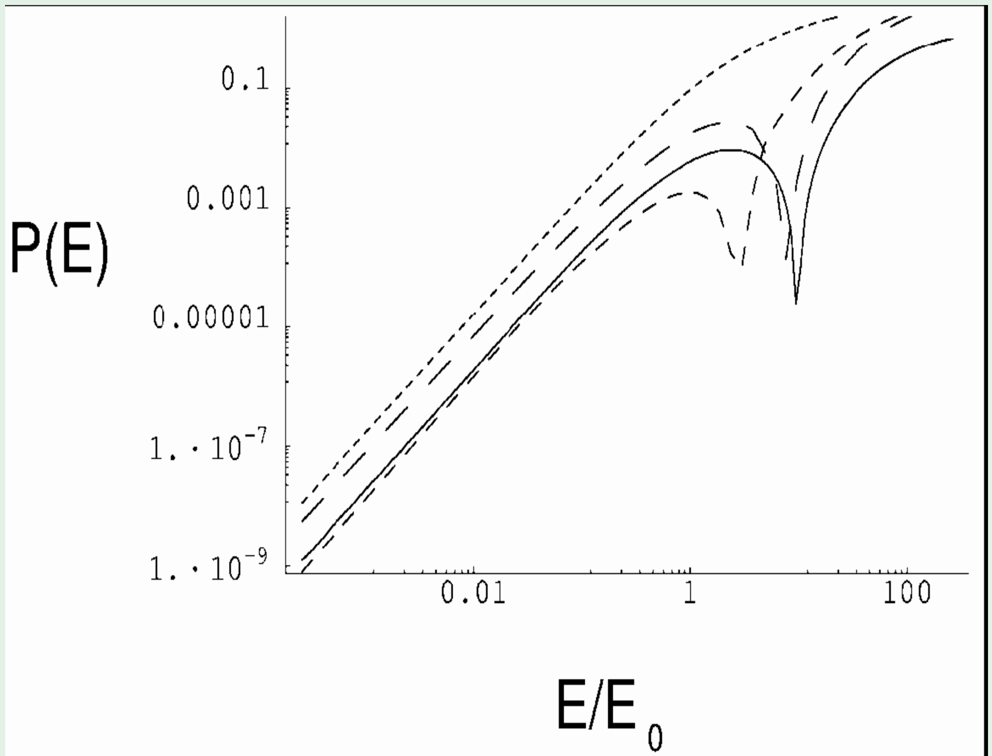
The function $\mathcal{E}(R)$ is the adiabatic eigenvalue.



The complex energy surface for the zero-range model, showing a branch point at $R =$(2.5918 , 2.9740 i). The heavy curve is one of the paths that contribute to the transition probability between the states in the hidden crossing theory.

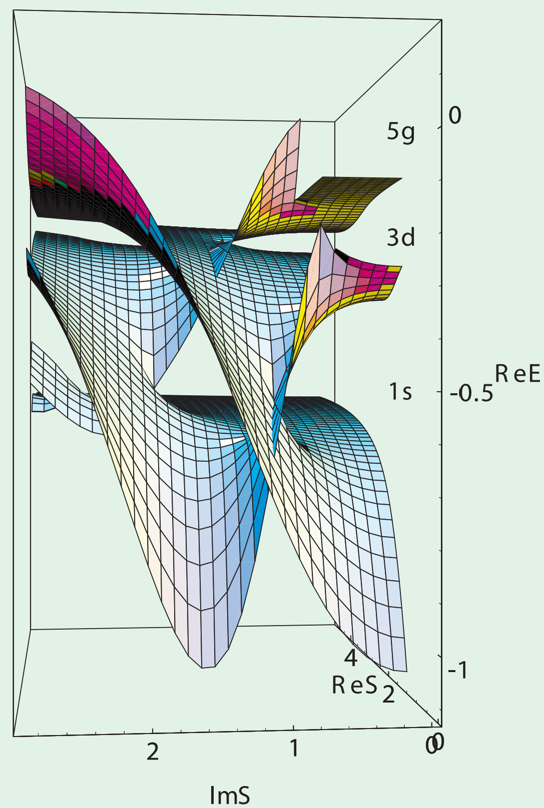
“Stuekelberg” phase

The “Stuekelberg” phase $\Delta_r(R_0)$ is closely related to the exact elastic scattering phase at the breakup threshold.



The transition probability for the reaction ^{4}He + ^{4}He + ^{4}He $\rightarrow$ ^{4}He + ^{4}He$_2$. The solid line is the coupled channel result, the intermediate dashed curve is the hidden crossing result, and the long dashed curve is with the Langer correction omitted, the short dashed curve is the ‘Stuekelberg” phase omitted. [E. Nielsen and J. H. Macek, Phys. Rev. Lett **83**, 1566 (1999)]

Riemann surface of H$^-$



Plot of $\mathrm{Re}E(R)$ vs $S = \sqrt{R}$ The integration path that gives the Wannier threshold law $P(E) \propto E^{\xi}$ with $\xi = \sqrt{\frac{12Z-1}{8z-2}} - \frac{1}{4}$ is also shown.

Conclusions

I. There are simple separable solutions when $a_\ell \to \infty$ for $\ell = 0, \;\; 1$ ZRPs, but not for $\ell \geq 2$.

2. There are Efimov effective potentials for $\ell = 0 \; ZRPs$ with $t_0 = 1.00625\ldots$.

3. Completely analytic solutions are found for $E = 0$. Results are in good accord with those obtained from the STM equation and EFT.

4. Results for $E < 0$ are very accurate.

5. There are analytic results for $E > 0$ in threshold laws.

All results can be found in Phys. Rev. A **72**, 032709 (2005) and Phys. Rev. A **73**, 032704 (2006)