Behavior of Wave Functions near the Thresholds

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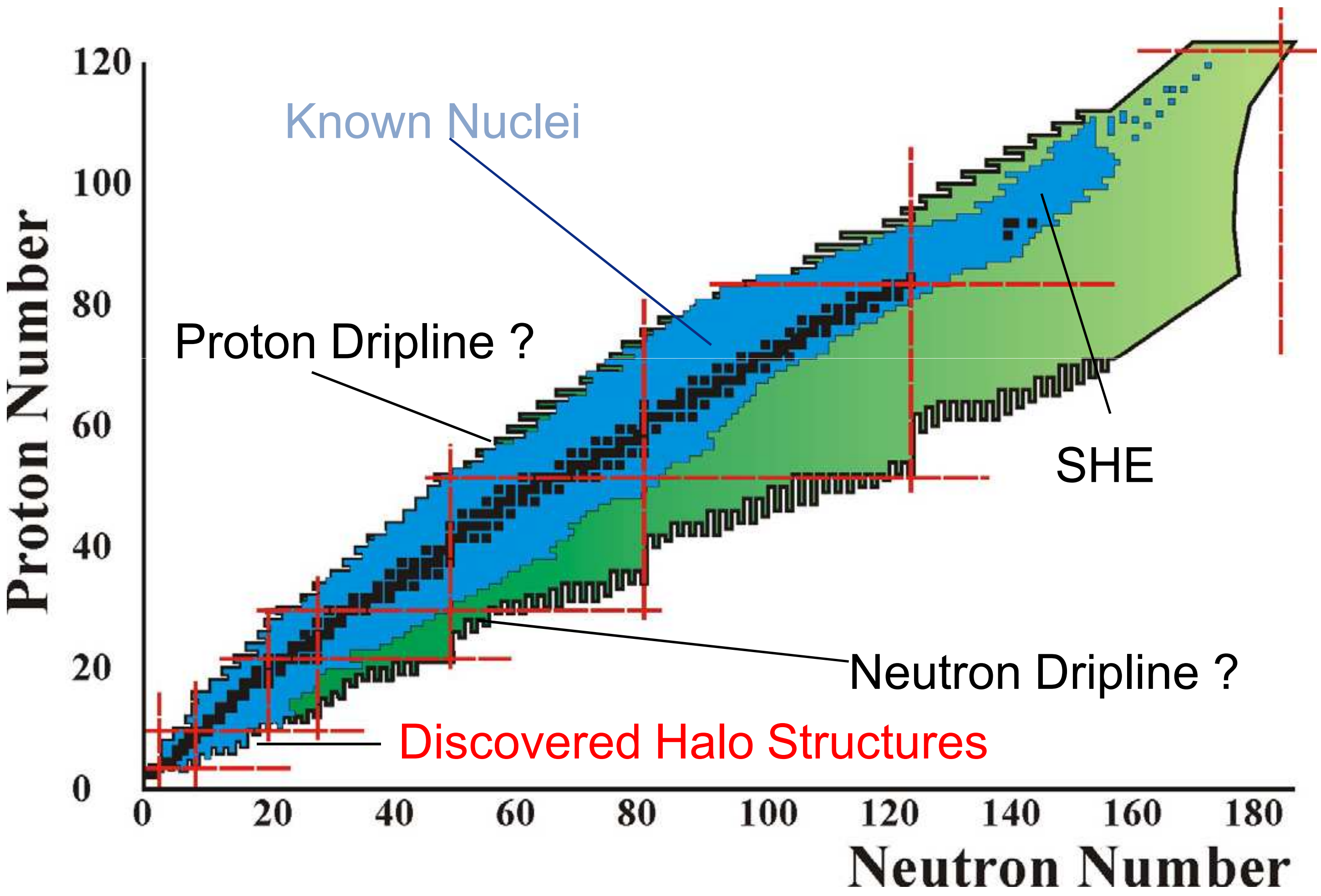
Plan of the Talk

- Patterns of near-threshold behavior and examples
- Basic definitions
- A short review of the Klaus and Simon method
- Examples of halo formation
- Bounds on the Green’s functions with repulsion
- Bound states at threshold in negative ions
- The case of $N \geq 4$ and open problems.

Nuclear Chart



The nucleus ^{11}Li lies on the drip line. Two neutrons form a halo

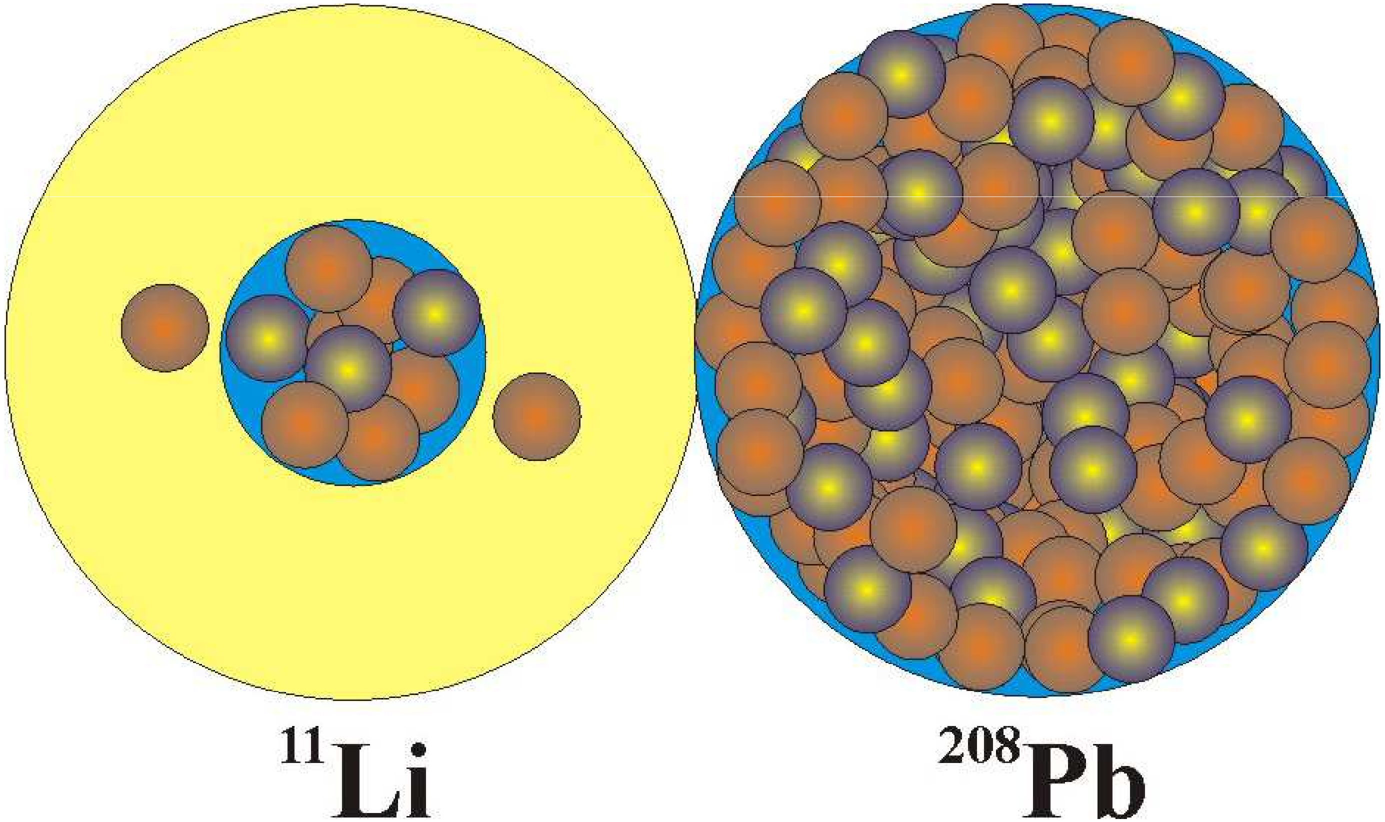
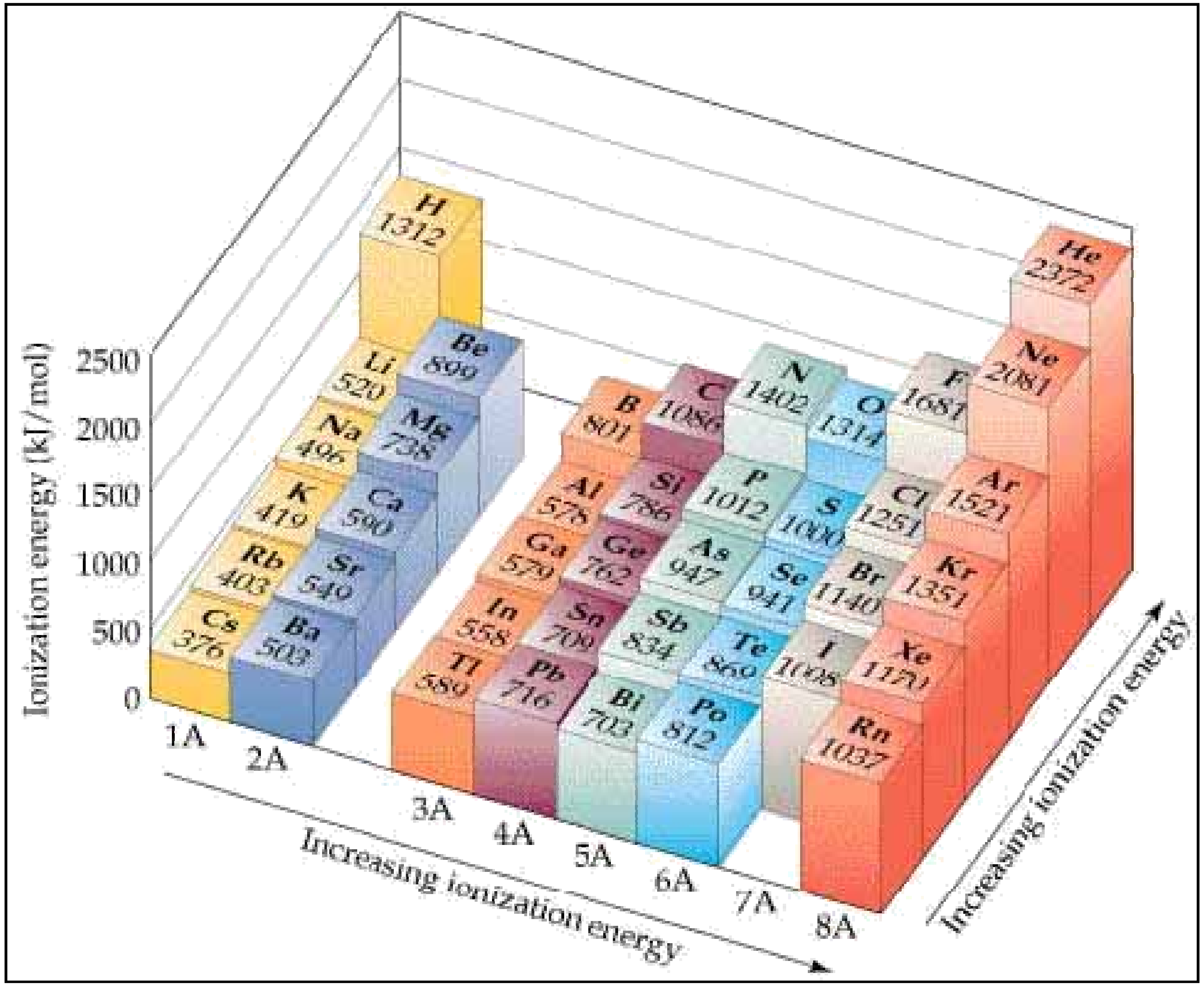


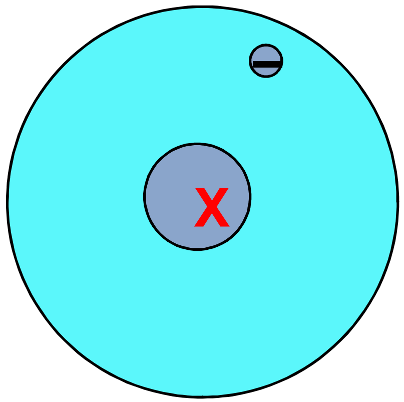
Table of Inonization energy for the first electron



Electron Affinities in kJ / Mol

Small compared to ionization energies (near-threshold behavior)

H −73							He >0
Li −60	Be >0	B −27	C −122	N >0	O −141	F −328	Ne >0
Na −53	Mg >0	Al −43	Si −134	P −72	S −200	Cl −349	Ar >0
K −48	Ca −2	Ga −30	Ge −119	As −78	Se −195	Br −325	Kr >0
Rb −47	Sr −5	In −30	Sn −107	Sb −103	Te −190	I −295	Xe >0



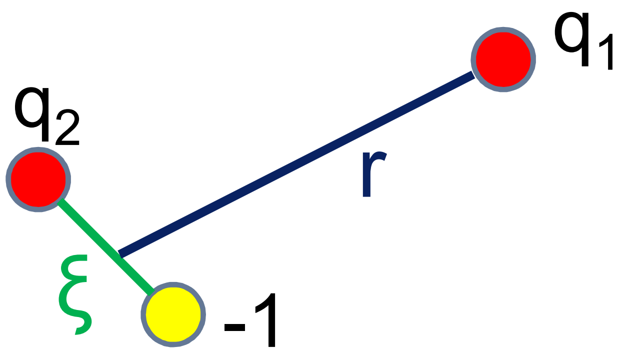
Stability diagram for three charges (-1, q_1 , q_2) with masses (1, m_1 , m_2)

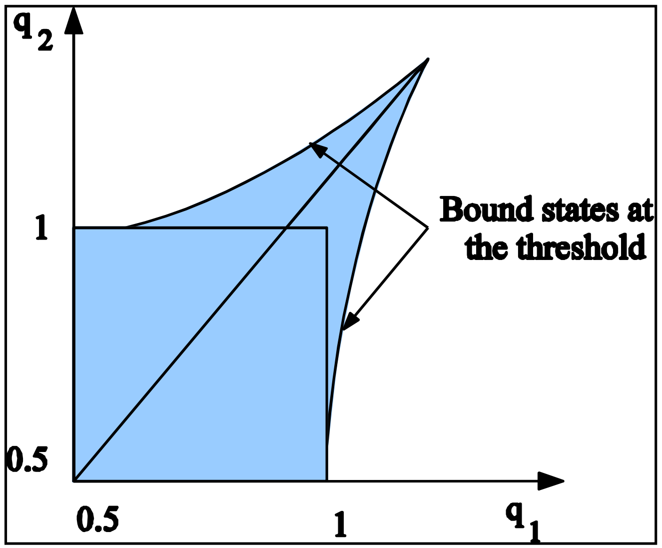
$$H(q_1, q_2) = H_{thr} + \frac{p_r^2}{2\mu} + W(r,\xi),$$

where

$$W(r,\xi) = -\frac{q_1}{q_2|(1-s)\xi - r|} + \frac{q_1}{|s\xi + r|}$$

$$H_{thr} = \frac{p_\xi^2}{4} - \frac{1}{|\xi|}$$

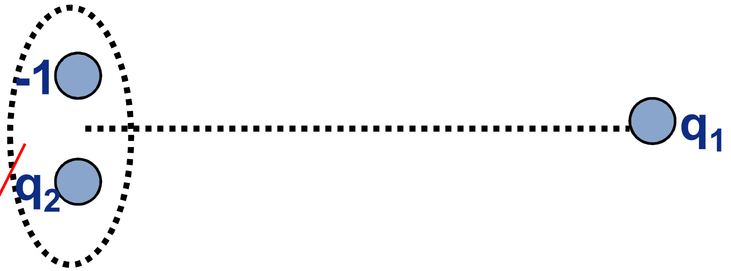




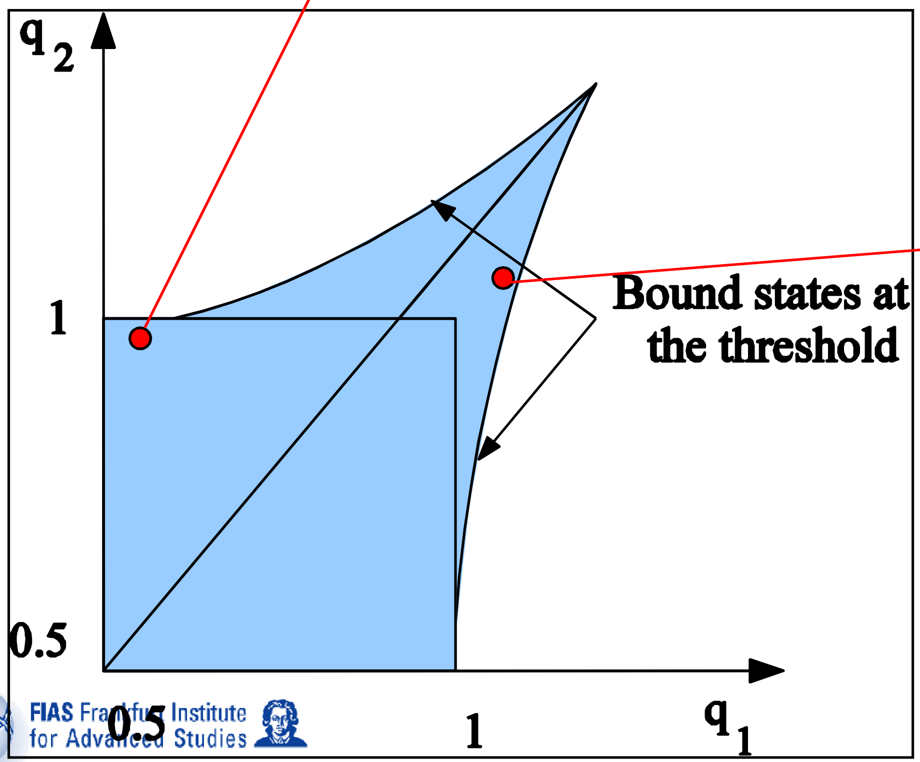
The line of equal thresholds:

$$\mu_{23} q_2^2 = \mu_{13} q_1^2$$

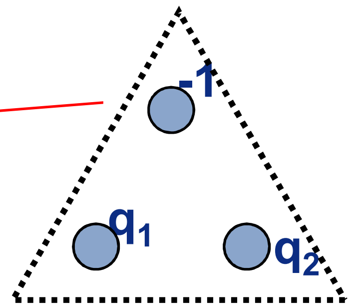
Stability diagram for three charges (-1, q_1 , q_2) with masses (1, m_1 , m_2)



Halo Structure !



On the arcs the wave function remains compact



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Proof of the halo structure

Suppose that the Hamiltonian

$$H(q_1,1) = H_{thr} + \frac{p_r^2}{2\mu} + W(r,\xi), \quad \text{where} \quad E_{thr} = -1, \quad H_{thr} = \frac{p_\xi^2}{4} - \frac{1}{|\xi|}$$

and

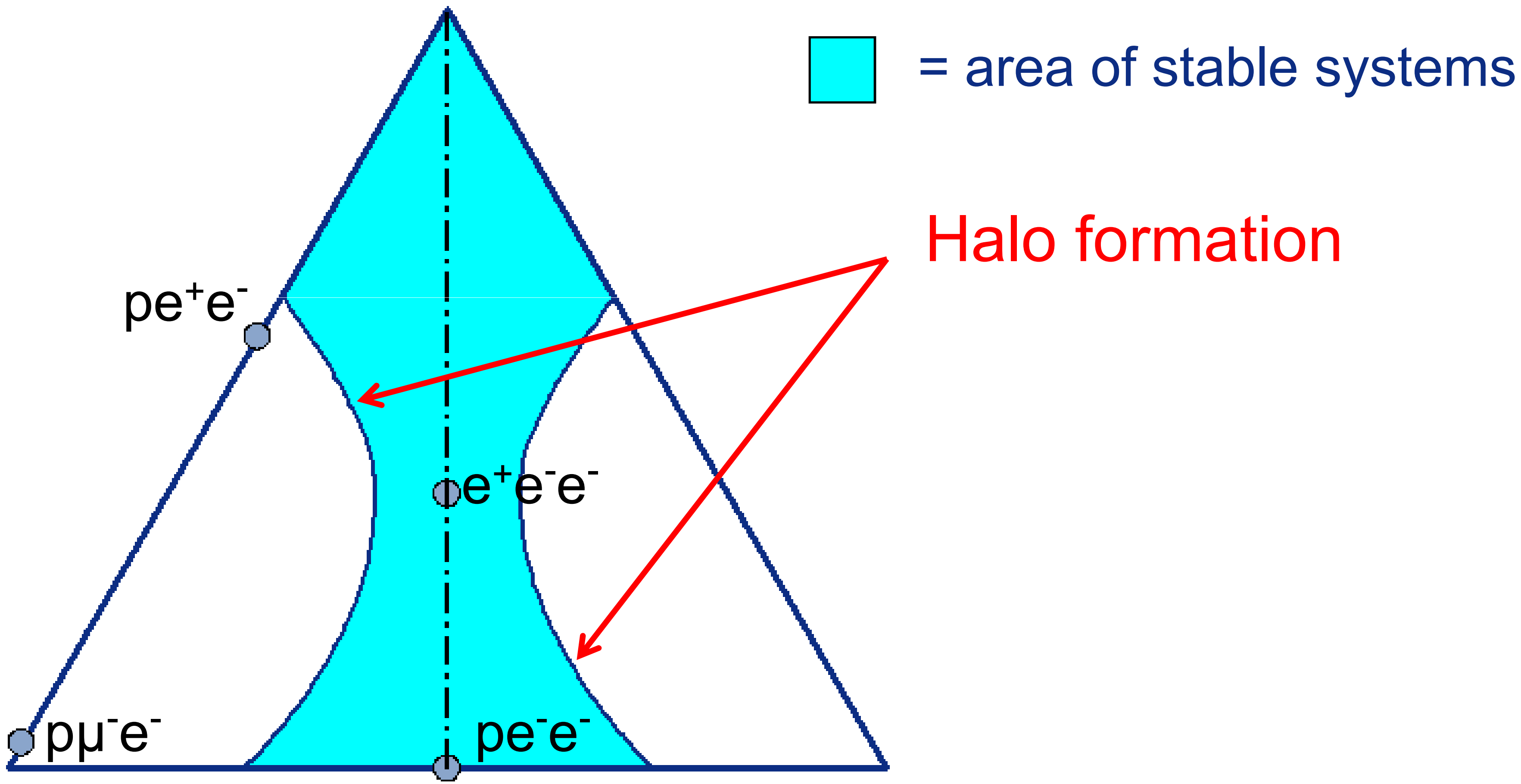
$$W(r,\xi) = -\frac{q_1}{|(1-s)\xi - r|} + \frac{q_1}{|s\xi + r|}$$

has a bound state at threshold $H(q_1,1)\phi_0 = -\phi_0$

Then $\langle\phi_0|W|\phi_0\rangle < 0$ **and the Hamiltonian** $H(q_1+\epsilon,1)$

must be stable for $\epsilon > 0$

The map of stable systems for three unit charges



How does E(λ) behave near λ = λcr?

For a negative short-range potential W one has

$$(-\Delta + \lambda W)\psi_k = -k^2\psi_k$$

Through a substitution $u_k = W^{1/2}\psi_k$ one gets

$$K u_k = -\lambda^{-1}(k) u_k,$$

where we define the integral operator

$$K(x,y) = \frac{e^{-k|x-y|}}{4\pi|x-y|} W^{1/2}(x) W^{1/2}(y)$$

Performing perturbation theory near $k = 0$ gives

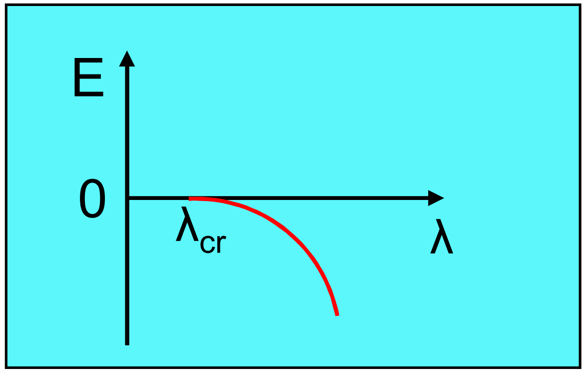
$$\lambda^{-1}(k) = \lambda_{cr}^{-1} + a_1 k + a_2 k^2 + \ldots.$$

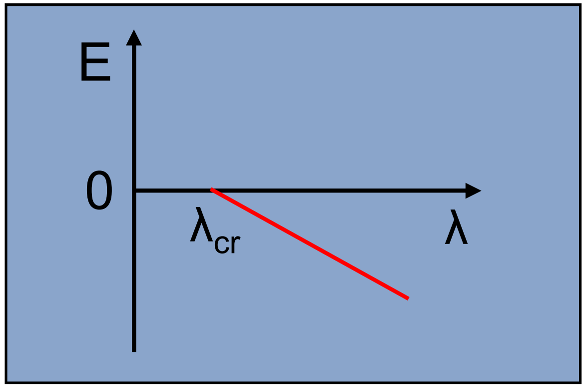
There are two possibilities for some c>0

$$E(\lambda) = -c(\lambda - \lambda_{cr})^2 + O((\lambda - \lambda_{cr})^3) \qquad (analytic)$$

$$E(\lambda) = -c(\lambda - \lambda_{cr}) + O((\lambda - \lambda_{cr})^{3/2}) \qquad (non - analytic)$$

By the Feynmann-Helman theorem $\langle \psi | W | \psi \rangle = dE/d\lambda$



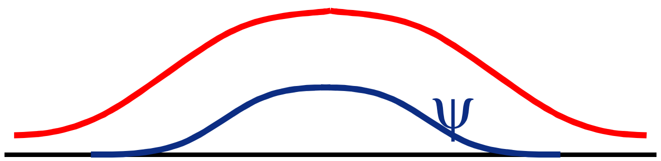


Formation of halo in the two-body system.

Corollary. *If there exist* $A, a > 0$ *such that* $|W| \leq Ae^{-a|x|}$ *and at* $\lambda = \lambda_{cr}$ *there is no zero-energy bound state then the following upper bound holds for the normalized bound state* ψ *having the energy* $E(\lambda)$ *in the neighborhood of* $E(\lambda_{cr}) = 0$

$$|\psi| \leq \frac{C|E|^{1/4} e^{-\sqrt{|E|}r}}{r},$$

where $C > 0$ *is some constant independent of* E*.*



Proof.

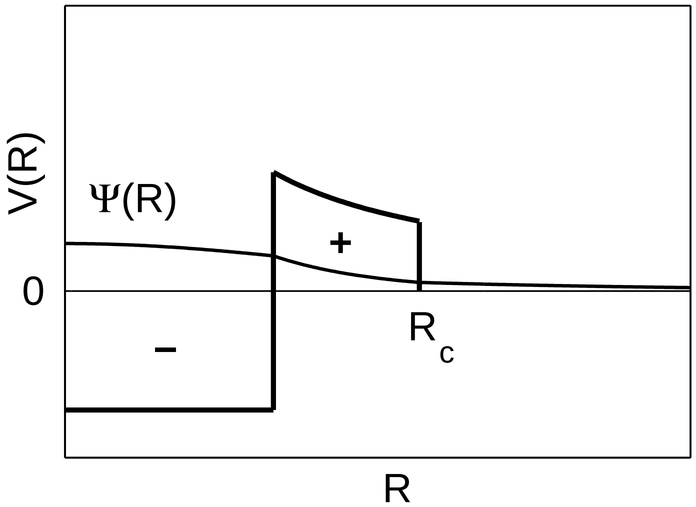
$$\psi(x) = -\lambda \int dy \, \frac{e^{-\sqrt{|E|}|x-y|} W(y)\psi(y)}{4\pi|x-y|}$$

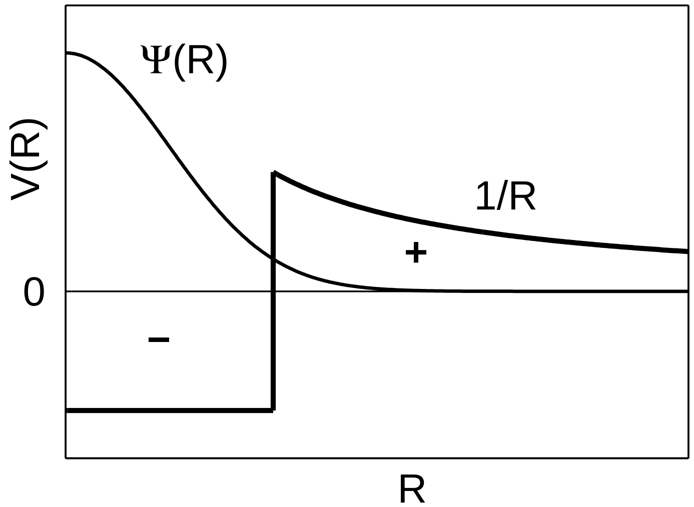
Using $|W| \leq Ae^{-a|x|}$ and applying the Schwarz inequality gives

$$|\psi| \leq \lambda \langle\psi||W||\psi\rangle^{1/2} \left[\int dy \, \frac{Ae^{-a|y|} e^{-2\sqrt{|E|}|x-y|}}{|x-y|^2} \right]^{1/2} \leq \lambda \langle\psi||W||\psi\rangle^{1/2} \frac{C' e^{-\sqrt{|E|}r}}{r}$$

On the other hand $\langle\psi||W||\psi\rangle / |E|^{1/2} = O(1)$ □

Behavior of the ground state near the drip-line





- For the Coulomb tail there is a bound state with E = 0
- Only S-states can spread
- For rigorous results see D. Bolle, F. Gesztesy and W.Schweiger, J. Math. Phys 26, 1661 (1985); M Ho®mann-Ostenhof, T Hoffmann-Ostenhof and B Simon, J. Phys. A 16, 1125 (1983); D. Gridnev and M. Garcia J. Phys. A 40 9003–9016 (2007) .

Connections between bound states at threshold and spreading

The Hamiltonian $H(Z)$ describes the system of N particles

$$H(Z) = H_0 + V(Z, x)$$
$$V(Z, x) = \sum_{1 \le i < j \le N} V_{ij}(Z; x_i - x_j),$$

where Z takes the values from the parameter sequence $Z_k \to Z_{cr}$. One defines the threshold as $E_{thr}(Z) := \inf \sigma_{ess}(H(Z))$.

Hamiltonian must satisfy the requirements

R1 $|V_{ij}(Z; y)| \le F(y)$ for all $Z \in \mathcal{Z}$, where $F(y) \in L^2(\mathbb{R}^3)$.

R2 $\forall f(x) \in C_0^\infty(\mathbb{R}^{3N-3})$: $\lim_{Z_k \to Z_{cr}} \big\| \big[V(Z_k) - V(Z_{cr})\big] f \big\| = 0$.

R3 for all Z_k there are $E(Z_k) \in \mathbb{R}$, $\psi(Z_k) \in D(H_0)$ such that $H(Z_k)\psi(Z_k) = E(Z_k)\psi(Z_k)$, where $\|\psi(Z_k)\| = 1$ and $E(Z_k) < E_{thr}(Z_k)$.

R4 $\lim_{Z_k \to Z_{cr}} E(Z_k) = \lim_{Z_k \to Z_{cr}} E_{thr}(Z_k) = E_{thr}(Z_{cr})$.

Connections between bound states at threshold and spreading

Theorem (essentially Zhislin). *Let $(H(Z), \mathcal{Z})$ be a Hamiltonian satisfying R1-4. If the sequence $\psi(Z_k)$ defined in R3 does not fully spread then $H(Z_{cr})$ has a bound state at the threshold*

$$H(Z_{cr})\psi_0 = E_{thr}(Z_{cr})\psi_0, \quad \textit{where} \quad \psi_0 \in D(H_0) \subset L^2(\mathbb{R}^{3N-3})$$

The following theorems are helpful

Theorem. *Suppose $f_n \in D(H_0)$, $f_n \stackrel{w}{\to} \phi_0$ and $\|H_0 f_n\|$ are uniformly norm-bounded. Then $\|f_n - \phi_0\| \to 0$.*

Theorem. *Let $f_n \in L^2(\mathbb{R}^n)$ be a normalized sequence of functions, with the property that every weakly converging subsequence converges also in norm. Then f_n does not spread.*

Theorem. *Suppose that the sequence of functions $f_n \in L^2(\mathbb{R}^n)$ is uniformly norm-bounded and $|f_n|$ is non-decreasing $|f_n| \leq |f_{n+1}|$. Then f_n does not spread.*

Upper Bounds for the Green's functions (two-body case)

The Schrödinger equation $H_0 + \lambda W \Psi = -k^2 \Psi$ can be rewritten as

$$\Psi = (H_0 + \lambda W_+)^{-1} W_- \Psi, \quad \text{where} \quad W = W_+ - W_-; \quad W_+ = \max(0, W)$$

If $\lambda W_+ \geq \eta$ this gives the upper bound

$$|\Psi| \leq (H_0 + \eta)^{-1} W_- |\Psi|$$

One looks for the upper bound on the integral kernel of $G = (H_0 + \eta)^{-1}$ for some special form of η

$$\eta(A, R_0; x) = \begin{cases} 0 & \text{if } r < R_0 \\ A r^{-2} & \text{if } r \geq R_0, \end{cases}$$

Note that if $G_1 = [H_0 + \eta_1]^{-1}$ and $G_2 = [H_0 + \eta_2]^{-1}$ then $G_1(x, y) \leq G_2(x, y)$ pointwise when $\eta_1 \geq \eta_2$

Upper Bounds for the Green's functions (two-body case)

Use the trick to find $\tilde{A}(s)$ and $\tilde{R}_0(s)$ such that

$$\eta(A, R_0; x) \geq \eta(\tilde{A}(s), \tilde{R}_0(s); x - s)$$

Then

$$G(A, R_0; x, y) \leq G(\tilde{A}(s), \tilde{R}_0(s); x - s, y - s) \quad \text{for all} \quad s$$

Simply setting $s = y$ one gets the upper bound

$$G(A, R_0; x, y) \leq G(\tilde{A}(y), \tilde{R}_0(y); x - y, 0)$$

And $G(A, R_0; x, 0)$ is easy to find because it is spherically symmetric

$$[H_0 + \eta]G(A, R_0; x, 0) = \delta(x)$$

Examples of the Bounds

If G_k is defined as

$$G_k = \left[p^2 + \frac{3+\delta}{4|x|^2}\chi_{\{x|\ |x|\geq n\}} + k^2\right]^{-1},$$

Then one can write the bound

$$G_k(x,y)\chi_{\{y|\ |y|\leq n\}} \leq \frac{\chi_{\{y|\ |y|\leq n\}}}{4\pi|x-y|} \times \begin{cases} 1 & \text{if } |x-y| \leq \tilde{R}_0 \\ C_\delta n^{\tilde{a}}|x-y|^{-\tilde{a}} & \text{if } |x-y| \geq \tilde{R}_0 \end{cases},$$

where $\tilde{a}$ and $\tilde{R}_0$ are defined through

$$\tilde{a} = \frac{1}{2} + \frac{\min(1,\delta)}{20}$$
$$\tilde{R}_0 = \frac{20}{\min(1,\delta)}n$$

Examples of the Bounds

The case of a Coulomb-like potential

$$\tilde{G}_k(a) = \left[-\Delta + \left(\frac{a^2}{4} |x|^{-1} + \frac{a}{4} |x|^{-3/2} \right) \chi_{\{x|\ |x| \geq 1\}} + k^2 \right]^{-1}$$

$$\tilde{G}_k(a;x,y)\chi_{\{|y|\leq n\}} \leq \frac{1}{4\pi|x-y|} \times \begin{cases} 1 & \text{for } |x-y| \leq 2n \\ \exp\left\{ \frac{a}{2}\left(\sqrt{2n} - \sqrt{|x-y|}\right) \right\} & \text{for } |x-y| > 2n, \end{cases}$$

This makes the wave functions fall off as $\exp(-\sqrt{r})$

Absence of spreading for the two-cluster break up.

The Hamiltonian for the case of a two-cluster break up

$$H = H_{thr}(\xi, Z) + \frac{p_r^2}{2\mu} + W(r, \xi, Z)$$

where H_{thr} is the Hamiltonian of internal motion in the clusters $\mathfrak{C}_{1,2}$. One needs additional requirements (H_a denotes various two-cluster partitions)

R5 For all $Z \in \mathcal{Z}$ there exist a normalized bound state $\phi_{thr}(\xi, Z) \in D(H_{thr})$ and a constant $|\Delta\epsilon| > 0$ independent of Z such that $H_{thr}(Z)\phi_{thr}(\xi, Z) = E_{thr}(Z)\phi_{thr}(\xi, Z)$ and

$$\big(1 - P_{thr}(Z)\big)\Big[H_{thr}(Z) - E_{thr}(Z)\Big] \geq |\Delta\epsilon|\big(1 - P_{thr}(Z)\big)$$
$$\Big[H_{a\geq 2}(Z) - E_{thr}(Z)\Big] \geq |\Delta\epsilon|,$$

where $P_{thr}(Z) = 1 \otimes \phi_{thr}(\phi_{thr}, \cdot)$ is a projection operator.

R6 For all $Z \in \mathcal{Z}$ there are $A, q > 0$ independent of Z such that the bound state ϕ_{thr} defined in $R5$ satisfies the following inequality $|\phi_{thr}(\xi, Z)| \leq Ae^{-q|\xi|}$.

Absence of spreading for the two-cluster break up.

Theorem. *Suppose that $(H(Z), \mathcal{Z})$ satisfies R1-6 and for all $Z \in \mathcal{Z}$ the potentials satisfy the following inequality*

$$2\mu W \geq \frac{3+\delta}{4|r|^2} \quad \text{if} \quad |r| \geq C_0 + C_1|\xi|^p$$

where $\delta, C_{0,1}, p$ are fixed positive constants. Then: (a) for $Z_k \to Z_{cr}$ the sequence $\psi(Z_k)$ defined by R3 does not spread. (b) $H(Z_{cr})$ has at least one bound state at the bottom of the continuous spectrum.

Consider the Hamiltonian of an infinitely heavy atomic nucleus charge Z containing N electrons

$$H_N(Z) = H_0 - \sum_{i=1}^{N} \frac{Z}{|x_i|} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \tag{1}$$

The total number of particles is $N+1$ (the electrons are numbered from 1 to N and the nucleus is the particle number $N+1$).

Theorem. *Suppose that $Z_{cr} \in (N-2, N-1)$. Then $H_N(Z_{cr})\mathcal{P}_N$ has a bound state at the bottom of the continuous spectrum.*

New Results and open problems

➢ **Neither halos nor the Efimov effect exist for the number of clusters larger than 4 (the proof to be presented on the next conference).**

Some Open Problems

➢ **Prove rigorously that halos are formed in the ground state of 3 particles.**

➢ **Is a retardation possible in the three cluster break up? In other words, could it be that $\langle W_{12} \rangle / \langle W_{13} \rangle$ goes to zero?**