Eulogy for point interactions
The double well potential
The double point-well potential
The non linear double point-well potential

Nonlinear self-trapping via concentrated nonlinearities

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Geometria è Fisica, a Geometrical Vision
of Physics

Dedicated to Beppe Marmo
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Eulogy for point interactions

Many particle systems

The formal $c \to \infty$ limit of the $: \Phi^4 :$ field theory gives, in each sector with a fixed number of particles, a theory of non relativistic quantum particle interacting via point interactions.

Yet, no (non relativistic) N body, three dimensional point interaction hamiltonian, bounded from below, was ever found for $N > 2$.

The unbounded hamiltonians show low energy eigenvalues, characterized by "trimer" eigenfunctions supported on large spacial regions (Efimov effect) experimentally observed.

The problem to find a three body point interaction bounded from below and showing Efimov effect is still unsolved

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Eulogy for point interactions

Fermions do not interact among them via point interactions, but systems of M fermions interacting via zero range forces with N fermions of different kind present interesting stability issues.

There are maximal values of M and N and of the mass ratios above which the hamiltonians are unbounded from below (something to do with stability of nuclei?)

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## Eulogy for point interactions

One particle systems

The point interaction potentials may be generalized to point scatterers with an internal quantum structure making available models of macroscopic quantum environments.

Any kind of Schrödinger operator can be approximated with point interaction hamiltonians.

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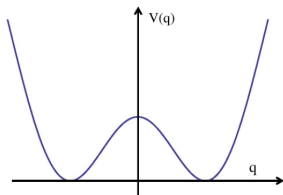
Two close eigenvalues
with corresponding symmetric
and antisymmetric eigenfunctions

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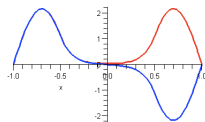
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The most popular case: the ammonia molecule
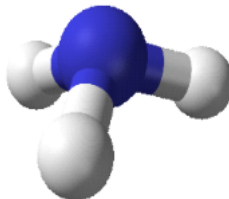
In the case of nitrogen the barrier to inversion is low enough for inversion to occur at an observable rate (and in fact it is observed in liquid ammonia). Nevertheless, the nitrogen inversion is generally absent whenever the molecule is part of a large organic structure.

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Mathematical molecular modeling addressed the interaction with the outside structure as an effective non-linear potential superimposed to the double well potential. It was proved that the non linear interaction destroys the beating effect.

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The self-adjoint operator $H_{\underline{\gamma},Y}$, with $\underline{\gamma} = \{\gamma_1, \gamma_2\}$ $\gamma_i \in \mathbb{R}$, characterized by two point interactions placed symmetrically with respect to the origin in $Y = \{y_1, y_2\}$, $|y_i| = a$ and $d = 2a$, with strength respectively γ_1 and γ_2, is defined as follow:

$$D(H_{\underline{\gamma},Y}) = \left\{\psi \in L^2(\mathbf{R}) \mid \psi = \phi^\lambda + \sum_{i,j=1}^{2} \left(\Gamma_{\underline{\gamma}}^\lambda\right)_{ij}^{-1} \phi^\lambda(y_i) G^\lambda(\cdot - y_i)\right\},$$

with $\phi^\lambda \in H^2(\mathbf{R}^3)$

$$(H_{\underline{\gamma},Y} + \lambda)\psi = (-\Delta + \lambda)\phi^\lambda$$

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where

$$G_\lambda(x) = \frac{e^{-\sqrt{\lambda}|x|}}{2\sqrt{\lambda}}$$

$$\left(\Gamma_{\underline{\gamma}}^\lambda\right)_{ij} = -\frac{1}{\gamma_i}\,\delta_{ij} - G^\lambda(y_i - y_j)$$

and the positive real λ is chosen large enough to make the matrix Γ_{ij}^λ invertible.

The parameter $\gamma_i \in \mathbb{R}$ is the inverse of the scattering length and it is related to the strength of the interaction at the point y_i.

The integral kernel of the resolvent $(H + \lambda)^{-1}$ reads

$$(H_{\underline{\gamma},Y}+\lambda)^{-1}(\underline{x},\underline{x}') = G^\lambda(\underline{x}-\underline{x}')+\sum_{i,j=1}^2 \left(\Gamma_{\underline{\gamma}}^\lambda\right)_{ij}^{-1} G^\lambda(\underline{x}-\underline{y}_i)G^\lambda(\underline{x}'-\underline{y}_j)$$

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The resolvent of $H_{\underline{\gamma}, Y}$ is a finite rank perturbation of the free laplacian resolvent operator. From the kernel representation of the resolvent spectral and scattering properties of the operator $H_{\underline{\gamma}, Y}$ are easily obtained in the case of interactions of the same strength ($\gamma_i = \gamma$).

The eigenvalues are associated to polar singularities of the resolvent. Specifically, the energy $-\lambda$ will be a negative eigenvalue of $H_{\underline{\gamma}, Y}$ if

$$\det \left(\Gamma^\lambda_{\underline{\gamma}} \right) = 0$$

In the case of two point interactions of the same strength the condition reads

$$\det \left[\begin{pmatrix} \frac{1}{\gamma} + \frac{1}{2\sqrt{\lambda}} & G^\lambda(d) \\ G^\lambda(d) & \frac{1}{\gamma} + \frac{1}{2\sqrt{\lambda}} \end{pmatrix} \right] = 0$$

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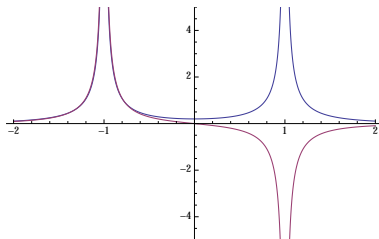The non linear double point-well potential

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For $\gamma < -\frac{1}{2d}$ there are two solutions $\lambda_{0,1}$ to the previous equation. The corresponding eigenfunctions are

$$\psi_0(x) = N_0 \left(G_{\lambda_0}(x - y) + G_{\lambda_0}(x + y) \right)$$

$$\psi_1(x) = N_1 \left(-G_{\lambda_1}(x - y) + G_{\lambda_1}(x + y) \right)$$

where N_0 and N_1 are explicitly computable normalization factors.

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It is possible to construct a state strongly localized on the left well by the following superposition of the previous states

$$\psi^L = \frac{1}{\sqrt{2}} \left(\psi_0 + \psi_1 \right)$$

This state will evolve in time as follows:

$$\psi_{beat}^L(x, t) = \frac{1}{\sqrt{2}} \left(e^{-\imath \lambda_0 t} \psi_0(x) + e^{-\imath \lambda_1 t} \psi_1(x) \right)$$

with a probability density given by

$$\mathcal{P}(x, t) = \frac{1}{2} \left(|\psi_0(x)|^2 + |\psi_1(x)|^2 + \psi_0(x)\psi_1(x) \cos\left((\lambda_1 - \lambda_0) \, t \right) \right)$$

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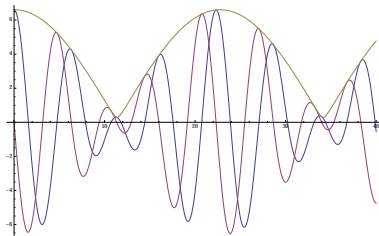The non linear double point-well potential
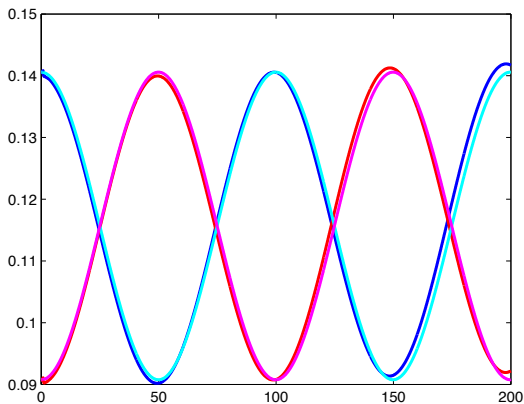
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ψ_{beat}^L is an oscillating function with period $T = \dfrac{2\pi}{\lambda_1 - \lambda_0}$ In particular the values assumed by the function $\psi_{beat}^L(x, t)$ in the centers of the two wells evolve in the following way

$$q_1^L(t) \equiv \psi(t, -a) = N_0 e^{-\imath\lambda_0 t} + N_1 e^{-\imath\lambda_1 t}$$
$$q_2^L(t) \equiv \psi(t, +a) = N_0 e^{-\imath\lambda_0 t} - N_1 e^{-\imath\lambda_1 t}$$

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For any initial condition $(\psi_0)(x)$ the evolution problem can be analyzed in an alternative way. Making the ansatz

$$\psi(t,x) = (\mathcal{U}(t)\psi_0)(x) - \imath\,\gamma \sum_{i=1}^{2} \int_0^t ds\, U(t-s : x - y_j)\psi(s,y_j)$$

one sees that it satisfies the Schrödinger equation for the two point-well hamiltonian if and only if the two charges satisfy the system of Volterra integral equations

$$
\begin{cases}
q_+(t) + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_+(s)}{\sqrt{t-s}}\,ds + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_-(s)}{\sqrt{t-s}}\, e^{\imath\frac{a^2}{t-s}}\,ds \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad = (\mathcal{U}(t)\,\psi_0)(a) \\[2ex]
q_-(t) + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_-(s)}{\sqrt{t-s}}\,ds + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_+(s)}{\sqrt{t-s}}\, e^{\imath\frac{a^2}{t-s}}\,ds \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad = (\mathcal{U}(t)\,\psi_0)(-a)
\end{cases}
$$

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Asymmetric double well
The two point interactions are again placed symmetrically in
$Y = \{y_1, y_2\}$ with $|y_i| = a$, but $\gamma_1 < \gamma_2$. and $|y_1 - y_2| = 2a \equiv d$.
The equation for the eigenvalues $-\lambda < 0$ reeds in this case

$$\det \Gamma_{(\gamma_1, \gamma_2)}(\lambda) = \det \left[\begin{pmatrix} \frac{1}{\gamma_1} + \frac{1}{2\sqrt{\lambda}} & -\frac{1}{2\sqrt{\lambda}} e^{\sqrt{\lambda}|y_2-y_1|} \\ -\frac{1}{2\sqrt{\lambda}} e^{\sqrt{\lambda}|y_2-y_1|} & \frac{1}{\gamma_2} + \frac{1}{2\sqrt{\lambda}} \end{pmatrix} \right] = 0.$$

Explicitly

$$\left(\frac{1}{\gamma_1} + \frac{1}{2\sqrt{\lambda}} \right) \left(\frac{1}{\gamma_2} + \frac{1}{2\sqrt{\lambda}} \right) - \left(\frac{1}{2\sqrt{\lambda}} \right)^2 e^{-2\sqrt{\lambda}d} = 0$$

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The number of positive solutions depends on the values of γ_i and $2a = |y_2 - y_1|$. With $\gamma_1 < \gamma_2 < 0$ there are two solutions if
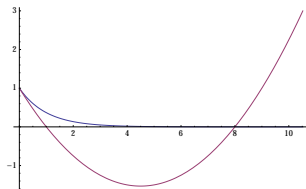
$$\frac{1}{|\gamma_1|} + \frac{1}{|\gamma_2|} < d$$

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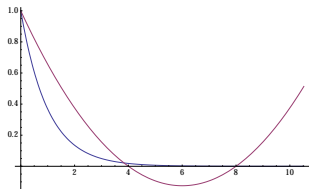
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or one solution if

$$\frac{1}{|\gamma_1|} + \frac{1}{|\gamma_2|} > d$$

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Assume that both $\gamma's$ are negative, $1/|\gamma_2| < d$ and that $|\gamma_1| \gg |\gamma_2|$ in such a way that two eigenvalues are present: The eigenfunction relative to the lowest eigenvalue $E = -\lambda_0 < 0$ has always the form

$$\psi_0(x) = c_1 G^{\lambda_0}(x - y_1) + c_2 G^{\lambda_0}(x - y_2)$$

where the coefficients (c_1, c_2) are the components of the of the matrix $\Gamma_{\underline{\gamma}}^{\lambda_0}$ eigenvector relative to the eigenvalue zero and can be chosen to be strictly positive. Explicitly

$$\left(\frac{c_1}{c_2}\right)^2 = \frac{\gamma_1}{\gamma_2} \frac{1 + \frac{\gamma_2}{2\sqrt{\lambda_0}}}{1 + \frac{\gamma_1}{2\sqrt{\lambda_0}}}$$

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Under the assumptions we made on γ there will be a second eigenvalue $E_1 > E_0$ with a corresponding eigenfunction:

$$\psi_1(x) = c_3 \, G^{\lambda_1}(x - y_1) + c_4 \, G^{\lambda_1}(x - y_2)$$

An explicit computation of the coefficient c_3 and c_4 and of the solution of the evolution equation shows that, as expected, there are no beating states in this case

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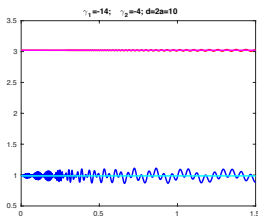
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Concentrated nonlinearities

The extension to the case of concentrated nonlinear interactions was developed in the last decade. It was used in modeling several quantum systems like Josephson junctions and rotating Bose condensates.

Formally a concentrated nonlinearity can be obtained taking time dependent strengths of point interactions proportional to the local modulus of the wave function

$$\gamma_j(t) = \gamma z^\sigma, \qquad z = |\psi(t, y_j)|$$

and considering the non autonomous problem

$$\imath \frac{\partial}{\partial t} \psi(t, x) = H_{\underline{\gamma}(t), Y} \psi(t, x)$$

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From general theory we know that if we choose an initial data $\psi_0(x) \in H^1(\mathbb{R})$, then the corresponding Cauchy problem have a unique solution which is global in time if $\gamma < 0$ and $\sigma < 1$.

Moreover it is proved that there are initial data $\psi_0^B(x)$ such that the solution of the Cauchy problem is blowing up in finite time if $\gamma < 0$ and $\sigma \geq 1$.

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The nonlinear evolution problem can be analyzed in its integral form

$$\psi(t,x) = (\mathcal{U}(t)\psi_0)(x) - \imath\,\gamma \sum_{j=1}^{2} \int_0^t ds\, U(t-s: x-y_j)|\psi(s,y_j)|^{2\sigma_j}\psi(s,y_j)$$

where $\mathcal{U}(t)$ is the one dimensional free unitary group

$$(\mathcal{U}(t)\phi)(x) = \int_{\mathbb{R}} dy\, \mathcal{U}(t; x-y)\phi(y) = \frac{1}{\sqrt{4\pi\imath t}} \int_{\mathbb{R}} dy e^{\imath|x-y|^2/4t}\phi(y).$$

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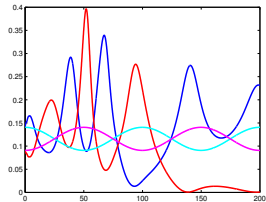
The coupled equations for the charges read as

$$
\begin{cases}
q_+(t) + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_+(s)\,|q_+(s)|^{2\sigma}}{\sqrt{t-s}}\,ds + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_-(s)\,|q_-(s)|^{2\sigma}}{\sqrt{t-s}}\,e^{\imath\frac{a^2}{t-s}}ds \\
\hspace{7cm} = (\mathcal{U}(t)\,\psi_0)(a) \\[2mm]
q_-(t) + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_-(s)\,|q_-(s)|^{2\sigma}}{\sqrt{t-s}}\,ds + \frac{\gamma}{2}\sqrt{\frac{\imath}{\pi}} \int_0^t \frac{q_+(s)\,|q_+(s)|^{2\sigma}}{\sqrt{t-s}}\,e^{\imath\frac{a^2}{t-s}}\,ds \\
\hspace{7cm} = (\mathcal{U}(t)\,\psi_0)(-a)
\end{cases}
$$

where $(\mathcal{U}(t)\,\psi_0)(x)$ denotes the free evolution of the initial condition.

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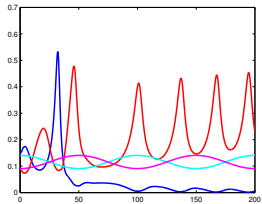The double point-well potential
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We are interested in the solution of this system when $\psi_0 = \psi_{beat}^L(t)$.

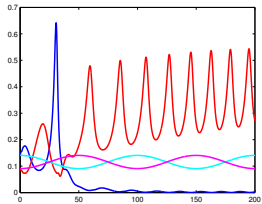Eulogy for point interactions
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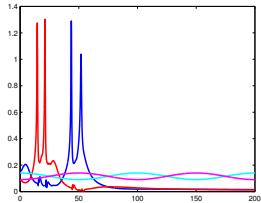# The double point-well potential

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Notice that superimposing a non linear asymmetric potential to the double well potential one forces the symmetry breaking from the outside.

I presented a case of a symmetric non linear double well potential and showed that the symmetric non linearity is responsible of the symmetry breaking.

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You did not change much in these last 46 years

Please go on in this way