# 40–Multiparticle Interactions of Zero–Range Potentials

by

Joseph Macek

University of Tennessee and

Oak Ridge National Laboratory

Presented at the workshop on Critical Stability,
Ettore Majorama Centre for Scientific Culture
12-18 October 2008

The interaction of three He atoms is the prototype for the interaction of three bosons when there is a loosely bound $He_2$ dimer. In this case the impulse approximation is accurate over a large energy range and gives the expression

$$\sigma_{\mathrm{breakup}} = 2\sigma^{(2)}_{\mathrm{elastic}}$$

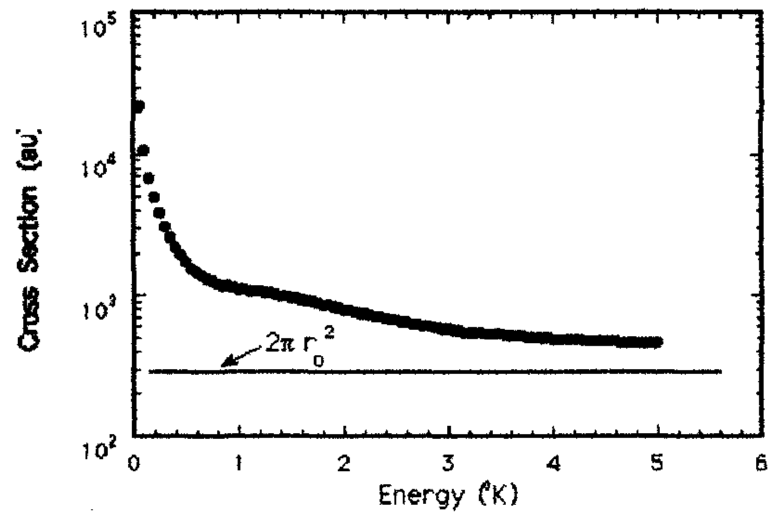



**FIGURE 1.** Cross section for the process $He + He_2 \to He + He + He$ in the impulse approximation. The horizontal line corresponds to the limit cross section for the hard core of the He-He potential with $r_0 = 4.5au$.

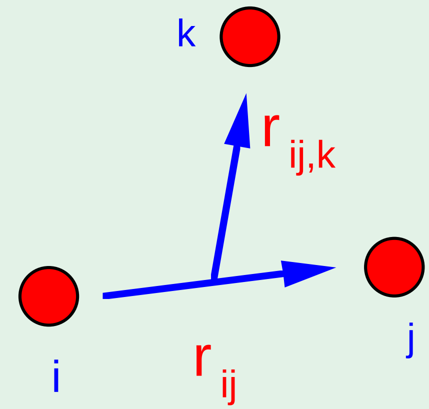
Two-body zero-range (or contact) pseudopotentials are defined as

3

$$v(r) = 2\pi \frac{(\ell+1)[(2\ell-1)!!]}{[(2\ell)!!]} a^{2\ell+1} \frac{\delta^3(\boldsymbol{r})}{r^\ell} \frac{\partial^{2\ell+1}}{\partial r^{2\ell+1}} r^{\ell+1}$$

Alternatively one can use ZRP boundary conditions

$$\lim_{r\to 0}\left[\frac{(2\ell+1)!!}{(2\ell-1)!!}\frac{d^{2\ell+1}(r^{\ell+1}\Psi)}{dr^{2\ell+1}} - \frac{r^{\ell+1}}{a_\ell^{2\ell+1}}\Psi\right] = 0,$$




The Schrödinger equation is separable in standard independent particle coordinates $\boldsymbol{r}_{ij}$, $\boldsymbol{r}_{ij,k}$, 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 boundary conditions separate in the limit as $a_0 \to \infty$ and an analytic solutions gives the Efimov states. For finite $a_0$ numerical methods are employed.

## Hyperspherical coordinates

N particle coordinates (mass scaled): $\{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_{N-1}\} \to \left\{R, \hat{\boldsymbol{R}}\right\}$

$\hat{\boldsymbol{R}} =$ unit vector in $3(N-1)$ dimensions. $R^2 = \sum_i^{N-1} r_i^2 =$ hyper-radius in $3(N-1)$ dimensions.

$$H = T_R + \frac{\Lambda^2_{\hat{\boldsymbol{R}}}}{2R^2}$$

Define basis functions $S(\nu; \hat{\boldsymbol{R}})$ according to

$$\left(\frac{\Lambda^2_{\hat{\boldsymbol{R}}}}{2R^2}\right) S(\nu; \hat{\boldsymbol{R}}) = \frac{(\lambda + 3N - 5)\lambda}{2R^2} S(\nu; \hat{\boldsymbol{R}})$$

For three particles one may find $S(\nu, \hat{\boldsymbol{R}})$ in closed form.

In hyperspherical coordinates there are cross derivatives between $x = r/R = \sin\alpha$ and $R$

$$\frac{\partial}{\partial r} = \frac{1-x^2}{R}\frac{\partial}{\partial x} + x\frac{\partial}{\partial R}$$

even in the limit as $x \to 0$ for general $\ell$. For $\ell = 0$ and $\ell = 1$, however the boundary conditions become

$$\frac{(2\ell+1)!!}{(2\ell-1)!!}\frac{\partial^{2\ell+1}(x_k^{\ell+1}\Psi)}{\partial x_k^{2\ell+1}} = \left(\frac{R}{a_\ell}\right)^{2\ell+1} x_k^{\ell+1}\Psi, \quad k = 1,\ 2,\ 3.$$

In the limit that $a \to \infty$ the equations separate and one can find the Thomas solutions $\Psi \approx R^{\nu_j - 2}$ as $R \to 0$ where $\nu_j$ is a root of

$$\lim_{x\to 0}\frac{(2\ell+1)!!}{(2\ell-1)!!}\frac{d^{2\ell+1}(x_k^{\ell+1}\Psi)}{dx_k^{2\ell+1}} = 0$$

## ZRP continued



Set $\lim_{R\to 0}\Psi(\boldsymbol{R}) \to R^{\nu-2}S(\nu,\hat{\boldsymbol{R}})$ where $S(\nu,\hat{\boldsymbol{R}})$ is a solution of

$$\Lambda^2_{\hat{\boldsymbol{R}}}S(\nu,\hat{\boldsymbol{R}}) = \nu(\nu+4)S(\nu,\hat{\boldsymbol{R}})$$

For $\ell = 0$ bosons one has

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

and the boundary conditions become

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

For $a_0 \to \infty$ or $R \to 0$ only allowed values of $\nu = \nu_j$ are roots of the equation

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

.

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

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

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

**Issues:** The roots $\nu_0 = \pm i t_0$, $t_0 = 1.0062...$ 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

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

There are an infinite number of three-body bound states for such potentials. Exact solutions confirm that the oscillatory solutions cannot be discarded.

What about $\ell \neq 0$ and spin $s = 1/2$ fermions?

## Fermions

To treat fermions we must include spin in the angular function $S(\nu,\hat{\boldsymbol{R}})$

$$S(\nu,\hat{\boldsymbol{R}},\sigma)=\sum_{k=1}^{3} f_{l_x l_y}(\alpha_k) Y_{\ell_x \ell_y LM}(\hat{\boldsymbol{x}}_k,\hat{\boldsymbol{y}}_k)\chi^{S}_{M_S}(ijk)$$

The boundary conditions must now be satisfied for every possible spin coupling. For $s-$ wave psuedopotentials $\chi(ijk)$ has the coupling $((\frac{1}{2}\frac{1}{2})0,\frac{1}{2})\frac{1}{2}$ and one finds that $\nu_j$ is a root of

$$\nu\cos\nu\frac{\pi}{2}-\frac{4}{\sqrt{3}}\sin\nu\frac{\pi}{6}=0$$

All of the roots of this equation are real so there is neither an Efimov nor Thomas effect. All three-body threshold dynamics are determined by the two-body scattering length $a_0$. When $a_0\rightarrow\infty$ then $\Psi(\boldsymbol{R})=S(\nu,\hat{\boldsymbol{R}},\sigma)Z_{\nu_j}(KR)$ is an exact solution. There are an infinite number of such solutions corresponding to the infinite number of separation constants (genaralized angular momenta) $\nu_j$. There are no three-body bound states.

For $\ell = 1^+$ the angular factor is $\boldsymbol{x}_k \times \boldsymbol{y}_k$ which is unchanged under cyclic permutations of $ijk$ and therefore factors out of the boundary conditions. Since the space part is antisymmetric under interchange of any two coordinates, the spin coupling must be ((1/2,1/2)1,1/2),1/2 or ((1/2,1/2)1, 1/2),3/2. The latter coupling corresponds to spin polarized fermions and in this case one finds that the boundary conditions for $a_\ell \to \infty$ become

$$\cos\nu\frac{\pi}{2} + 2\,{}_2F_1\left(-\frac{\nu}{2}+2, \frac{\nu}{2}+2; \frac{5}{2}; \frac{1}{4}\right) = 0$$

This equation has only real roots so that there neither an Efimov nor a Thomas effect. For the first coupling scheme with total spin equal to$1/2$, the boundary condition gives the equation

$$\cos\nu\frac{\pi}{2} - {}_2F_1\left(-\frac{\nu}{2}+2, \frac{\nu}{2}+2; \frac{5}{2}; \frac{1}{4}\right) = 0$$

This equation has complex roots $it_0$ with $t_0 = \pm 0.6668\ldots$. Accordingly there is both a Thomas effect and (possibly) an Efimov effect.

## Exact solution for $a_0 > 0$

14 We have seen that Efimov states correspond to exact separable solutions of the three-body Schrödinger equation with ZRPs where the scattering length $a_\ell \to \infty$.

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

When the $a_\ell$ is finite (not infinite) then the boundary conditions require a superposition of separable functions

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

. It follows from the boundary conditions that $A(\nu)$ is given by the three-term recurrence relation (TTR)[PRA, **72**, 032709 (2005)]:

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

with

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

## Exact solution for $a_0 > 0$ and $E \neq 0$



The magnitude of the $S_{00}$ is

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

where $P = A_0/(2\sinh t_0)$. The three-body recombination rate is

$$K_3 = C_3 \sin^2\Delta_r \frac{\hbar}{m} a^4$$

with $C_3 = 2^7\pi^2(4\pi - 3\sqrt{3})/\sinh^2 t_0 = \quad 67.1177\ldots$. The approximate hidden crossing theory gets

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

in surprisingly good agreement with the exact result where $\Delta_r \approx t_0 \ln(R_0/a) + 1.588$

## Approximate solution (Hyperspherical closed-coupling)

$$H = T_R + \frac{\Lambda^2_{\hat{\boldsymbol{R}}}}{2R^2} + V(\boldsymbol{R})$$

Define basis functions $\Phi(R;\hat{\boldsymbol{R}})$ according to

$$\left(\frac{\Lambda^2_{\hat{\boldsymbol{R}}}}{2R^2} + V(\boldsymbol{R})\right)\Phi(R;\hat{\boldsymbol{R}}) = \frac{\nu(R)^2 - (3N-5)}{2R^2}\Phi(R;\hat{\boldsymbol{R}})$$

For ZRP $\nu(R)$ is determined by the boundary conditions which give an equation of the form

$$f_\ell(\nu(R)) = R^{2\ell+1}M$$

where $M = k^{2\ell+1}\cot\delta \approx -\frac{1}{a^{2\ell+1}}$. The hidden crossing theory uses the effective potential $(\nu(R)^2 - 1/4)/2R^2$ to find approximate bound states and $S-$matrix elements. We have seen that the approximate solutions are fairly accurate. Use the adiabatic picture to analyze various generalizations of the ZRP's.

## Generalizations of the ZRP's

1. Use a multichannel ZRP (Oleg Kartavtsev, Few-Body Systems,**31**, 249 (2002)) $M$ becomes a matrix. Results are promising but one quickly finds that a large number of channels are involved.

2. Include energy dependence. Why? When the first term in the effective range expansion $-1/a^{2\ell+1}$ vanishes then the higher order terms are important. We can use the adiabatic theory to see if these terms make a significant difference to our conclusions about threshold effects.

To include energy dependence in the adiabatic picture we use the replacement $k^2 \to \frac{\nu(R)^2 - \ell_x(\ell_x+1)/3 - \ell_y(\ell_y+1)}{R^2}$ and consider

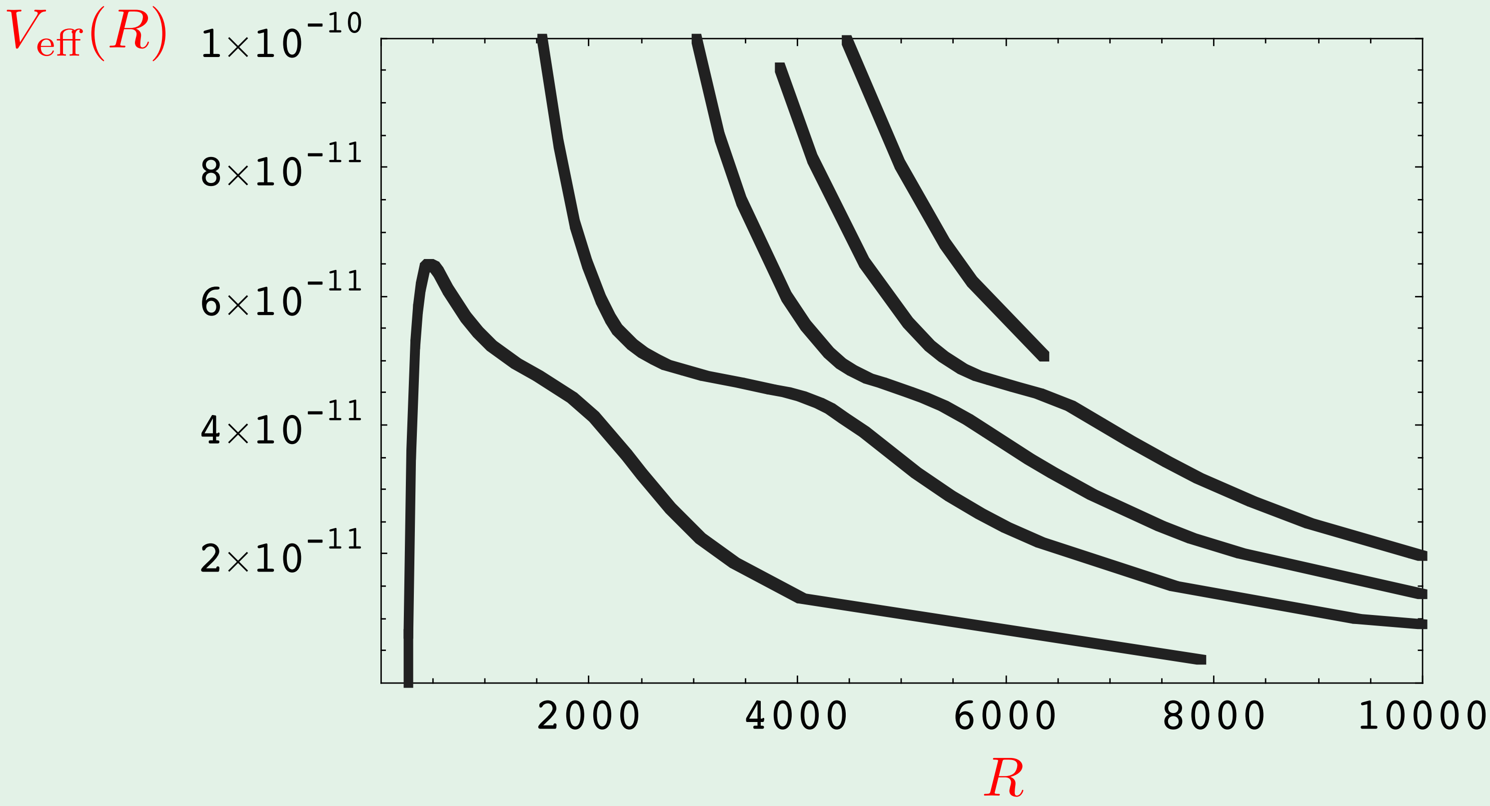
$$f(\nu(R)) = R^{2\ell+1} M(k^2) = -\left(\frac{R}{a}\right)^{2\ell+1} + O(R^{2\ell-1})$$

For $\ell = 0$ the effective range term in $RM(k^2)$ is of the order of $1/R$ so it has little effect on threshold quantities.

For $\ell = 1$, the effective range term in $R^3 M(k^2)$ is of the order of $R$ and cannot be ignored. If this term is not zero, there are no $\ell = 1$ Efimov states. In order to have Efimov states for $\ell = 1$ the p-wave $M(k^2)$ must be of the order of $k^4$ for small $k$. Not possible for local short-range potentials.

3. Energy dependence allows one to model resonances

$$M = k^{2\ell+1}\cot\delta = (E_r - E)/\gamma$$

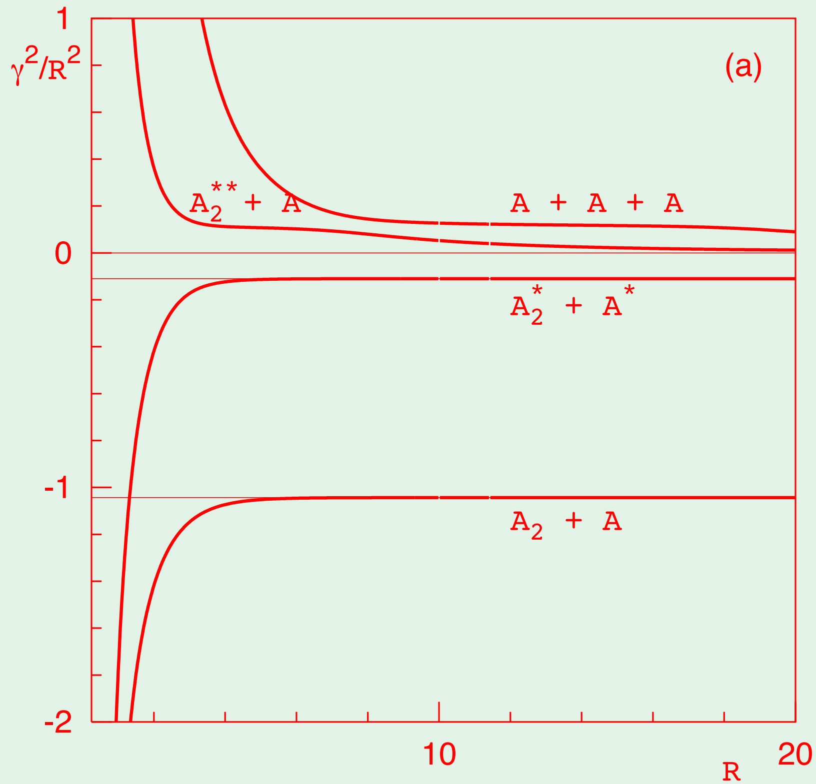


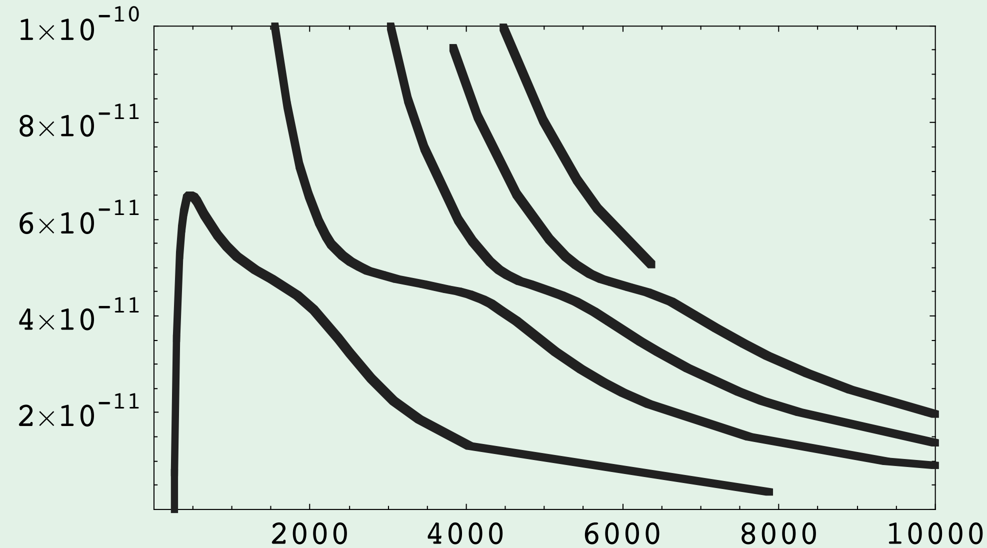
# Problems with energy-dependent potentials

First problem: Solutions of the S-equation are not orthogonal.

Second problem: Multiparticle $S-$ matrix is not defined.

Solution: Introduce energy dependence naturally. (e.g. Oleg Kartavstev's multichannel model)



## Conclusions

1. Contact interactions are usefully treated in hyperspherical coordinates.

2. Exact solutions and good approximate solutions are available.

3. p-wave states [unnatural parity] are interesting, but need a correct way to handle energy dependence.

4. Contact interactions for $\ell > 0$ are not actually contact interactions since the limit $r \to 0$ cannot be taken everywhere (e. g. in evaluating normalization constants).

5. Multichannel ZRP's appear to be the only way to correctly treat energy dependence with contact interactions.