MULTICHANNEL CONTACT INTERACTIONS

Generalizing contact interactions for a multichannel case is relatively straightforward. We now define (for s-wave interactions):

$$\boxed{\hat{V}_s(r) = \frac{4\pi\hbar^2}{2\mu}\,\underline{A}\,\delta(\vec{r})\,\frac{d}{dr}(r)}$$

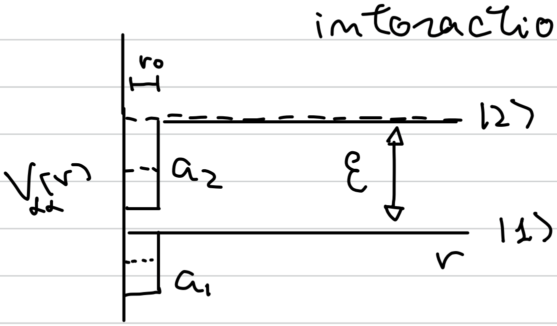
where $(A)_{\alpha\nu} = a_{\alpha\nu}$ is the scattering length matrix.
For this interaction, the Bethe-Peierls boundary condition is

$$\boxed{\left.\frac{d}{dr}u_{\alpha\nu}\right|_{r=0} = -\sum_{\alpha'}\frac{1}{a_{\nu\alpha'}}\,u_{\alpha'\nu} = -\sum_{\alpha'} M_{\nu\alpha'}\,u_{\alpha'\nu}}$$

A detailed analysis can be found in Ross & Shaw Ann. Phys. 13, 147 (1961). Here, we will simply use these results to illustrate some of the characteristics of multichannel scattering.

EXAMPLE:

Two channel problem with contact interactions:



($r_0 \to 0$) Contact interaction:

$$\hat{V}(r) = \frac{4\pi\hbar^2}{2\mu}\begin{pmatrix} a_1 & 1/\beta \\ 1/\beta & a_2 \end{pmatrix}\delta(\vec{r})\,\frac{d}{dr}\,r$$

There are 3 physically distinct regimes one can explore in this problem:

↳ (continue) →

(1) $E<0$: In this case all channels are closed and we want to analyse the molecular spectrum of the system.

what do we expect?

- $(a_1<0,\ a_2<0)$: no bound states
- $(a_1>0,\ a_2<0)$: one bound state

not very interesting

- $(a_1>0,\ a_2>0)$: one or two bound states if $\mathcal{E} < \hbar^2/2\mu a_2^2$

(2) $0\leq E<\mathcal{E}$: In this case, channel $|1\rangle$ is open while channel $|2\rangle$ is closed. We want analyse the resonant and scattering properties of the system. Note that since there is no open (exit) channels other than the incoming channel, scattering will occur in the absence of inelastic transitions.

what do we expect? (irrespective to a_1)

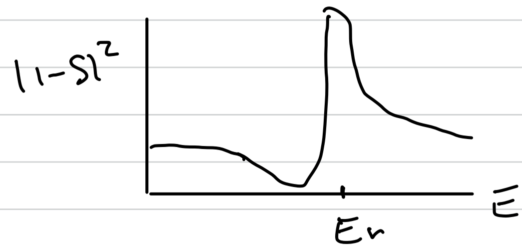
- $a_2<0$: no molecular state in channel (not much to see)
- $a_2>0$: there is a molecular state in channel 2 with energy, if there is no couplings,

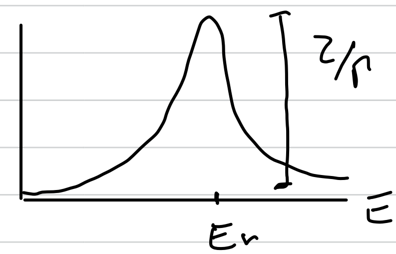
$$E_{bare} = \mathcal{E} - \frac{\hbar^2}{2\mu a_2^2} \qquad \text{(bare state energy)}$$

this molecular state will manifest in scattering if we vary E or $\mathcal{E}$. If we vary E, while $\mathcal{E}$ is fixed, and $\mathcal{E} > \hbar^2/2\mu a^2$, we should expect that for values of $E \approx E_{bare}$ scattering observables should display resonant effect. In that case we can analyse the corresponding Fano lineshapes, as well as, the time delay to obtain important properties of the resonant state

(Varying E)

Fano Lineshape Time delay

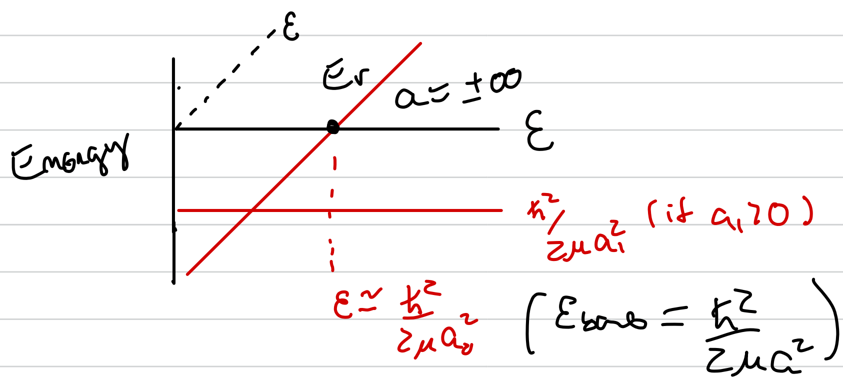




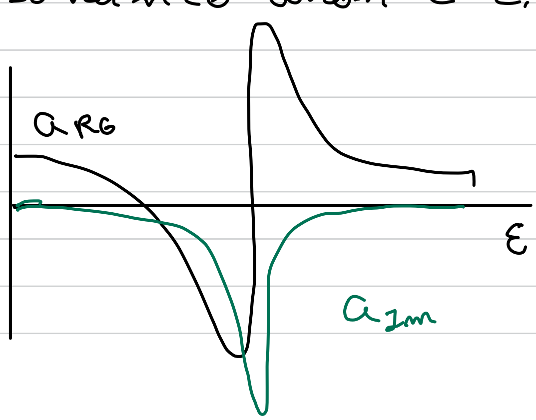
By varying $\mathcal{E}$, and keeping $E=0$, we can "move" the resonant state and change the scattering properties of the system. In fact, if the energy of the resonant state is brought near $E=0$, the s-wave scattering length will go through a pole (Feshbach resonance).

(Varying $\mathcal{E}$ ($E=0$))

Fano-Feshbach resonance



(3) $E > \mathcal{E}$: For this case both channels $|1\rangle$ and $|2\rangle$ are open. As a result, both elastic and inelastic process can happen. In that case the scattering length will be complex and it won't diverge near a resonance when $E=\mathcal{E}$;



Let's then get some calculations to explore these scenarios more carefully.

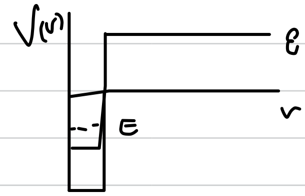
CASE (1) $E<0$: For this case, since both channels are closed, the general solution can be written as

$$u_{E0}(r) = u_{E0}^{(1)}(r)\,|1\rangle + u_{E0}^{(2)}(r)\,|2\rangle$$

with components given by

$$u_{E0}^{(1)}(r) = A\, e^{-\kappa r}$$

$$u_{E0}^{(2)}(r) = B\, e^{-\tilde{\kappa} r}$$



where $\kappa^2 = 2\mu|E|/\hbar^2$ and $\tilde{\kappa}^2 = 2\mu(\varepsilon+|E|)/\hbar^2 = k_\varepsilon^2 + \kappa^2$. We want to use the Bethe-Peierls boundary conditions in order to determine the of κ:

$$\frac{d}{dr}\begin{pmatrix} u_{E0}^{(1)} \\ u_{E0}^{(2)} \end{pmatrix}\Bigg|_{r=0} = -\begin{pmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{pmatrix}\begin{pmatrix} u_{E0}^{(1)} \\ u_{E0}^{(2)} \end{pmatrix}\Bigg|_{r=0}$$

$$\begin{pmatrix} -\kappa A \\ -\tilde{\kappa} B \end{pmatrix} = -\begin{pmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \qquad \begin{pmatrix} 1/a_1 - \kappa & \beta \\ \beta & 1/a_2 - \tilde{\kappa} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = 0$$

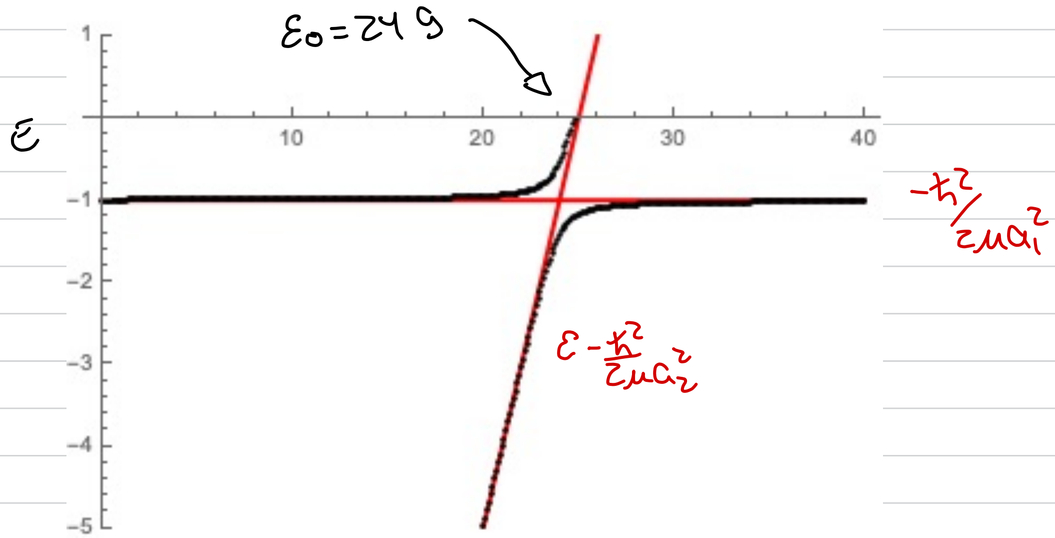
Quantization Condiction: ($\det = 0$)

$$\boxed{\left(\frac{1}{a_1} - \kappa\right)\left(\frac{1}{a_2} - \sqrt{\kappa^2 + k_\varepsilon^2}\right) - \beta^2 = 0}$$

SIDE NOTE: Does it make sense? setting $\beta=0$, there are two solutions (if $a_1>0$ and $a_2>0$)

$$\kappa = 1/a_1 \rightsquigarrow \boxed{E = -\frac{\hbar^2}{2\mu a_1^2}} \qquad \sqrt{\kappa^2 + k_\varepsilon^2} = 1/a_2 \Rightarrow \boxed{E = \varepsilon - \frac{\hbar^2}{2\mu a_2^2}}$$

In order to find the solutions of the quantization condition one needs to solve it numerically.
For $a_1 = 1$, $a_2 = 0.2$, $\beta = 0.1$ (assuming $\mu = \frac{m}{2} = 1/2$), one obtain:



⊛ CASE (2) $0 < E < \mathcal{E}$ note that there is only one open channel, whose solution can be expressed as

$$u_{E0}(r) = u_{E0}^{(1)}(r)\,|1\rangle + u_{E0}^{(2)}(r)\,|2\rangle$$

with components given by

$$u_{E0}^{(1)}(r) = A \sin(kr + \delta) \qquad \text{(open channel)}$$

$$u_{E0}^{(2)}(r) = B\, e^{-\kappa r} \qquad \text{(closed channel)}$$

where $\kappa^2 = 2\mu(\mathcal{E} - E)/\hbar^2 = k_{\mathcal{E}}^2 - k^2$. We now want to use the Bethe-Peierls boundary conditions in order to determine the phase-shift δ:

$$\frac{d}{dr}\begin{pmatrix} u_{E0}^{(1)} \\ u_{E0}^{(2)} \end{pmatrix}\Bigg|_{r=0} = -\begin{pmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{pmatrix}\begin{pmatrix} u_{E0}^{(1)} \\ u_{E0}^{(2)} \end{pmatrix}\Bigg|_{r=0}$$

$$\begin{pmatrix} k\cos\delta \\ -\kappa D \end{pmatrix} = -\begin{pmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{pmatrix}\begin{pmatrix} \sin\delta \\ D \end{pmatrix}$$

where $D = B/A$. We can solve the above equation for $\tan\delta$, and find:

$$\boxed{\tan\delta(E) = -k\left(\frac{1}{a_1} - \frac{a_2\beta^2}{1-a_2K}\right)^{-1}} \qquad [K^2 = k_\mathcal{E}^2 - k^2]$$

SCATTERING LENGTH (vary $\mathcal{E}$ and fix $E=0$)

In order to determine the scattering length we now just need to calculate $a = -\lim_{k\to 0}\tan\delta/k$, which leads to

$$\boxed{a = \left(\frac{1}{a_1} - \frac{a_2\beta^2}{1-a_2k_\mathcal{E}}\right)^{-1}}$$

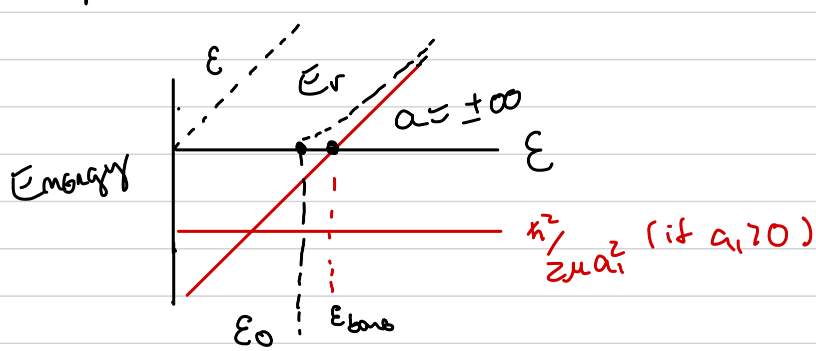
which diverges whenever $a_2 > 0$ and $a_1a_2\beta^2 < 1$ (important) at $\mathcal{E} = \mathcal{E}_0$, where

$$\boxed{\mathcal{E}_0 = (1-a_1a_2\beta^2)^2\frac{\hbar^2}{2\mu a_2^2}}$$

Note that the resonance occurs for a value of $\mathcal{E}$ which is shifted from the bare state crossing ($\mathcal{E}_{bare} = \hbar^2/2\mu a_2^2$) such that

$$\mathcal{E}_0 - \mathcal{E}_{bare} = -\left[a_1a_2\beta^2(2-a_1a_2\beta^2)\right]\frac{\hbar^2}{2\mu a_2^2} < 0$$

reflecting the interchannel interaction, controled by the β parameter.



We can fit the values of $a(\mathcal{E})$ accordingly to the Wigner-Breit formula

$$a(\mathcal{E}) \simeq \left(1 + \frac{\Delta\mathcal{E}}{\mathcal{E}-\mathcal{E}_0}\right) a_{bg}$$

where the resonance width $\Delta\mathcal{E}$ is defined as the difference between the values of $\mathcal{E}$ in which $a=\infty$ $(\mathcal{E}=\mathcal{E}_0)$ and $a=0$ $(\mathcal{E}=\hbar^2/2\mu c^2)$ leading to

$$\boxed{\Delta\mathcal{E} = -a_1 a_2 \beta^2 \left(2 - a_1 a_2 \beta^2\right) \frac{\hbar^2}{2\mu a_2^2}}$$

and background scattering length, a_{bg}, by the value of $a(\mathcal{E}\to\infty)$, leading to

$$\boxed{a_{bg} = a_1}$$

RESONANT STRUCTURE (fix $\mathcal{E}$ and vary E)

In order to analyse the resonant structure of the system we can look for the Fano lineshapes

$$F(k) = |1-S|^2/4 = |1-e^{2i\delta}|^2/4 = \sin^2\delta$$

$$\boxed{F(k) = \frac{k^2}{\left(\frac{1}{a_1} - \frac{a_2\beta^2}{1-a_2\kappa}\right)^2 + k^2}}$$

$[\kappa^2 = k_{\mathcal{E}}^2 - k^2]$

In order to obtain some of the resonance properties we now compare the above expression to the standard Fano lineshape, i.e.,

$$F(q,\tilde{\varepsilon}) = \frac{1}{(1+q^2)} \frac{(q+\tilde{\varepsilon})^2}{1+\tilde{\varepsilon}^2} \qquad \text{where } \tilde{\varepsilon} = \frac{E-E_{res}}{\Gamma_{res}/2}$$

Recall that this expression is valid for isolated resonances.
Recall also the following properties:

Minimum: $F(q,\mathcal{E})=0$: $E = E_{res} - q\,\Gamma_{res}/2 = E_{min}$

Maximum: $F(q,\mathcal{E}) = 1$: $E = E_{res} + \frac{\Gamma_{res}}{2q} = E_{max}$

Off-Res: $\mathcal{E}\to\infty$: $F(q,\mathcal{E}) = \frac{1}{1+q^2}$

$E_{max} - E_{min} = \frac{\Gamma}{2}\left(q+\frac{1}{q}\right)$

For our case, we obtain

Minimum: $F(k)=0$: $1 - a_2 K = 0$

$$1 - a_2\left(k_{\mathcal{E}}^2 - k^2\right)^{1/2} = 0$$

$$\boxed{E_{min} = \mathcal{E} - \frac{\hbar^2}{2\mu a_2^2}}$$

Maximum: $F(k) = 1$: $\left(\frac{1}{a_1} - \frac{a_2\beta^2}{1-a_2K}\right) = 0$

$$\boxed{E_{max} = \mathcal{E} - \frac{\hbar^2}{2\mu a_2^2} + \frac{\hbar^2}{\mu}\left(\frac{a_1}{a_2}\beta^2\right)\left(1 - a_1a_2\beta^2\right)}$$

Off-Res: If $|\mathcal{E} - E_{res}/\Gamma/2| \gg 1$, we can assume that at $E=\mathcal{E}$ $F(k)$ to be off-resonance. In that case

$$\frac{k_{\mathcal{E}}^2}{\left(\frac{1}{a_1} - a_2\beta^2\right)^2 + k_{\mathcal{E}}^2} = \frac{1}{1+q^2} \;\Rightarrow\; \boxed{q = \frac{\left(1 - a_1a_2\beta^2\right)}{a_1 k_{\mathcal{E}}}}$$

Using the equations above we can find E_{res} and Γ_{res}

$$E_{res} = \mathcal{E} - \frac{\hbar^2}{2\mu a_2^2} + \frac{\hbar^2}{2\mu a_2}\,\frac{a_1\beta^2\left(2 - a_1a_2\beta^2\right)\left(1 - a_1a_2\beta^2\right)^2}{\left[1 - 2a_1a_2\beta^2 + a_1^2\left(k_{\mathcal{E}}^2 + a_2^2\beta^4\right)\right]}$$

$$\simeq \mathcal{E} - \frac{\hbar^2}{2\mu a^2} + \frac{\hbar^2}{2\mu a_2^2}\left(\frac{2a_1a_2\beta^2}{1 + a_1^2k_{\mathcal{E}}^2}\right) \approx E_{bare} \qquad (a_1a_2\beta \ll 1)$$

$$\Gamma_{res} = + \frac{a_1^2 k_\varepsilon \beta^2 (2 - a_1 a_2 \beta^2)(1 - a_1 a_2 \beta^2)}{a_2 (1 - 2 a_1 a_2 \beta^2 + a_1^2 (k_\varepsilon^2 + a_2^2 \beta^4))} \frac{\hbar}{\mu}$$

$$\simeq + \left[\frac{4 a_1 k_\varepsilon (a_1 a_2 \beta^2)}{1 + a_1^2 k_\varepsilon^2} \right] \frac{\hbar^2}{2 \mu a_2^2} \approx 0 \quad (a_1 a_2 \beta \ll 1)$$

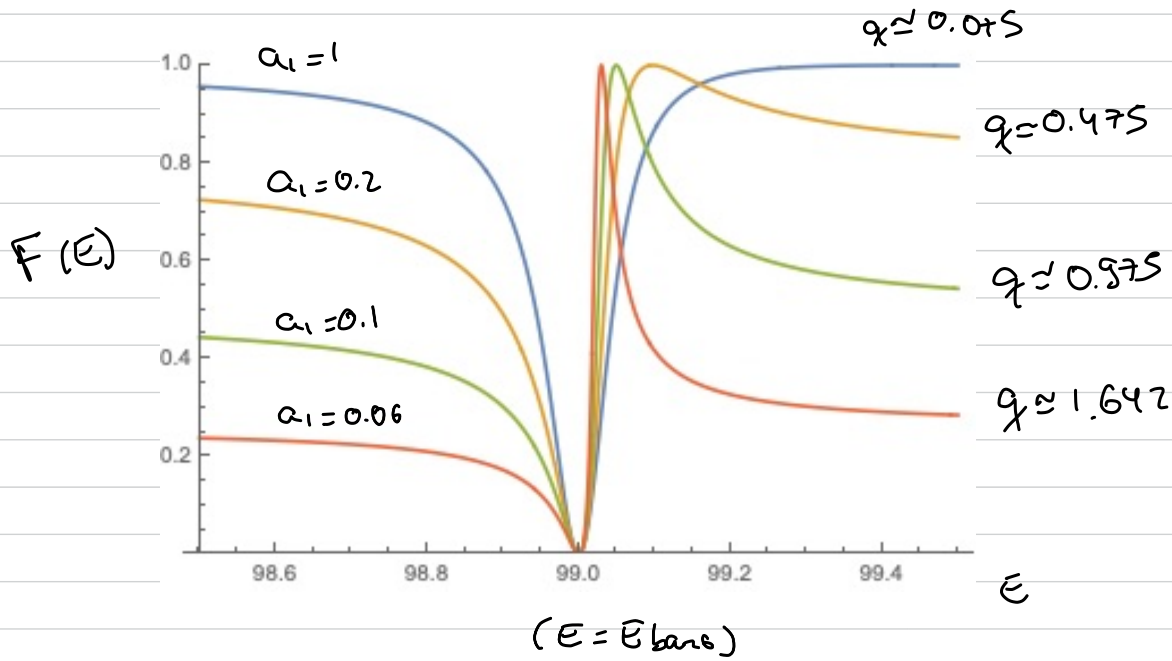
Recall that these expressions are only valid if $|\varepsilon - E_{res} / \Gamma/2| \gg 1$, $E_{res}/\Gamma_{res} \gg 1$ and $a_1 a_2 \beta^2 < 1$

SIDE NOTE: It is pretty straight forward to calculate the time delay once we know $\tan\delta(E)$:

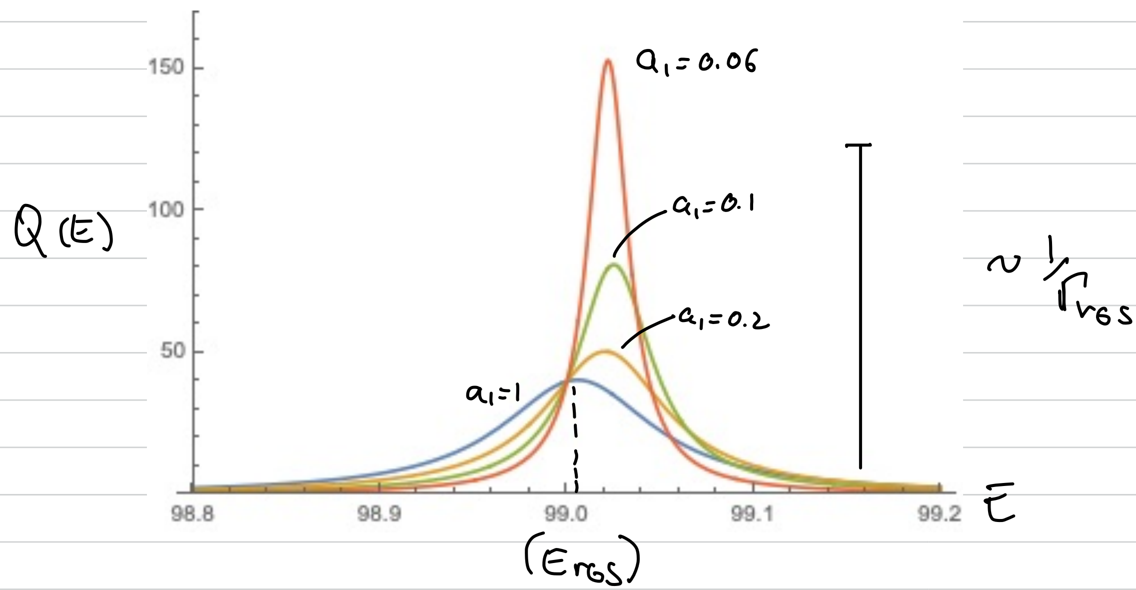
$$Q(E) = -2\hbar \frac{d}{dE} \delta(E) \simeq \frac{\hbar \Gamma_{res}}{(E - E_{res})^2 + (\Gamma_{res}/2)^2}$$

EX: vary E, for different values of a_1, and $a_2 = 1$, $\beta = 0.5$ and $\varepsilon = 100$ (off-resonance regime)

(Fano lineshapes)

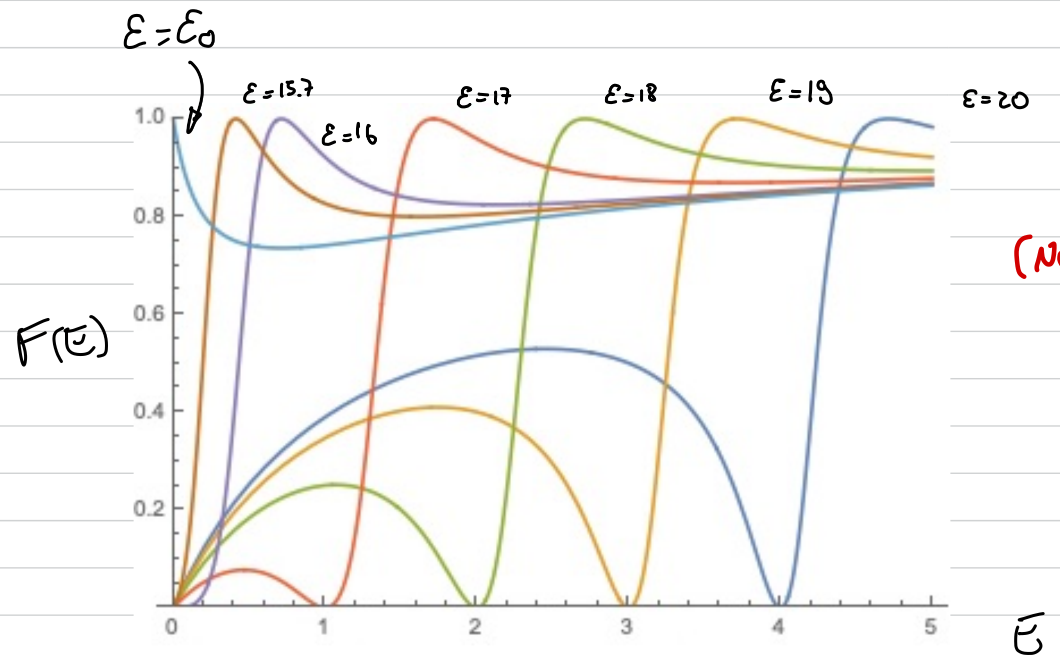


(time delay)



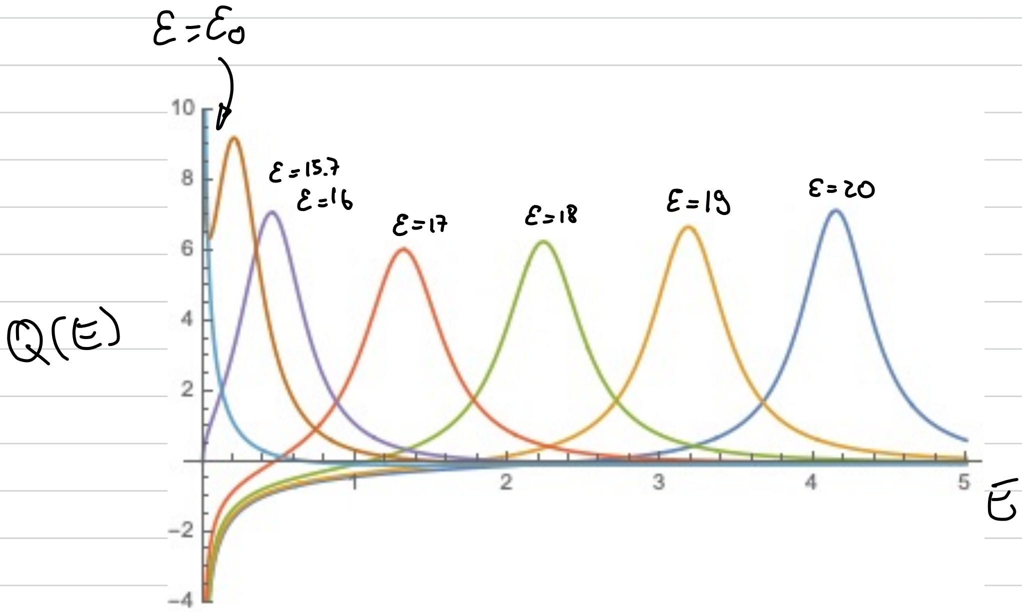
Ex: vary E, for different values of $\varepsilon \approx \varepsilon_0$ ($= 15.2881$) (near-resonance regime), and $a_1 = 1$, $a_2 = 0.25$, $\beta = 0.3$

(Fano lineshapes)



(NOT A FANO LINESHAPE)

(time delay)



(NOT A LORENTZIAN)

Note that when approaching $\mathcal{E}=\mathcal{E}_0$, Γ_{res} first increases but at some point $\Gamma_{res} \to 0$ as $\mathcal{E} \to \mathcal{E}_0$.

⊛ CASE (3): $E \geq \mathcal{E}$. In this case, our problem will have two open channels. This will allows for both elastic and inelastic processes.

The $r \neq 0$ radial solution is now written as

$$\underline{u}(r) = \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} - \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \begin{pmatrix} g_1 & 0 \\ 0 & g_2 \end{pmatrix}$$

where K_{ij}, is the K-matrix elements and

$$f_1 \sim \sin(k_1 r) \qquad g_1 \sim -\cos(k_1 r)$$
$$f_2 \sim \sin(k_2 r) \qquad g_2 \sim -\cos(k_2 r)$$

with

$$k_1^2 = 2\mu(\mathcal{E}+E)/\hbar^2$$
$$k_2^2 = 2\mu E/\hbar^2 = k^2$$

The idea here, is the same than before. We want to apply the Bethe-Peierl's boundary condition, and solve for K_{ij}:

$$\frac{d}{dr}\begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} = -\begin{pmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{pmatrix}\begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}\Big|_{r=0}$$

Once that is done we can use the following relations to find the scattering length

$$S = \frac{1+iK}{1-iK} \rightarrow S_{\alpha\alpha} = e^{2i\delta_\alpha}$$

$$\delta_\alpha = \frac{\ln(S_{\alpha\alpha})}{2i}$$

Knowing the phase-shift we get $\underline{a}$ by:

$$a = -\lim_{k\to 0}\frac{\tan\delta_\alpha}{k} \qquad (k_1 = k_\varepsilon \text{ as } E\to 0)$$

$$= \frac{a_2(1+ia_1k_\varepsilon)}{1+ia_1k_\varepsilon - a_1a_2\beta^2}$$

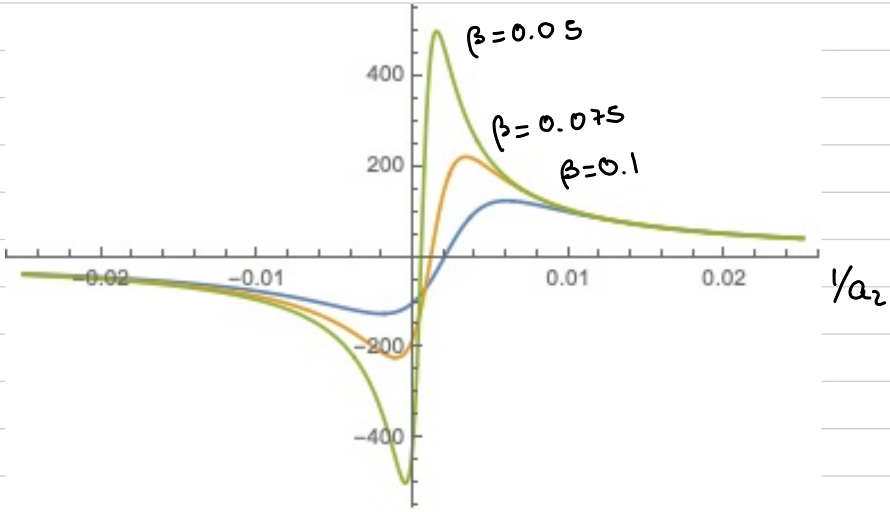
$$\boxed{Re[a] = \frac{a_2[(1-a_1a_2\beta^2)+a_1^2k_\varepsilon^2]}{(1-a_1a_2\beta^2)^2+a_1^2k_\varepsilon^2}}$$

$$\boxed{Im[a] = -\frac{a_1^2a_2^2\beta^2k_\varepsilon}{(1-a_1a_2\beta^2)+a_1^2k_\varepsilon^2}} < 0$$

Reality check:

$$\left.\begin{matrix} \beta = 0; \\ k_\varepsilon = \infty \end{matrix}\right\} \rightarrow Re[a] = a_2 \quad Im[a] = 0$$

EXAMPLE: $Re[a]$ $(a_1 = 1, k_\varepsilon = 2)$



$Im[a]$