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PERTURBATION OF EMBEDDED EIGENVALUE BY A NEAR-LYING RESONANCE

The case of quantum-mechanical system (including electronic molecules) is considered where Hamiltonian allows a separation, in particular by the Faddeev method, of a weakly coupled channel. Width (i. e. the imaginary part) of the resonance generated by a discrete spectrum eigenvalue of the separated channel is studied in the case where main part of the Hamiltonian gives itself another resonance. It is shown that if real parts of these resonances coincide and, at the same time, a coupling between the separated and main channels is sufficiently small then the width of the resonance generated by the separated (molecular) channel is inversely proportional to the width of the main (nuclear) channel resonance. This phenomenon being a kind of universal law, may play an important role increasing the "cold fusion" probability in electronic molecules whose nuclear constituents have narrow pre-threshold resonances.

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I. INTRODUCTION

It is usually accepted that properties of electronic molecules are determined exclusively by Coulombic forces acting between nuclei and electrons and the strong interaction between nuclear constituents plays a negligible role. Surely, with respect to the nuclear channels, electronic molecule is indeed observed as a very stable object but it is evident nevertheless that any molecular level (corresponding to the Coulomb interactions only) looks in fact as an eigenvalue embedded into continuous spectrum of a sub-Hamiltonian of the molecule describing its nuclear constituents. If there are no special reasons, this means that a coupling between the molecular and nuclear channels turn the molecular levels into resonances* (see, e. g., Refs. [**?**] – [**?**] and references cited therein). Of course, the coupling is extremely small due to a wide Coulombic repulsive barrier between nuclei and short-range character of nuclear interaction. Therefore, widths of such resonances giving a probability of a fusion of the nuclear constituents of the molecule, are extremely small, too. However, we will show the situation turns out to be rather different in the case where nuclear subsystem of a molecule has a sufficiently narrow near-threshold (more precisely, pre-threshold) resonance. A number of concrete examples concerning the nuclear systems forming near-threshold resonance states may be extracted e. g., from the data presented in Ref. [**?**]. Among them are even such intrigue systems as $p\,p\,^{16}\mathrm{O}$ and $p\,^{17}\mathrm{O}$ [**?**], [**?**] i. e. the nuclear constituents of the usual water molecule H_2O or hydroxyl ions OH^- based on the more rare isotope $^{17}\mathrm{O}$. Possibility of influence of near-threshold nuclear resonances on the molecular properties was recently indicated in Ref. [**?**] where an estimation of overlap integrals between ansatz molecular and resonance nuclear wave functions was made for the molecules LiD and H_2O. There exists also a well-known example [**?**] of muon catalyzed fusion of deuteron and triton in the $dt\mu$ molecule where a near-threshold nuclear resonance plays a decisive role.

Although we have in mind, first of all, the molecular systems (which can include instead of electrons another light negative-charged particles like muons) we deal in the paper with more general Hamiltonians. The only thing we use is a possibility of a separation in them of weakly coupled ("molecular") channels giving initial eigenvalues ("molecular"energies) embedded into continuous spectrum of respective rest ("nuclear") Hamiltonians. So that these eigenvalues turn automatically into "molecular" resonances when a coupling between the separated "molecular" and rest "nuclear" channels is switched on.

For all the models concerned we prove the following statement.

If the "nuclear" channel itself has a narrow resonance with a real part

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*By resonance we understand a complex value of energy (in an unphysical sheet) where analytic continuation of the resolvent kernel (or its matrix element between suitable states [**?**]) has a pole. Such poles turn out usually to be poles of the scattering matrix continued, too.

being nearly the same as the initial "molecular" energy then *the width* (i. e. the imaginary part) *of the resulting "molecular" resonance turns out to be inversely proportional to the "nuclear" width* [and increases in this regime till its value acquires an order of the (decreasing) "nuclear" one]. In other words, the more narrow is the "nuclear" resonance, the more wide is the "molecular" one. Consequently, a large increase of the decay rate of the "molecular" state may be observed in the case concerned, in a contrast to the cases where such near-lying "nuclear" resonances with small widths are absent.

We deliberately consider in the paper certain abstract Hamiltonians since, on the one hand, this consideration exposes more clearly a mechanism of the effect of interplay between the resonance widths. On the other hand, our consideration shows that such an enhancement of decay of a resonance state due to a presence of another closed resonance makes a sense of an universal law working in a wide class of quantum-mechanical systems. The same effect has to take place also in various problems of classical condensed matter, optics and electronics etc., in all the cases description of which may be reduced to spectral problems for model three-channel or two-channel operators like (1) and (22) or more general Hamiltonians of the form (33).

We start, in Section II, with an explicitly solvable matrix model (1) which demonstrates as clearly as possible a mechanism and the effect of interplay between the resonance widths. The model corresponds to a system of arbitrary nature allowing to separate a main channel with continuous spectrum and two additional weakly coupled one-dimensional channels giving, in absence of coupling, two discrete spectrum eigenvalues embedded into continuous spectrum of the main channel. In the case of a molecule, the latter are considered as trial energies for the nuclear and molecular resonances.

If the molecular state may be considered usually as weakly coupled with nuclear channels and, therefore, its separation into a molecular resonance channel like channel 2 in the Hamiltonian (1) may be done comparatively easy, such a separation of the nuclear resonance channel like channel 1 in this Hamiltonian, may turn out to be difficult. This is why we specially consider in Section III another model Hamiltonian (22) with explicit separation of the "molecular" resonance channel only.

Section IV is devoted to consideration of a model including realistic sub-Hamiltonians for nuclear subsystems of N-atomic molecules with $N \geq 2$. In this case, a separation of the molecular resonance channel is realized in framework of an approach motivated by the Faddeev method [**?**], [**?**].

In Section **??** we consider a time evolution of the molecular state in a presence again of the narrow nuclear pre-threshold resonance. There is shown in this section that in a wide time interval, decay of the molecular state does have a standard exponential character [**?**]. The decay is obliged first of all to the open nuclear channels and its rate is ruled just by the inverse width of the nuclear resonance.

II. HAMILTONIAN WITH EXPLICIT SEPARATION OF BOTH RESONANCE CHANNELS

First, we introduce a three-channel Hilbert space $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2$, the sum of a "main" Hilbert space $\mathcal{H}_0$ (channel 0) and two one-dimensional spaces $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}$ (channels 1 and 2, respectively). Elements of the space $\mathcal{H}$ are represented as "vectors" $u = \begin{pmatrix} \mathrm{u}_0 \\ \mathrm{u}_1 \\ \mathrm{u}_2 \end{pmatrix}$ with $u_0 \in \mathcal{H}_0$ and u_1, u_2, complex numbers, $u_1, u_2 \in \mathbb{C}$. Inner product $\langle\,\cdot\,,\,\cdot\,\rangle$ in $\mathcal{H}$ is naturally defined via inner product $\langle\,\cdot\,,\,\cdot\,\rangle$ in $\mathcal{H}_0$ as $\langle u, v\rangle = \langle u_0, v_0\rangle + u_1\overline{v}_1 + u_2\overline{v}_2$.

We deal with Hamiltonian h acting in $\mathcal{H}$ as a 3×3 (operator) matrix,

$$h = \begin{pmatrix} \mathrm{h}_0 \\ \quad \mathrm{b}_{01} \\ \mathrm{b}_{02} \\ \langle\,\cdot\,, b_{01}\rangle \\ \lambda_1 \\ \mathrm{b}_{12} \\ \langle\,\cdot\,, b_{02}\rangle \\ \overline{b}_{12} \\ \lambda_2 \end{pmatrix} \tag{1}$$

with h_0, a self-adjoint operator in the main Hilbert space $\mathcal{H}_0$ and λ_1, λ_2, the real numbers. The vectors b_{01} and b_{02} of the space $\mathcal{H}_0$ realize a coupling of the channels 1 and 2 corresponding to the initial eigenvalues λ_1 and λ_2 with the main channel $\mathcal{H}_0$. The complex number b_{12} describes an immediate coupling between the channels 1 and 2.

If the coupling between the channels in h is absent, $b_{01} = b_{02} = 0$ and $b_{12} = 0$, spectrum of the Hamiltonian h consists of the operator h_0 spectrum and two additional discrete spectrum eigenvalues λ_1 and λ_2 (which are interpreted as trial values respectively, for nuclear resonance and molecule energy). We suppose that the Hamiltonian h_0 has a continuous spectrum denoted by $\sigma_c(h_0)$, and the eigenvalues λ_1 and λ_2 are embedded into this spectrum. It is assumed also that λ_1, λ_2 are not threshold points of the spectrum $\sigma_c(h_0)$ and in a wide vicinity of λ_1, λ_2 this spectrum is absolutely continuous. If the coupling between the channels becomes non-trivial, the eigenvalues λ_1 and λ_2 may go out on unphysical sheet(s) of the energy plane turning into resonances. The latter are considered as poles of analytic continuation on unphysical energy sheets of the resolvent kernel $r(z) = (h - z)^{-1}$ or its matrix elements taken between suitable states.

We suppose here that the resolvent $r_0(z) = (h_0 - z)^{-1}$ does not have such poles in a sufficiently wide neighborhood $\mathcal{D}$ of the points λ_1 and λ_2 in unphysical sheet(s) and the matrix elements $\beta_{jk}(z) \equiv \langle r_0(z) b_{0j}, b_{0k}\rangle$, $j, k = 1, 2$, allow analytical continuation in z at least on this neighborhood $\mathcal{D}$ and

$$c_{\mathcal{D}}^{(j)} = \inf_{z\in\mathcal{D}} |\,\mathrm{Im}\langle r_0(z)\hat{b}_{0j}, \hat{b}_{0j}\rangle| > 0, \quad C_{\mathcal{D}} = \max_{j,k} \sup_{z\in\mathcal{D}} |\langle r_0(z)\hat{b}_{0j}, \hat{b}_{0k}\rangle| < \infty$$

where $\hat{b}_{0j} = b_{0j}/\|b_{0j}\|$, $j = 1, 2$, and the values of $c_{\mathcal{D}}^{(j)}$ and $C_{\mathcal{D}}$ for given $\hat{b}_{0j}$ and $\hat{b}_{0k}$, depend only on $\mathcal{D}$. So that for given (and fixed) "structure functions" $\hat{b}_{0j}$ one has the following estimates:

$$c_{\mathcal{D}}^{(j)}\|b_{0j}\|^2 \leq |\operatorname{Im}\beta_{jj}(z)| \leq \tilde{C}_{\mathcal{D}}^{(j)}\|b_{0j}\|^2 \quad \text{and} \quad |\beta_{jk}(z)| \leq C_{\mathcal{D}}\|b_{0j}\|\|b_{0k}\| \qquad (2)$$

where $\tilde{C}_{\mathcal{D}}^{(j)} = \sup\limits_{z\in\mathcal{D}} |\operatorname{Im}\langle r_0(z)\hat{b}_{0j}, \hat{b}_{0j}\rangle|$, $\quad c_{\mathcal{D}}^{(j)} \leq \tilde{C}_{\mathcal{D}}^{(j)} \leq C_{\mathcal{D}}$.

Let us consider the spectral problem $hu = zu$,

$$\begin{array}{l} (\mathrm{h}_0 - z)u_0 + \mathrm{b}_{01}u_1 + \mathrm{b}_{02}u_2 = 0 \\ \langle u_0, b_{01}\rangle + (\lambda_1 - z)u_1 + \mathrm{b}_{12}u_2 = 0 \\ \langle u_0, b_{02}\rangle + \overline{b}_{12}u_1 + (\lambda_2 - z)u_2 = 0 \end{array} \qquad (3)$$

for the Hamiltonian h. Expressing the component $u_0 = -r_0(z)b_{01}u_1 - r_0(z)b_{02}u_2$ from the first equation (3) and substituting it into the rest equations, one comes immediately to an equivalent scalar system including the components u_1 and u_2 only,

$$\begin{cases} [\lambda_1 - z - \beta_{11}(z)]u_1 + [\mathrm{b}_{12} - \beta_{12}(z)]u_2 = 0 \\ [\overline{b}_{12} - \beta_{21}(z)]u_1 + [\lambda_2 - z - \beta_{22}(z)]u_2 = 0. \end{cases} \qquad (4)$$

Therefore, the system (4) and, hence, the problem (3) is solvable in $\mathcal{H}$ if and only if the energy z satisfies the "quadratic" equation

$$(\lambda_1 - z - \beta_{11})(\lambda_2 - z - \beta_{22}) - (b_{12} - \beta_{12})(\overline{b}_{12} - \beta_{21}) = 0. \tag{5}$$

It is easy to check that exactly the left part of the equation (5) is present as a denominator in the expression for the resolvent $r(z)$. Obviously, this equation has no solutions z with $\operatorname{Im} z \neq 0$ in the physical sheet. Otherwise, such z were the discrete spectrum eigenvalues of h. However, this is impossible since the Hamiltonian h is a self-adjoint operator. Therefore the equation (5) may be solvable only in real axis and/or in unphysical sheet(s) of the energy Riemann surface of $r_0(z)$.

At the beginning, let us consider, a special case where $b_{12} = 0$ and, say, $b_{0j} \neq 0$ but $b_{0k} = 0$, $k \neq j$. In this case, the eigenvalue λ_k stays fixed. At the same time the equation (5) turns into

$$z = \lambda_j - \langle r_0(z) b_{0j}, b_{0j} \rangle. \tag{6}$$

If $\|b_{j0}\|$ is small enough, to prove existence of solutions in a vicinity of $z = \lambda_j$, one can apply to the equation (6) the fixed point theorem. Since, by supposition, λ_j is not a threshold point of $\sigma_c(h_0)$, the equation (6) gives us two resonances (see, e. g., [?], [?]) looking in a first order of perturbation series as

$$z_j^{(\pm)} \underset{\|b_{j0}\| \to 0}{=} \lambda_j - \langle r_0(\lambda_j \mp i0) b_{0j}, b_{0j} \rangle + o(\|b_{j0}\|^2), \tag{7}$$

and being situated, respectively, in lower and upper half-planes of unphysical sheet(s) neighboring with the physical one in a vicinity of the point $z = \lambda_j$. The real, $E_R^{(j)}$, and imaginary, $\Gamma_R^{(j)}/2$, parts of the resonances $z_j^{(\pm)}$, $z_j^{(\pm)} = E_R^{(j)} \pm i\frac{\Gamma_R^{(j)}}{2}$, are given by

$$\begin{aligned} E_R^{(j)} &= \lambda_j - \operatorname{Re}\langle r_0(\lambda_j + i0) b_{0j}, b_{0j} \rangle + o(\|b_{j0}\|^2), \\ \Gamma_R^{(j)} &= 2 \operatorname{Im}\langle r_0(\lambda_j + i0) b_{0j}, b_{0j} \rangle + o(\|b_{j0}\|^2). \end{aligned} \tag{8}$$

For analysis of the general three-channel equation (5), it is convenient to resolve it for given $\beta_{jk} = \langle r_0(z) b_{0j}, b_{0k} \rangle$ as a quadratic equation with respect to z:

$$z = \frac{\lambda_1 + \lambda_2 - \beta_{11} - \beta_{22}}{2} \pm \sqrt{\left(\frac{\lambda_1 - \lambda_2 - \beta_{11} + \beta_{22}}{2}\right)^2 + (b_{12} - \beta_{12})(\overline{b}_{12} - \beta_{21})} \tag{9}$$

We suppose the resonances generated by the both eigenvalues λ_1 and λ_2, are narrow. This means that the coupling of the channels in (1) must be weak, i. e. the previous conditions of a "very small" $\|b_{0j}\|$, j=1,2, as well as the condition of a "very small" $|b_{12}|$ are valid. So, the solvability of the equations (9) in unphysical sheet(s) may be proved again using the fixed point theorem.

Here, we consider two cases:

1. $C_{\mathcal{D}}\|b_{0j}\|\|b_{0k}\| \ll |\lambda_2-\lambda_1|$ for all $j,k=1,2$ and $\|b_{12}\| \ll |\lambda_2-\lambda_1|$. One can see easily in this case the equations (9) give two pairs of solutions which are practically independent on each other and these solutions are expressed by formulae like (7).

2. The case where $\lambda_1 \approx \lambda_2$, but nevertheless

$$|(b_{12}-\beta_{12})(\overline{b}_{12}-\beta_{21})| \ll |\lambda_1-\lambda_2-\beta_{11}+\beta_{22}|^2. \tag{10}$$

Namely this case is of most interest for us in the context of the main topic of the work. We have in mind that the Hamiltonians

$$h_1 = \begin{pmatrix} \mathrm{h}_0 & \mathrm{b}_{01} \\ \langle\,\cdot\,, b_{01}\rangle & \lambda_1 \end{pmatrix} \quad \text{and} \quad h_2 = \begin{pmatrix} \mathrm{h}_0 & \mathrm{b}_{02} \\ \langle\,\cdot\,, b_{02}\rangle & \lambda_2 \end{pmatrix} \tag{11}$$

are as if modelling, respectively, the nuclear subsystem of a molecule forming a resonance state and the molecule itself in absence of the nuclear resonance. Leading terms of the "nuclear" and "molecular" resonances $z_1^{(\pm)}$ and $z_2^{(\pm)}$ generated by the respective Hamiltonians h_1 and h_2 are given by (7). According to (2) their widths (8) satisfy inequalities

$$c_{\mathcal{D}}^{(1)}\|b_{01}\|^2 \le \Gamma_R^{(1)}/2 \le \tilde{C}_{\mathcal{D}}^{(1)}\|b_{01}\|^2 \quad \text{and} \quad c_{\mathcal{D}}^{(2)}\|b_{02}\|^2 \le \Gamma_R^{(2)}/2 \le \tilde{C}_{\mathcal{D}}^{(2)}\|b_{02}\|^2.$$

Since the molecular width $\Gamma_R^{(2)}$ is usually much more small, $\Gamma_R^{(2)} \ll \Gamma_R^{(1)}$, as compared to the nuclear one, $\Gamma_R^{(1)}$, one may require

$$C_{\mathcal{D}}\|b_{02}\|^2 \ll c_{\mathcal{D}}^{(1)}\|b_{01}\|^2. \tag{12}$$

The channel $\mathcal{H}_1$ belongs to the pure nuclear part of the system. This means that, if there are no special reasons, its constant of coupling $|b_{12}|$ with the molecular channel $\mathcal{H}_2$ must have the same order of magnitude as $\|b_{02}\|$, i. e.

$$|b_{12}| \sim \|b_{02}\| \quad (\text{and, thereby,} \quad C_{\mathcal{D}}|b_{12}|^2 \ll c_{\mathcal{D}}^{(1)}\|b_{01}\|^2). \tag{13}$$

¿From the beginning, we assume for convenience the "coupling constant" $\|b_{01}\|$ to be so small that

$$C_{\mathcal{D}}\|b_{01}\| < 1 \tag{14}$$

i. e. the "nuclear" resonances $z_1^{(\pm)}$ are as narrow as $\Gamma_R^{(1)} < \tilde{C}_{\mathcal{D}}^{(1)}/C_{\mathcal{D}}^2$.

In the condition (12) we have

$$|\lambda_1-\lambda_2-\beta_{11}+\beta_{22}|^2 \approx |\lambda_1-\lambda_2-\beta_{11}|^2 \ge [\mathrm{Im}\,\beta_{11}(z)]^2 \approx$$
$$\approx [\mathrm{Im}\,\beta_{11}(\lambda_1+i0)]^2 \approx \left(\frac{\Gamma_R^{(1)}}{2}\right)^2 \ge \left(c_{\mathcal{D}}^{(1)}\right)^2 \|b_{01}\|^4. \tag{15}$$

At the same time,

$$|(b_{12}-\beta_{12})(\overline{b}_{12}-\beta_{21})| \leq (|b_{12}|+C_{\mathcal{D}}\|b_{01}\|\|b_{02}\|)^2.$$

Since the conditions (13) and (14) take place, we get

$$(|b_{12}|+C_{\mathcal{D}}\|b_{01}\|\|b_{02}\|)^2 \sim \|b_{02}\|^2(1+C_{\mathcal{D}}\|b_{01}\|)^2 \leq (c_{\mathcal{D}}^{(2)})^{-1}\Gamma_R^{(2)}. \tag{16}$$

Let us suppose further that the "nuclear" resonances $z_1^{(\pm)}$ is in fact as narrow that

$$\Gamma_R^{(1)} \ll 1/c_{\mathcal{D}}^{(2)}. \tag{17}$$

Then, as follows from the estimates (15) and (16), the condition (10) is obviously satisfied if

$$\Gamma_R^{(2)} \ll c_{\mathcal{D}}^{(2)}\left(\Gamma_R^{(1)}\right)^2. \tag{18}$$

Now, using the expression $\sqrt{1+\varepsilon}=1+\dfrac{\varepsilon}{2}+O(\varepsilon^2)$ at $|\varepsilon|\ll 1$, one can rewrite the equations (9) for z in $O(\|b_{01}\|^2)$-vicinity of λ_1 and $\lambda_2=\lambda_1+O(\|b_{01}\|^2)$ as

$$\begin{aligned} z &= \frac{\lambda_1+\lambda_2-\beta_{11}-\beta_{22}}{2} \pm \\ &\pm \frac{\lambda_1-\lambda_2-\beta_{11}+\beta_{22}}{2}\left[1+\frac{2(b_{12}-\beta_{12})(\overline{b}_{12}-\beta_{21})}{(\lambda_1+\lambda_2-\beta_{11}-\beta_{22})^2}+O(\varepsilon^2)\right] \end{aligned} \tag{19}$$

with $\varepsilon \sim \left(c_{\mathcal{D}}^{(2)}\right)^{-1}\Gamma_R^{(2)}/\left(\Gamma_R^{(1)}\right)^2$. It follows from (19) that in the conditions above, the equations (9) have solutions

$$z_{\rm nucl}^{(\pm)} = \lambda_1-\beta_{11}(\lambda_1\mp i0)+o(\|b_{01}\|^2)+\frac{|b_{12}|^2}{\lambda_1-\lambda_2-\beta_{11}(\lambda_1\mp i0)}\left[1+O(\varepsilon^2)\right]$$

and

$$z_{\rm mol}^{(\pm)} = \lambda_2-\beta_{22}(\lambda_2\mp i0)+o(\|b_{02}\|^2)-\frac{|b_{12}|^2}{\lambda_1-\lambda_2-\beta_{11}(\lambda_1\mp i0)}\left[1+O(\varepsilon^2)\right] \tag{20}$$

Due to (13) and (18) we have

$$\frac{|b_{12}|^2}{|\lambda_1-\lambda_2-\beta_{11}(\lambda_1\pm i0)|}\le 2\cdot\frac{|b_{12}|^2}{\Gamma_R^{(1)}}\sim 2\cdot\frac{\|b_{02}\|^2}{\Gamma_R^{(1)}}\le\frac{\Gamma_R^{(2)}}{c_{\mathcal{D}}^{(2)}\Gamma_R^{(1)}}=$$
$$=\Gamma_R^{(1)}\cdot\frac{\Gamma_R^{(2)}}{c_{\mathcal{D}}^{(2)}\left(\Gamma_R^{(1)}\right)^2}\ll\Gamma_R^{(1)}.$$

Therefore, the resonances $z_{\rm nucl}^{(\pm)}$ are only weakly perturbed initial "nuclear" resonances $z_1^{(\pm)}$ with practically the same width $\Gamma_R^{(1)}$. In a contrast to $z_{\rm nucl}^{(\pm)}$, a difference between widths of the resonances $z_{\rm mol}^{(\pm)}$ and $z_2^{(\pm)}$ in the case concerned can be very large. Such a situation takes place if the initial "molecular" energy λ_2 coincides with real part of the "nuclear" resonances $z_1^{(\pm)}$,

$$\lambda_2=E_R^{(1)}\approx\lambda_1-\operatorname{Re}\beta_{11}(\lambda_1+i0).$$

and, in accordance with (20),

$$z_{\rm mol}^{(\pm)}\cong E_R^{(1)}\pm 2i\frac{|b_{12}|^2}{\Gamma_R^{(1)}}.$$

The width $\Gamma_R^{(m)}$ of the resonances $z_{\rm mol}^{(\pm)}$,

$$\Gamma_R^{(m)}=2|\operatorname{Im}z_{\rm mol}^{(\pm)}|\cong 4\cdot\frac{|b_{12}|^2}{\Gamma_R^{(1)}},$$

being small, $\Gamma_R^{(m)}\ll\Gamma_R^{(1)}$, is nevertheless much more large than $\Gamma_R^{(2)}\cong 2\operatorname{Im}\beta_{22}(\lambda_2+i0)$. Indeed, due to (13) and (17) we find

$$\Gamma_R^{(m)}\sim\frac{\|b_{02}\|^2}{\Gamma_R^{(1)}}\sim\Gamma_R^{(2)}\cdot\frac{1/c_{\mathcal{D}}^{(2)}}{\Gamma_R^{(1)}}\gg\Gamma_R^{(2)}. \tag{21}$$

This completes the proof of our statement in the case of three-channel Hamiltonians, concerning a crucial influence of a narrow "nuclear" resonance on the width of the "molecular" level: *if the "molecular" energy λ_2 coincides with the real part $E_R^{(1)}$ of the "nuclear" resonance then the "molecular" width $\Gamma_R^{(m)}$ is* **inversely proportional** *to the width $\Gamma_R^{(1)}$ of this resonance and, thereby, for a small $\Gamma_R^{(1)}$, $\Gamma_R^{(1)}\ll 1/c_{\mathcal{D}}^{(2)}$, it can be very large compared with such a width, $\Gamma_R^{(2)}$, in absence of the "nuclear" resonance.*

To get a feeling of the $c_{\mathcal{D}}^{(2)}$ value in a molecular case, let us suppose the Hamiltonian h_0 describes indeed a few-nucleon system (constituted by nuclei of the molecule). Then the kernel of the resolvent component $r_0^c(z)$ corresponding to the continuous spectrum of h_0 allows, say, in configuration space

$\mathbb{R}^n$ (the dimension n is determined by number of the nucleons), the following representation [?]

$$r_0^c(X, X', z) = \sum_{\mathrm{A}} \int_{\mathbb{R}^{n_{\mathrm{A}}}} dp_{\mathrm{A}} \, \frac{U_{\mathrm{A}}(X, p_{\mathrm{A}}) \overline{U}_{\mathrm{A}}(X', p_{\mathrm{A}})}{E_{\mathrm{A}} + p_{\mathrm{A}}^2 - z}$$

where X, X' stand for points of $\mathbb{R}^n$ and A, for multi-indices (see Ref. [?], §4 of Chapter I) numerating the scattering channels. Notations U_{A} are used for respective channel wave functions (kernels of the wave operators) and E_{A}, for thresholds. The channel dimensions n_{A} are determined by numbers of clusters (nuclei) in respective initial scattering states.

In the case, the coupling vectors b_{02} have to be considered as functions $b_{02}(X)$ belonging to a subspace corresponding to a specific symmetry of the molecule concerned. Calculating a jump of the kernel $r_0^c(X, X', z)$ when z crosses the real axis at the point λ_2 one finds the following estimation for $c_{\mathcal{D}}^{(2)}$

$$\begin{aligned} c_{\mathcal{D}}^{(2)} &\sim \mathrm{Im}\langle r_0^c(\lambda_2 + i0)\hat{b}_{02}, \hat{b}_{02}\rangle = \\ &= \sum_{\mathrm{A}:\ E_{\mathrm{A}} < \lambda_2} \pi \, [\lambda_2 - E_{\mathrm{A}}]^{(n_{\mathrm{A}}-2)/2} \int_{S^{n_{\mathrm{A}}-1}} d\hat{p}_{\mathrm{A}} \, |\langle \hat{b}_{02}, U_{\mathrm{A}}(\sqrt{\lambda_2 - E_{\mathrm{A}}}\hat{p}_{\mathrm{A}})\rangle|^2 \end{aligned}$$

where $S^{n_{\mathrm{A}}-1}$ stands for the unit sphere in $\mathbb{R}^{n_{\mathrm{A}}}$, $\hat{p}_{\mathrm{A}} \in S^{n_{\mathrm{A}}-1}$.

III. TWO-CHANNEL HAMILTONIAN WITH EXPLICIT SEPARATION ONLY OF A "MOLECULAR" RESONANCE CHANNEL

In the present section we consider a Hamiltonian h in the Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathbb{C}$ defined (cf. Section II) as a matrix

$$h = \begin{pmatrix} \mathrm{h}_1 & \mathrm{b} \\ \langle \cdot \,, b\rangle & \lambda_2 \end{pmatrix} \qquad (22)$$

where h_1 stands now for a main ("nuclear") Hamiltonian acting in a Hilbert space $\mathcal{H}_1$ and λ_2, $\lambda_2 \in \mathbb{R}$, again for a trial "molecular" energy. A vector $b \in \mathcal{H}_1$ realizes a coupling between the channels. Evidently, the Hamiltonian (1) is a particular case of the Hamiltonian (22).

If $b \neq 0$, the eigenvalue λ_2 turns into resonances z being solutions of the equation like (6),

$$z = \lambda_2 - \beta(z) \qquad (23)$$

with $\beta(z) = \langle r_1(z)b, b\rangle$, $r_1(z) = (h_1 - z)^{-1}$. In a contrast to Section II we assume here that the "nuclear" resonance[†] closed to λ_2, is present immediately in the channel 1, i. e. the function $\beta(z)$ continued in an unphysical sheet sticked in vicinity of λ_2 with the physical one, say, along upper rim of the cut, has a pole $z_1 = E_R^{(1)} - i\dfrac{\Gamma_R^{(1)}}{2}$, with $E_R^{(1)} \in \mathbb{R}$, $\Gamma_R^{(1)} > 0$. For the sake of simplicity we suppose that this pole is simple, so that in this vicinity

$$\beta(z) = \frac{a}{z - z_1} + \beta^{\mathrm{reg}}(z) \tag{24}$$

with a holomorphic function $\beta^{\mathrm{reg}}(z)$. For a fixed "structure function" $\hat{b} = b/\|b\|$ we have $|a| = C_a\|b\|^2$ with a constant $C_a > 0$ determined by the residue at $z = z_1$ of the resolvent $r_1(z)$ continued. Note that this residue is expressed in terms of respective resonance wave functions, the so-called Gamow vectors, corresponding to the resonance z_1 [see below formula (**??**)]. In fact, we suppose that this resonance corresponds to a kind of an "almost eigenstate" of the Hamiltonian h_1, i. e. a limit procedure is possible, in principle, with respect to a certain parameter (or parameters) inside of h_1 in which $\Gamma_R^{(1)} \to 0$ and the resonance turns into usual eigenvalue with eigenvector $\psi_1 \in \mathcal{H}_1$. In other words we suppose that

$$C_a = C_a^{(0)} + o(1) \quad \text{as} \quad \Gamma_R^{(1)} \to 0 \tag{25}$$

and $C_a^{(0)} \equiv \langle\hat{b}, \psi_1\rangle\langle\psi_1, \hat{b}\rangle \neq 0$. An example of such a situation with $C_a^{(0)} = 1$ was already demonstrated in the previous section with the Hamiltonians (11). The limit procedure (25) will be discussed in more detail in Section **??**.

Analogously to a, we represent the regular term $\beta^{\mathrm{reg}}(z)$ as $\beta^{\mathrm{reg}}(z) = \|b\|^2 f(z)$ with a factor $f(z)$ depending only on $\hat{b}$. We shall suppose the vector $\hat{b}$ to be such that, in a sufficiently wide domain $\mathcal{D}$ about λ_2 concerned, in the unphysical sheet, the function $f(z)$ is bounded, $C_{\mathcal{D}} = \sup_{z\in\mathcal{D}} |f(z)| < \infty$, and $c_{\mathcal{D}} = \inf_{z\in\mathcal{D}} |\operatorname{Im} f(z)| > 0$. Therefore $|\beta^{\mathrm{reg}}(z)| \leq C_{\mathcal{D}}\|b\|^2$ and $c_{\mathcal{D}}\|b\|^2 \leq |\operatorname{Im}\beta^{\mathrm{reg}}(z)| \leq \tilde{C}_{\mathcal{D}}\|b\|^2$ where $\tilde{C}_{\mathcal{D}} = \sup_{z\in\mathcal{D}} |\operatorname{Im} f(z)|$, $\tilde{C}_{\mathcal{D}} \leq C_{\mathcal{D}}$.

A substitution of the representation (24) for $\beta(z)$ into equation (23) turns the latter into "quadratic" equation

$$(z - \lambda_2)(z - z_1) + a + (z - z_1)\beta^{\mathrm{reg}}(z) = 0$$

[†]More precisely, two resonances. Since the Hamiltonian h_1 is a self-adjoint operator its resolvent obeys in the physical sheet the symmetry condition $[r_1(z)]^* = r_1(\overline{z})$. Then, it immediately follows from the uniqueness principle of analytic continuation, if z_1 is a resonance in a sheet neighboring with the physical one then the conjugate point $\overline{z}_1$ is also a resonance with the same multiplicity (but maybe in another sheet).

with "solutions"

$$z = \frac{\lambda_2 + z_1 - \beta^{\rm reg}}{2} \pm \sqrt{\left(\frac{\lambda_2 - z_1 - \beta^{\rm reg}}{2}\right)^2 - a}. \qquad (26)$$

The equations (26) are quite analogous to the equations (9) being suitable for applying the fixed point theorem when proving a solvability of (23).

We shall suppose that the coupling between channels in the Hamiltonian (22) is so weak that

$$\left| \; \beta^{\rm reg}(z)|_{z\in\mathcal{D}} \right| \le C_{\mathcal{D}}\|b\|^2 \ll \Gamma_R^{(1)} \quad \text{and} \quad |a| = C_a\|b\|^2 \ll \left(\Gamma_R^{(1)}\right)^2. \qquad (27)$$

This means

$$\frac{|a|}{\left|\lambda_2 - z_1 - \; \beta^{\rm reg}(z)|_{z\in\mathcal{D}}\right|^2} = \frac{|a|}{\left|\lambda_2 - E_R^{(1)} + i\dfrac{\Gamma_R^{(1)}}{2} - \; \beta^{\rm reg}(z)|_{z\in\mathcal{D}}\right|^2} \approx$$

$$\approx \frac{|a|}{\left|\lambda_2 - E_R^{(1)}\right|^2 + \left(\dfrac{\Gamma_R^{(1)}}{2}\right)^2} \le \frac{4|a|}{\left(\Gamma_R^{(1)}\right)^2} \le \frac{4C_a\|b\|^2}{\left(\Gamma_R^{(1)}\right)^2} \ll 1. \qquad (28)$$

Note that if the resonance z_1 was absent in the channel 0 and in such a case, one had $\beta(z) \equiv \beta^{\rm reg}(z)$, then the eigenvalue λ_2 had generated, in the lower half-plane $\operatorname{Im} z \le 0$, the resonance $z_2 = E_R^{(2)} - i\Gamma_R^{(2)}/2$ (see Section II) with the width $\Gamma_R^{(2)} \approx 2\operatorname{Im}\beta^{\rm reg}(\lambda_2 + i0)$ satisfying inequalities

$$c_{\mathcal{D}}\|b\|^2 \le \Gamma_R^{(2)}/2 \le \tilde{C}_{\mathcal{D}}\|b\|^2.$$

Therefore, we can compare (in terms of the "pure nuclear", $\Gamma_R^{(1)}$, and "pure molecular", $\Gamma_R^{(2)}$, widths) the case where a "nuclear" resonance, z_1, is present, with an opposite case where such a resonance is absent. In particular, the second condition (27) follows from the requirement, analogous to (18),

$$C_a\Gamma_R^{(2)} \ll c_{\mathcal{D}}\left(\Gamma_R^{(1)}\right)^2.$$

It follows from the relations (26) considered together with the estimates (27) and (28) that the domain $\mathcal{D}$ includes (at $\operatorname{Im} z < 0$) only two roots $z_{\rm nucl}$ and $z_{\rm mol}$ of the equation (23) with leading terms given by

$$z_{\rm nucl} \cong z_1 + \frac{a}{\lambda_2 - z_1 - \beta^{\rm reg}(z_1)} \cong z_1 + \frac{a}{\lambda_2 - z_1}, \qquad (29)$$

$$z_{\rm mol} \cong \lambda_2 - \beta^{\rm reg}(\lambda_2 + i0) - \frac{a}{\lambda_2 - z_1 - \beta^{\rm reg}(\lambda_2 + i0)} \cong \lambda_2 - \frac{a}{\lambda_2 - z_1}. \qquad (30)$$

Due to the second condition (27) we have $\left|\dfrac{a}{\lambda_2 - z_1}\right| \ll \Gamma_R^{(1)}$ and, thereby, the resonance $z_{\rm nucl}$ represents only a very weak perturbation of the initial "nuclear" resonance z_1. At the same time, a situation with the "molecular" resonance is crucially different (cf. Section II).

In particular, if the "molecular" energy λ_2 coincides with the real part $E_R^{(1)}$ of the "nuclear" resonance z_1 then $z_{\rm mol} = E_R^{(m)} - i\dfrac{\Gamma_R^{(m)}}{2}$ with $E_R^{(m)} \cong \lambda_2 - 2\dfrac{\operatorname{Im} a}{\Gamma_R^{(1)}}$ and

$$\Gamma_R^{(m)} \cong 4\frac{|\operatorname{Re} a|}{\Gamma_R^{(1)}}, \quad \operatorname{Re} a < 0. \tag{31}$$

Since $|\operatorname{Re} a| \sim C_a \|b\|^2 \sim \dfrac{C_a}{c_{\mathcal{D}}}\Gamma_R^{(2)}$, one finds for $\Gamma_R^{(m)}$ the estimate

$$\Gamma_R^{(m)} \sim \Gamma_R^{(2)} \cdot \frac{C_a/c_{\mathcal{D}}}{\Gamma_R^{(1)}}. \tag{32}$$

It should be noted in this place that, due to the consideration (25) of the resonance z_1 as an "almost eigenvalue", the ratio $C_a = |a|/\|b\|^2$ is separated from zero, $C_a \geq C > 0$, as $\Gamma_R^{(1)} \to 0$. With this remark, it follows from the estimations (31) and (32) as in Section II, that, in the case of a narrow "nuclear" resonance with a width $\Gamma_R^{(1)} \ll C_a/c_{\mathcal{D}}$, one has to observe a large rise, proportional just to the factor $\dfrac{C_a/c_{\mathcal{D}}}{\Gamma_R^{(1)}}$ [cf. formula (21)], of the "molecular" width as compared to the case where such a resonance is absent.

Concluding the section we note that if the conditions (27) do not fulfil i. e. the coupling between channels in the Hamiltonian (22) is not small as compared to the "nuclear" width $\Gamma_R^{(1)}$ then it follows from (26) that the molecular width $\Gamma_R^{(m)}$ acquires itself an order of $\Gamma_R^{(1)}$. We do not consider this case in the paper since such a situation seems to be unreachable in electronic molecules.

IV. CONSIDERATION OF A REAL MOLECULE

In this section we will prove the main statements of previous sections but for a "model-free" Hamiltonian. Namely, we consider now the Hamiltonian

$$H = h_0 + v_1 + v_2 \tag{33}$$

in a Hilbert space $\mathcal{H}_0$ with a self-adjoint main operator h_0. The potentials v_1 and v_2, symmetric operators, are supposed to be such that the operator H is also self-adjoint as well as the operators $h_1 = h_0 + v_1$ and $h_2 = h_0 + v_2$ in the same domain $\mathbf{D} \subset \mathcal{H}_0$.

We consider such H in particular as a realistic Hamiltonian for the nuclear subsystem of a N-atomic molecule, $N \geq 2$. The part h_0 will include in this case a sum of the kinetic energy operator and Coulomb interactions inside of the nuclear subsystem. The term v_1 will describe a strong interaction and v_2, an additional effective interaction between the nuclear constituents due to electrons. By $\mathcal{H}_0$ we understand a subspace corresponding to a specific symmetry of the molecule (and thereby, of its nuclear subsystem, too). This is why we assume that continuous spectra of the operators h_0, h_1 and h_2 fill semi-infinitive intervals, respectively, $\sigma_c(h_0) = \sigma_c(h_2) = (E_0, +\infty)$ and $\sigma_c(h_1) = (E_1, +\infty)$ and the lower boundary (lower threshold) E_1 of the continuous spectrum $\sigma_c(h_1)$ of h_1 is situated below than that, E_0, of h_0 and h_2: $E_1 < E_0$. The "molecular" Hamiltonian h_2 is supposed to have a simple isolated eigenvalue λ_2, $\lambda_2 < E_0$, with an eigenfunction $\varphi_2 \in \mathcal{H}_0$, $h_2\varphi_2 = \lambda_2\varphi_2$, $\|\varphi_2\| = 1$. For the sake of simplicity we suppose that all the discrete spectrum‡ of h_2 consists of this point λ_2 only. At the same time, as in the previous sections, we assume that the ("pure nuclear") channel described by the Hamiltonian h_1, has a narrow resonance $z_1 = E_R^{(1)} - i\dfrac{\Gamma_R^{(1)}}{2}$, $E_R^{(1)} \in \mathbb{R}$, $\Gamma_R^{(1)} > 0$, closed to the threshold E_0 so that $E_R^{(1)} \approx \lambda_2$.

In principle, one could reduce the Hamiltonian H to the matrix models (1) or (22) using a standard projection procedure. For example, to obtain from H the three-channel Hamiltonian (1) one can introduce a state $\tilde{\varphi}_1 \in \mathcal{H}_0$, $\|\tilde{\varphi}_1\| = 1$, being a good approximation of the nuclear resonance wave function $\varphi_1^{\rm res}$ [see below formula (**??**)] at least at nuclear distances so that $\langle h_1\tilde{\varphi}_1, \tilde{\varphi}_1\rangle \approx E_R^{(1)}$. Then one ortogonalizes the functions $\tilde{\varphi}_1$ and φ_2 obtaining new orthonormal vectors ψ_1 and ψ_2 closed respectively, to $\tilde{\varphi}_1$ and φ_2. Considering the projectors $P_1 = \psi_1\langle\,\cdot\,,\psi_1\rangle$, $P_2 = \psi_2\langle\,\cdot\,,\psi_2\rangle$ and $P_0 = I - P_1 - P_2$, one rewrites the Hamiltonian H as a matrix operator, $H' = \{P_iHP_j\}$, $i,j = 0,1,2$, corresponding to the decomposition $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2$. The operator H' (and, of course, the Hamiltonian H itself) turns out evidently to be unitary equivalent exactly to the operator (1) with $\lambda_j = \langle H\psi_j, \psi_j\rangle$, $b_{12} = \langle H\psi_1, \psi_2\rangle$ and $b_{0j} = P_0H\psi_j$. The 00-component of the matrix (1) stays the same, P_0HP_0, as in H'. Unfortunately, the separation described of the resonance channels is approximate and resolvent of the operator P_0HP_0 has to keep poles (with rest, rather "small", residues) at the molecular and nuclear resonances (corresponding to the total Hamiltonian H). Account of this circumstance, in analysis of the type (5) or (23) equations, requires an additional, and cumbersome, consideration. To make an exact (and rather simple) separation in H of the nuclear and molecular channels, we propose another natural approach

‡Here, in the case of a real molecule one has to take in mind only the discrete spectrum corresponding to the subspace $\mathcal{H}_0$ above of a specific symmetry of the molecule.

motivated by the Faddeev method [?], [?].

A. Separation of the molecular resonance channel in the Faddeev approach

A study of the spectral properties of the Hamiltonians decomposed like H in a sum of a main Hamiltonian (usually the kinetic energy operator) and few perturbations of a rather arbitrary nature (in the example of three-body problems these ones are usually two-body potentials) can be reduced to an investigation of the Faddeev matrix operator (associated with the respective Faddeev equations [?], [?]) on its "physical" invariant subspace (see Ref. [?] and Refs. cited therein).

The Faddeev matrix corresponding to the decomposition (33) looks as

$$H_F = \begin{pmatrix} \mathrm{h}_0 + v_1 & \mathrm{v}_1 \\ \mathrm{v}_2 & \mathrm{h}_0 + v_2 \end{pmatrix} = \begin{pmatrix} \mathrm{h}_1 & \mathrm{v}_1 \\ \mathrm{v}_2 & \mathrm{h}_2 \end{pmatrix} \tag{34}$$

being considered as operator in the Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}_0$.

The Hamiltonian (34) represents a particular case of the general 2×2 matrix operators (with components h_1 and h_2 generally independent on v_1 and v_2), some aspects of spectral theory for which may be found in Refs. [?] and [?].

In the special case of $h_1 = h_0 + v_1$ and $h_2 = h_0 + v_2$ considered, one can check that

$$(H_F - z)^{-1} = (h_0 - z)^{-1}\mathbf{I} - (h_0 - z)^{-1} \begin{pmatrix} \mathrm{v}_1 & \mathrm{v}_1 \\ \mathrm{v}_2 & \mathrm{v}_2 \end{pmatrix} (H - z)^{-1} \tag{35}$$

with $\mathbf{I}$, the identity operator in $\mathcal{H}$. This allows one to conclude that although the operator H_F is non-symmetric but nevertheless it has a pure real spectrum. Moreover, one can show (see [?]) that the spectrum of H_F consists of the ("physical") spectrum of H and ("spurious") spectrum of h_0. Eigenfunctions Ψ of the initial Hamiltonian H are expressed via eigenfunctions $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ of the Faddeev operator H_F corresponding to its "physical" spectrum as $\Psi = \psi_1 + \psi_2$.

It follows also from the identity (35) that if a resonance appears as a pole of analytic continuation of the resolvent kernel $(H - z)^{-1}$ than it has to be