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PERTURBATION OF EMBEDDED EIGENVALUE BY A NEAR-LYING RESONANCE

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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. [1] – [5] 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. [6]. Among them are even such intrigue systems as $pp^{16}O$ and $p^{17}O$ [7], [8] i. e. the nuclear constituents of the usual water molecule H_2O or hydroxyl ions OH^- based on the more rare isotope ^{17}O. Possibility of influence of near-threshold nuclear resonances on the molecular properties was recently indicated in Ref. [9] 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 [10] 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 [5]) 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 [11], [12].

In Section V 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 [13]. 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" $u = \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix}$ 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 $\langle u, v \rangle = \langle u_0, v_0 \rangle + u_1 \bar{v}_1 + u_2 \bar{v}_2$.

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

$$h = \begin{pmatrix} h_0 & b_{01} & b_{02} \\ \langle \cdot, b_{01} \rangle & \lambda_1 & b_{12} \\ \langle \cdot, b_{02} \rangle & \bar{b}_{12} & \lambda_2 \end{pmatrix} \tag{1}$$

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

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

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:

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

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

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

$$
\begin{array}{rcl}
(h_0 - z)u_0 + & b_{01}u_1 + & b_{02}u_2 = 0 \\
\langle u_0, b_{01}\rangle + (\lambda_1 - z)u_1 + & b_{12}u_2 = 0 \\
\langle u_0, b_{02}\rangle + & \overline{b}_{12}u_1 + (\lambda_2 - z)u_2 = 0
\end{array}
\tag{3}
$$

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,

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

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 $\mathrm{Im}\,z \neq 0$ 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., [14], [15]) 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 $z_j^{(\pm)}$, $z_j^{(\pm)} = E_R^{(j)} \pm i\dfrac{\Gamma_R^{(j)}}{2}$, are given by

$$E_R^{(j)} = \lambda_j - \mathrm{Re}\langle r_0(\lambda_j + i0)b_{0j}, b_{0j}\rangle + o(\|b_{j0}\|^2),$$

$$\Gamma_R^{(j)} = 2\,\mathrm{Im}\langle r_0(\lambda_j + i0)b_{0j}, b_{0j}\rangle + o(\|b_{j0}\|^2). \tag{8}$$

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:

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

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. $C_D\|b_{0j}\|\|b_{0k}\| \ll |\lambda_2 - \lambda_1|$ 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

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

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

$$h_1 = \begin{pmatrix} h_0 & b_{01} \\ \langle\,\cdot\,, b_{01}\rangle & \lambda_1 \end{pmatrix} \quad \text{and} \quad h_2 = \begin{pmatrix} h_0 & b_{02} \\ \langle\,\cdot\,, b_{02}\rangle & \lambda_2 \end{pmatrix} \tag{11}$$

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

$$c_D^{(1)}\|b_{01}\|^2 \leq \Gamma_R^{(1)}/2 \leq \tilde{C}_D^{(1)}\|b_{01}\|^2 \quad \text{and} \quad c_D^{(2)}\|b_{02}\|^2 \leq \Gamma_R^{(2)}/2 \leq \tilde{C}_D^{(2)}\|b_{02}\|^2.$$

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

$$C_D\|b_{02}\|^2 \ll c_D^{(1)}\|b_{01}\|^2. \tag{12}$$

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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.

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

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

$$C_{\mathcal{D}}\|b_{01}\| < 1 \qquad (14)$$

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

$$|\lambda_1 - \lambda_2 - \beta_{11} + \beta_{22}|^2 \approx |\lambda_1 - \lambda_2 - \beta_{11}|^2 \geq [\operatorname{Im}\beta_{11}(z)]^2 \approx$$

$$\approx [\operatorname{Im}\beta_{11}(\lambda_1 + i0)]^2 \approx \left(\frac{\Gamma_R^{(1)}}{2}\right)^2 \geq \left(c_{\mathcal{D}}^{(1)}\right)^2 \|b_{01}\|^4. \qquad (15)$$

At the same time,

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

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

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

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

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

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

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

Now, using the expression $\sqrt{1 + \varepsilon} = 1 + \frac{\varepsilon}{2} + O(\varepsilon^2)$ 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

$$z = \frac{\lambda_1 + \lambda_2 - \beta_{11} - \beta_{22}}{2} \pm$$

$$\pm \frac{\lambda_1 - \lambda_2 - \beta_{11} + \beta_{22}}{2}\left[1 + \frac{2(b_{12} - \beta_{12})(\bar{b}_{12} - \beta_{21})}{(\lambda_1 + \lambda_2 - \beta_{11} - \beta_{22})^2} + O(\varepsilon^2)\right] \qquad (19)$$

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

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

and

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

(20)

Due to (13) and (18) we have

$$\frac{|b_{12}|^2}{|\lambda_1 - \lambda_2 - \beta_{11}(\lambda_1 \pm i0)|} \leq 2 \cdot \frac{|b_{12}|^2}{\Gamma_R^{(1)}} \sim 2 \cdot \frac{\|b_{02}\|^2}{\Gamma_R^{(1)}} \leq \frac{\Gamma_R^{(2)}}{c_D^{(2)}\Gamma_R^{(1)}} =$$

$$= \Gamma_R^{(1)} \cdot \frac{\Gamma_R^{(2)}}{c_D^{(2)}\left(\Gamma_R^{(1)}\right)^2} \ll \Gamma_R^{(1)}.$$

Therefore, the resonances $z_{\text{nucl}}^{(\pm)}$ are only weakly perturbed initial "nuclear" resonances $z_1^{(\pm)}$ with practically the same width $\Gamma_R^{(1)}$. In a contrast to $z_{\text{nucl}}^{(\pm)}$, a difference between widths of the resonances $z_{\text{mol}}^{(\pm)}$ 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 $z_1^{(\pm)}$,

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

and, in accordance with (20),

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

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

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

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

$$\Gamma_R^{(m)} \sim \frac{\|b_{02}\|^2}{\Gamma_R^{(1)}} \sim \Gamma_R^{(2)} \cdot \frac{1/c_D^{(2)}}{\Gamma_R^{(1)}} \gg \Gamma_R^{(2)}.$$

(21)

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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 $\Gamma_R^{(1)}$, $\Gamma_R^{(1)} \ll 1/c_D^{(2)}$, 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 $c_D^{(2)}$ 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 [12]

$$r_0^c(X, X', z) = \sum_A \int_{\mathbb{R}^{n_A}} dp_A \, \frac{U_A(X, p_A)\overline{U}_A(X', p_A)}{E_A + p_A^2 - z}$$

where X, X' stand for points of $\mathbb{R}^n$ and A, for multi-indices (see Ref. [12], §§2–4 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 $c_D^{(2)}$

$$c_D^{(2)} \sim \text{Im}\langle r_0^c(\lambda_2 + i0)\hat{b}_{02}, \hat{b}_{02}\rangle =$$

$$= \sum_{A:\, E_A < \lambda_2} \pi \, [\lambda_2 - E_A]^{(n_A - 2)/2} \int_{S^{n_A - 1}} d\hat{p}_A \, |\langle \hat{b}_{02}, U_A(\sqrt{\lambda_2 - E_A}\hat{p}_A)\rangle|^2$$

where $S^{n_A - 1}$ stands for the unit sphere in $\mathbb{R}^{n_A}$, $\hat{p}_A \in S^{n_A - 1}$.

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

$$h = \begin{pmatrix} h_1 & b \\ \langle \cdot, b \rangle & \lambda_2 \end{pmatrix} \tag{22}$$

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),

$$z = \lambda_2 - \beta(z) \tag{23}$$

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

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

with a holomorphic function $\beta^{\text{reg}}(z)$. 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 (42)]. 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 IV B.

Analogously to a, we represent the regular term $\beta^{\text{reg}}(z)$ as $\beta^{\text{reg}}(z) = \|b\|^2 f(z)$ with a factor $f(z)$ depending only on $\hat{b}$. We shall suppose the vector $\dot{b}$ to be such that, in a sufficiently wide domain $\mathcal{D}$ about λ_2 concerned, in

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[†]More precisely, two resonances. Since the Hamiltonian h_1 is a self-adjoint operator its resolvent obeys in the physical sheet the symmetry condition $[r_1(z)]^* = r_1(\bar{z})$. 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 $\bar{z}_1$ is also a resonance with the same multiplicity (but maybe in another sheet).

the unphysical sheet, the function $f(z)$ is bounded, $C_{\mathcal{D}} = \sup\limits_{z \in \mathcal{D}} |f(z)| < \infty$, and $c_{\mathcal{D}} = \inf\limits_{z \in \mathcal{D}} |\operatorname{Im} f(z)| > 0$. Therefore $|\beta^{\text{reg}}(z)| \leq C_{\mathcal{D}}\|b\|^2$ and $c_{\mathcal{D}}\|b\|^2 \leq |\operatorname{Im} \beta^{\text{reg}}(z)| \leq \tilde{C}_{\mathcal{D}}\|b\|^2$ where $\tilde{C}_{\mathcal{D}} = \sup\limits_{z \in \mathcal{D}} |\operatorname{Im} f(z)|$, $\tilde{C}_{\mathcal{D}} \leq C_{\mathcal{D}}$.

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

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

with "solutions"

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

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

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

This means

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

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

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

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

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_{nucl} and z_{mol} of the equation (23) with leading terms given by

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

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

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_{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 $z_{\text{mol}} = E_R^{(m)} - i\dfrac{\Gamma_R^{(m)}}{2}$ 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 real 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

$$H = h_0 + v_1 + v_2 \qquad (33)$$

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 φ_1^{res} [see below formula (42)] 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, $H' = \{P_i H P_j\}$, $i, j = 0, 1, 2$, corresponding to the decomposition $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2$. The operator H' (and,

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[‡]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.

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 $b_{0j} = P_0 H\psi_j$. The 00-component of the matrix (1) stays the same, $P_0 H P_0$, as in H'. Unfortunately, the separation described of the resonance channels is approximate and resolvent of the operator $P_0 H P_0$ 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 motivated by the Faddeev method [11], [12].

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 [11], [12]) on its "physical" invariant subspace (see Ref. [17] and Refs. cited therein).

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

$$H_F = \begin{pmatrix} h_0 + v_1 & v_1 \\ v_2 & h_0 + v_2 \end{pmatrix} = \begin{pmatrix} h_1 & v_1 \\ v_2 & h_2 \end{pmatrix} \qquad (34)$$

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. [18] and [19].

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

$$(H_F - z)^{-1} = (h_0 - z)^{-1}\mathbf{I} - (h_0 - z)^{-1}\begin{pmatrix} v_1 & v_1 \\ v_2 & v_2 \end{pmatrix}(H - z)^{-1} \qquad (35)$$

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 [17]) 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 such a pole as well for the resolvent $(H_F - z)^{-1}$. An inverse statement is also valid if the resonance is not a pole of respective continuation of the resolvent kernel $(h_0 - z)^{-1}$.

Let Q_2 be the projector on a subspace of $\mathcal{H}_2$ orthogonal to the "molecular" eigenfunction φ_2, $Q_2 = I - \varphi_2 \langle \cdot, \varphi_2 \rangle$. A separation of contributions to h_2 from the eigenvalue λ_2 and the rest spectrum allows us to rewrite the Hamiltonian (34) in the form very closed to the model (22). Namely, we rewrite this Hamiltonian as the matrix operator

$$H'_F = \begin{pmatrix} \tilde{H}_F & \mathbf{b}_{12} \\ \langle \cdot, \mathbf{b}_{21} \rangle & \lambda_2 \end{pmatrix} \tag{36}$$

considered in the Hilbert space $\tilde{\mathcal{H}} \oplus \mathbb{C}$ where $\tilde{\mathcal{H}} = \mathcal{H}_1 \oplus Q_2\mathcal{H}_2$. By $\tilde{H}_F$ we understand the operator in $\tilde{\mathcal{H}}$ defined as

$$\tilde{H}_F = \begin{pmatrix} h_1 & v_1 Q_2 \\ Q_2 v_2 & \tilde{h}_2 \end{pmatrix}$$

where $\tilde{h}_2$ stands for a part of the Hamiltonian h_2 in $Q_2\mathcal{H}_2$. The vectors $\mathbf{b}_{12}$ and $\mathbf{b}_{21}$ of the space $\tilde{\mathcal{H}}$ determining a coupling between the channels in (36), look as $\mathbf{b}_{12} = \begin{pmatrix} b_{12} \\ 0 \end{pmatrix}$ with $b_{12} = v_1\varphi_2$, $b_{12} \in \mathcal{H}_1$, and $\mathbf{b}_{21} = \begin{pmatrix} b_{21} \\ 0 \end{pmatrix}$ with $b_{21} = v_2\varphi_2$, $b_{21} \in \mathcal{H}_1$.

The resolvent $(H'_F - z)^{-1}$ of the reduced Faddeev operator H'_F may be written as

$$(H'_F - z)^{-1} = \begin{pmatrix} \tilde{R}_F(z) + \dfrac{\tilde{R}_F(z)\mathbf{b}_{12}\langle \tilde{R}_F(z)\cdot, \mathbf{b}_{21} \rangle}{D(z)} & -\dfrac{\tilde{R}_F(z)\mathbf{b}_{12}}{D(z)} \\ -\dfrac{\langle \tilde{R}_F(z)\cdot, \mathbf{b}_{21} \rangle}{D(z)} & \dfrac{1}{D(z)} \end{pmatrix} \tag{37}$$

where $\tilde{R}_F(z)$ stands for the resolvent of the Hamiltonian $\tilde{H}_F$, $\tilde{R}_F(z) = (\tilde{H}_F - z)^{-1}$, and $D(z)$, for the scalar function

$$D(z) = \lambda_2 - z - \tilde{\beta}(z) \tag{38}$$

with

$$\tilde{\beta}(z) = \langle \tilde{R}_F(z)\mathbf{b}_{12}, \mathbf{b}_{21} \rangle \equiv \langle g_1(z)b_{12}, b_{21} \rangle. \tag{39}$$

Here, $g_1(z)$ is a generalized resolvent of the operator $\tilde{H}_F$,

$$g_1(z) = (h_1 - z - v_1 Q_2 \tilde{r}_2(z) Q_2 v_2)^{-1} \tag{40}$$

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where $\tilde{r}_2(z) = (\tilde{h}_2 - z)^{-1}$.

Since the expression (36) represents an unitary equivalent form of the Faddeev operator H_F, singularities of the resolvent $(H'_F - z)^{-1}$ in the physical sheet have to coincide with those of $(H_F - z)^{-1}$, being located in the spectra of the Hamiltonians h_0 and/or H, i. e. in the real axis only. This is an advantage of the representation (37), in a contrast to the formula (35), to manifest explicitly that a perturbation of the molecular eigenvalue λ_2, in a presence of the nuclear channels, may be computed solving the equation $D(z) = 0$, or equivalent, the equation

$$z = \lambda_2 - \tilde{\beta}(z). \qquad (41)$$

According to the formulae (37) and (38), the roots of the latter turn out automatically to be poles of the resolvent $(H_F - z)^{-1}$. Hence, such roots in the physical sheet may exist in the real axis only. Searching for the roots of the equation continued in unphysical sheet(s), one can find, among them, resonance(s) engendered by the initial molecular eigenvalue λ_2.

B. Perturbation of the nuclear resonance due to a continuous spectrum component of the molecular Hamiltonian

Evidently, an analysis of the equation (41) in the case of "small" coupling vectors b_{12} and/or b_{21} may be carried out in the same way as the analysis of the analogous equation (23) in the previous section. And, if there exists a pole of $\tilde{\beta}(z)$ having a real part closed to λ_2, the effect of the inversely proportional growth of the "molecular" width as the "nuclear" width decreases, will appear again. We have a candidate for such a pole, the initial "pure nuclear" resonance z_1 which is, of course, perturbed due to the presence in $\tilde{H}_F$ of the extra channel with $\tilde{h}_2$. Now we will formulate certain sufficient conditions when such a perturbation of z_1 is small as compared to $\Gamma_R^{(1)}$. It should be noted that in real molecular systems such a property is very natural from physical reasons.

First we remind that the eigenvalue λ_2 is situated below the threshold E_0. Therefore, we consider analytic continuation of the resolvent kernel(s) $(H'_F - z)^{-1}$ and, thereby, the form $\tilde{\beta}(z)$ on unphysical sheet[§] neighboring below E_0 with the physical one in a vicinity of the point λ_2. The energy E_0 is, at the same time, a lower boundary of the continuous spectrum of h_2 and, thereby, of $\tilde{h}_2$. This means that the resolvent $\tilde{r}_2(z)$, included in (40), will stay during such a continuation in the physical sheet. Of course a domain $\mathcal{D}$ about λ_2 where the continuation is provided in the unphysical sheet concerned, will

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[§]In definitions of Ref. [16] for a three-body problem, this one is called a *two-body* sheet.

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be chosen to be "sufficiently small", with a diameter of order of $\Gamma_R^{(1)}$ and, to be separated from the ray $[E_0, +\infty)$.

Let us suppose that the analytic continuation of the resolvent kernel $r_1(z)$ in a vicinity of the resonance pole z_1 admits the representation with explicitly factorized residue,

$$r_1(z) = \frac{A\varphi_1^{\text{res}}\langle\,\cdot\,,\tilde{\varphi}_1^{\text{res}}\rangle}{z_1 - z} + \tilde{r}_1(z). \tag{42}$$

Here, the (generalized) eigenvectors (the so-called Gamow states) φ_1^{res} and $\tilde{\varphi}_1^{\text{res}}$ of the Hamiltonian h_1 are assumed to be specific (including in the coordinate representation only outgoing waves with exponentially increasing asymptotics) solutions of the Schrödinger equation $h_1\psi_1 = z\psi_1$, respectively at $z = z_1$ and $z = \bar{z}_1$. A complex number A is a "normalization" constant. The term $\tilde{r}_1(z)$ represents a regular at $z = z_1$ summand of r_1. Surely, as the resolvent kernel $r_1(z)$ itself, the terms of the representation (42) have to be understood in the unphysical sheet in a sense of the generalized functions (distributions) like e. g., in Ref. [16]. This means in particular that only sufficiently "good" elements (e. g., sufficiently quickly decreasing test functions in the coordinate representation) forming a dense subset $\mathcal{H}_1^{(0)}$ in $\mathcal{H}_1$, can be substituted instead of "$\cdot$" into the products $\langle\,\cdot\,,\varphi_1^{\text{res}}\rangle$ and $\langle\,\cdot\,,\tilde{\varphi}_1^{\text{res}}\rangle$.

The near-resonance representation of the Green function (42) is approved in the two-body problems e. g., in framework of the Jost formalism [20]. A possibility of such a representation in the three-body problems follows from the results of Ref. [16], at least in the case of the quickly decreasing, in the x-space, interactions and thereby, in the cases where one can cut the Coulombic potentials between nuclear constituents, say, at molecular distances.

As in Section III we assume that the resonance z_1 is a kind of a discrete spectrum eigenvalue going from the real axis. So that, a limit procedure is as if possible where $\Gamma_R^{(1)} \to 0$ and the Gamow states φ_1^{res} and $\tilde{\varphi}_1^{\text{res}}$ turn (in the weak sense) into a "normal" eigenfunction φ_1 (the same for both of them), i. e. for any $f \in \mathcal{H}_1^{(0)}$

$$\langle\varphi_1^{\text{res}}, f\rangle \longrightarrow \langle\varphi_1, f\rangle, \quad \langle\tilde{\varphi}_1^{\text{res}}, f\rangle \longrightarrow \langle\varphi_1, f\rangle \quad \text{and} \quad A \longrightarrow 1/\|\varphi_1\|^2 \tag{43}$$

as $\Gamma_R^{(1)} \to 0$.

Let the strong, v_1 and molecular, v_2, potentials be such that the product

$$w_{12}(z) \equiv v_1 Q_2 \tilde{r}_2(z) Q_2 v_2$$

is an uniformly bounded operator-valued function of $z \in \mathcal{D}$ with a finite and rather small norm

$$\|w_{12}\|_{\mathcal{D}} = \sup_{z \in \mathcal{D}} \|v_1 Q_2 \tilde{r}_2(z) Q_2 v_2\|.$$

At the same time, let the width $\Gamma_R^{(1)}$ satisfy the condition

$$\Gamma_R^{(1)} \ll E_R^{(1)} - E_1' \tag{44}$$

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where E_1' is the nearest from below (may be, differing from E_1) threshold of the continuous spectrum of h_1 (just such a situation is expected to take place in a real molecule). Then one can assume that a kernel of the normalized product $\hat{w}_{12}(z) = \dfrac{w_{12}(z)}{\|w_{12}\|}$ falls off in coordinate space as quickly that it may be applied, in condition (44), to $\varphi_1^{\mathbf{res}}$, $\tilde{\varphi}_1^{\mathbf{res}}$ and $\tilde{r}_1(z)$, so that, in particular, $\hat{w}_{12}(z)\varphi_1^{\mathbf{res}} \in \mathcal{H}_1^{(0)}$ and $\hat{w}_{12}^*(z)\tilde{\varphi}_1^{\mathbf{res}} \in \mathcal{H}_1^{(0)}$. One can assume, moreover, that the matrix element $\langle \hat{w}_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{\varphi}_1^{\mathbf{res}} \rangle$ makes a sense for $z \in \mathcal{D}$ as well as the cross products $\langle \hat{w}_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{r}_1(z) \cdot \rangle$, $\langle \hat{w}_{12}(z)\tilde{r}_1(z) \cdot, \tilde{\varphi}_1^{\mathbf{res}} \rangle$ and $\langle \hat{w}_{12}(z)\tilde{r}_1(z) \cdot, \tilde{r}_1(z) \cdot \rangle$ where one has to substitute, instead of "$\cdot$", the elements of a dense subset $\mathcal{H}_1^{(0)}$ mentioned above. We suppose further that the value of $\|w_{12}\|_{\mathcal{D}}$ is as small that, for a fixed $\hat{w}_{12}(z)$, the following estimate takes place

$$\sup_{z \in \mathcal{D}} |A\langle w_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{\varphi}_1^{\mathbf{res}} \rangle| \leq \|w_{12}\|_{\mathcal{D}} \cdot \sup_{z \in \mathcal{D}} |A\langle \hat{w}_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{\varphi}_1^{\mathbf{res}} \rangle| \ll \Gamma_R^{(1)}. \quad (45)$$

With these presuppositions one can prove already that a shift of the initial "nuclear" resonance z_1 due to a presence of the $\tilde{h}_2$ channel in $\tilde{H}_F$ is indeed very small as compared to the width $\Gamma_R^{(1)}$. To show this, we consider the Lippmann-Schwinger equation for the generalized resolvent $g_1(z)$,

$$g_1(z) = r_1(z) - r_1(z)w_{12}(z)g_1(z).$$

In the conditions above this equation may be continued in the domain $\mathcal{D}$ of the unphysical sheet concerned. To give an "explicit" representation for $g_1(z)$, we shall use a solution $\tilde{r}_1'(z)$ of another Lippmman-Schwinger equation in the same unphysical sheet,

$$\tilde{r}_1'(z) = \tilde{r}_1(z) - \tilde{r}_1(z)w_{12}(z)\tilde{r}_1'(z). \quad (46)$$

With a fixed $\hat{w}_{12}(z)$ and sufficiently small $\|w_{12}\|_{\mathcal{D}}$, the unique solvability of the last equation may be easily proved for $z \in \mathcal{D}$. One can show in fact that the solution of (46) belongs to a class of kernels satisfying the same conditions concerning the cross products with $w_{12}(z)$ as $\tilde{r}_1(z)$.

Then, representing the resolvent $r_1(z)$ in the form (42) one finds immediately that the generalized resolvent $g_1(z)$ looks as

$$g_1(z) = A\frac{[I - \tilde{r}_1'(z)w_{12}(z)]\varphi_1^{\mathbf{res}}\langle \cdot, \tilde{\varphi}_1^{\mathbf{res}} \rangle[I - w_{12}(z)\tilde{r}_1'(z)]}{F_1(z)} + \tilde{r}_1'(z) \quad (47)$$

with

$$F_1(z) = z_1 - z + A\langle w_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{\varphi}_1^{\mathbf{res}} \rangle + A\langle w_{12}(z)\tilde{r}_1'(z)w_{12}(z)\varphi_1^{\mathbf{res}}, \tilde{\varphi}_1^{\mathbf{res}} \rangle \quad (48)$$

It follows from the expression (47) that the initial nuclear resonance z_1 transforms into a solution z of the equation

$$F_1(z) = 0. \quad (49)$$

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Thus, due to (48), the resonance $\tilde{z}_1$ generated, instead of h_1, by the Hamiltonian $\tilde{H}_F$, has the following asymptotics (as $\|w_{12}\|_\mathcal{D} \to 0$):

$$\tilde{z}_1 = z_1 + A\langle w_{12}(z_1)\varphi_1^{\mathrm{res}}, \tilde{\varphi}_1^{\mathrm{res}}\rangle + O(\|w_{12}\|_\mathcal{D}^2),$$

and, thereby, according to the supposition (45) the perturbation of z_1 due to $\tilde{h}_2$ is small indeed,

$$|\tilde{z}_1 - z_1| \ll \Gamma_R^{(1)}.$$

C. Interplay between molecular and nuclear widths

Let us return now to the equation (41). Additional assumptions are accepted here that the nuclear, v_1, and molecular, v_2, potentials and the "molecular" eigenfunction φ_2 are such that the products $\langle b_{12}, \tilde{\varphi}_1^{\mathrm{res}}\rangle$ and $\langle \varphi_1^{\mathrm{res}}, b_{21}\rangle$ make a sense (i. e. the both functions b_{12} and b_{21} are elements of the dense subset $\mathcal{H}_1^{(0)}$ above) as well as the products $\langle w_{12}(z)\tilde{r}_1'(z)b_{12}, \tilde{\varphi}_1^{\mathrm{res}}\rangle$ and $\langle \tilde{r}_1'(z)w_{12}(z)\varphi_1^{\mathrm{res}}, b_{21}\rangle$, $z \in \mathcal{D}$. Then one can obviously rewrite the function $\tilde{\beta}(z)$ for $z \in \mathcal{D}$ exactly as (23),

$$\tilde{\beta}(z) = \frac{\tilde{a}}{z - \tilde{z}_1} + \tilde{\beta}^{\mathrm{reg}}(z).$$

Here, $\tilde{a}$ stands for a residue of this function at the pole $z = \tilde{z}_1$ and $\tilde{\beta}^{\mathrm{reg}}(z)$, for a regular part. Therefore, the equation (41) may be rewritten as (26), i. e.

$$z = \frac{\lambda_2 + \tilde{z}_1 - \tilde{\beta}^{\mathrm{reg}}}{2} \pm \sqrt{\left(\frac{\lambda_2 - \tilde{z}_1 - \tilde{\beta}^{\mathrm{reg}}}{2}\right)^2 - \tilde{a}}. \tag{50}$$

It follows from the representation (47) that for a given (and fixed) "structure functions" $\hat{w}_{12}(z)$, $\hat{b}_{12} = \dfrac{b_{12}}{\|b_{12}\|}$ and $\hat{b}_{21} = \dfrac{b_{21}}{\|b_{21}\|}$ the following asymptotical formulae keep true for $\tilde{a}$ and $\tilde{\beta}^{\mathrm{reg}}$ as $\|w_{12}\|_\mathcal{D} \to 0$:

$$\tilde{a} = a + O(\|w_{12}\|_\mathcal{D}\|b_{12}\|\|b_{21}\|), \quad \tilde{\beta}^{\mathrm{reg}}(z) = \beta^{\mathrm{reg}}(z) + O(\|w_{12}\|_\mathcal{D}\|b_{12}\|\|b_{21}\|) \tag{51}$$

where $a = -A\langle b_{12}, \tilde{\varphi}_1^{\mathrm{res}}\rangle\langle \varphi_1^{\mathrm{res}}, b_{21}\rangle$ and $\beta^{\mathrm{reg}}(z) = \langle \tilde{r}_1(z)b_{12}, b_{21}\rangle$.

We suppose that at least the function $b_{12} = v_1\varphi_2$ is so small[**] that

$$|\tilde{\beta}^{\mathrm{reg}}(z)| \approx |\langle \tilde{r}_1(z)b_{12}, b_{21}\rangle| \le C_\mathcal{D} \cdot \|b_{12}\| \cdot \|b_{21}\| \ll \Gamma_R^{(1)},$$

[**]Due to internuclear Coulombic barrier suppressing the molecular eigenfunction at nuclear distances

$$|\tilde{a}| \approx |a| = C_a \cdot \|\hat{b}_{12}\| \cdot \|\hat{b}_{21}\| \ll \left(\Gamma_R^{(1)}\right)^2. \tag{52}$$

Notations $C_\mathcal{D}$ and C_a make now the following sense:

$$C_\mathcal{D} = \sup_{z \in \mathcal{D}} |\langle \tilde{r}_1(z)\hat{b}_{12}, \hat{b}_{21}\rangle|, \quad C_a = |A| \cdot |\langle \hat{b}_{12}, \tilde{\varphi}_1^{\mathrm{res}}\rangle\langle \varphi_1^{\mathrm{res}}, \hat{b}_{21}\rangle|.$$

Repeating almost literally a discussion of the equations (26) in Section III we show that the equations (50) have only two solutions in the domain $\mathcal{D}$, z_{nucl} in the case of sign "−" and z_{mol} in the case of sign "+", leading terms of which are given by formulae (29) and (30).

If the molecular energy λ_2 "almost" coincides with the real part $E_R^{(1)}$ of the nuclear resonance z_1, $|E_R^{(1)} - \lambda_2| \ll \Gamma_R^{(1)}$, one gets

$$z_{\mathrm{nucl}} \cong z_1 - i\frac{2a}{\Gamma_R^{(1)}},$$

$$z_{\mathrm{mol}} \cong \lambda_2 + i\frac{2a}{\Gamma_R^{(1)}}. \tag{53}$$

It is evident that the pole z_{nucl}, being a weak [since, in view of (52), $|a|/\Gamma_R^{(1)} \ll \Gamma_R^{(1)}$] perturbation of the resonance z_1, belongs to the unphysical sheet concerned. Analogous assertion for the molecular resonance z_{mol} follows, in principle, from the statement above that the equation (41) can have at $\mathrm{Im}\, z > 0$ no solutions in the physical sheet. However, at least for small $\Gamma_R^{(1)}$, one can immediately check the inequality $\mathrm{Re}\, a < 0$ holds true guaranteeing a location of the resonance z_{mol} in the unphysical sheet. Indeed, we note that

$$\langle \varphi_1^{\mathrm{res}}, v_2\varphi_2\rangle = -\langle \varphi_1^{\mathrm{res}}, (h_0 - \lambda_2)\varphi_2\rangle =$$
$$= -\langle (h_0 - z_1)\varphi_1^{\mathrm{res}}, \varphi_2\rangle + (\lambda_2 - z_1)\langle \varphi_1^{\mathrm{res}}, \varphi_2\rangle =$$
$$= \langle v_1\varphi_1^{\mathrm{res}}, \varphi_2\rangle + (\lambda_2 - z_1)\langle v_1\varphi_1^{\mathrm{res}}, \varphi_2\rangle.$$

Therefore,

$$a = -A\langle v_1\varphi_2, \tilde{\varphi}_1^{\mathrm{res}}\rangle\langle \varphi_1^{\mathrm{res}}, v_1\varphi_2\rangle + A(z_1 - \lambda_2)\langle \varphi_2, v_1\tilde{\varphi}_1^{\mathrm{res}}\rangle\langle \varphi_1^{\mathrm{res}}, \varphi_2\rangle.$$

Remind, we suppose the nuclear resonance z_1 to be such that a limit procedure (43) is possible. This means

$$a \underset{\Gamma_R^{(1)} \to 0}{=} -\frac{|\langle \varphi_1, v_1\varphi_2\rangle|^2}{\|\varphi_1\|^2} + o(1) + i\frac{\Gamma_R^{(1)}}{2}\left(\frac{\langle v_1\varphi_2, \varphi_1\rangle\langle \varphi_1, \varphi_2\rangle}{\|\varphi_1\|^2} + o(1)\right) \tag{54}$$

So that

$$\mathrm{Re}\, a = -\frac{|\langle \varphi_1, v_1\varphi_2\rangle|^2}{\|\varphi_1\|^2} + o(1)$$

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is really negative, at least for sufficiently small widths $\Gamma_R^{(1)}$. (Of course, we exclude here the cases of an incidental degeneration where $\langle \varphi_1, v_1 \varphi_2 \rangle = 0$.) So that, according to (53), the width $\Gamma_R^{(m)}$ of the resonance z_{mol} depends on $\Gamma_R^{(1)}$ as $\Gamma_R^{(1)} \to 0$ exactly as (31), $\Gamma_R^{(m)} \cong 4 \dfrac{|\operatorname{Re} a|}{\Gamma_R^{(1)}}$.

To complete discussion of the equation (41), let us compare the behavior of $\Gamma_R^{(m)}$ in the presence of the nuclear near-threshold resonance z_1 with an opposite case where such a resonance is absent and, thus, the function $\tilde{\beta}(z)$, $\tilde{\beta}(z) \equiv \tilde{\beta}^{\text{res}}(z)$, is holomorphic in $\mathcal{D}$. In this case, the equation (41) has in $\mathcal{D}$ only one solution $z_R^{(2)}$, leading terms of which are given with account of second formula (51) by

$$z_R^{(2)} \cong \lambda_2 - \langle r_1(\lambda_2 + i0)b_{12}, b_{21} \rangle = \lambda_2 - \langle r_1(\lambda_2 + i0)v_1\varphi_2, v_2\varphi_2 \rangle.$$

Since $v_2\varphi_2 = -(h_2 - \lambda_2)\varphi_2$, one finds

$$z_R^{(2)} \cong \lambda_2 + \langle v_1\varphi_2, \varphi_2 \rangle - \langle r_1(\lambda_2 + i0)v_1\varphi_2, v_1\varphi_2 \rangle.$$

Therefore, the width $\Gamma_R^{(2)}$ of the resonance $z_R^{(2)}$ is given by

$$\Gamma_R^{(2)} \cong 2 \operatorname{Im} \langle r_1(\lambda_2 + i0)v_1\varphi_2, v_1\varphi_2 \rangle.$$

This means that one has, in presence of the nuclear resonance z_1, to compare the width $\Gamma_R^{(m)}$ with the value $|\operatorname{Im} \tilde{\beta}^{\text{res}}(\lambda_2 + i0)| \approx |\operatorname{Im} \langle \tilde{r}_1(\lambda_2 + i0)v_1\varphi_2, v_1\varphi_2 \rangle| \geq c_{\mathcal{D}}' \|b_{12}\|^2$ where $c_{\mathcal{D}}' = \inf_{z \in \mathcal{D}} |\langle \tilde{r}_1(z)\hat{b}_{12}, \hat{b}_{12} \rangle|$. As a result we come to (a rough) estimation like (32),

$$\Gamma_R^{(m)} \sim \Gamma_R^{(2)} \cdot \frac{C_a'/c_{\mathcal{D}}'}{\Gamma_R^{(1)}}. \tag{55}$$

with

$$C_a' = \frac{1}{\|b_{12}\|^2} |A\langle v_1\varphi_2, \tilde{\varphi}_1^{\text{res}} \rangle \langle \varphi_1^{\text{res}}, v_1\varphi_2 \rangle| \underset{\Gamma_R^{(1)} \to 0}{\cong} \frac{|\langle \hat{b}_{12}, \varphi_1 \rangle|^2}{\|\varphi_1\|^2}.$$

Again, as in Sections II and III we find that if the nuclear resonance is narrow, $\Gamma_R^{(1)} \ll C_a'/c_{\mathcal{D}}'$ then a large increasing of the molecular width, proportional just to the factor $\dfrac{C_a'/c_{\mathcal{D}}'}{\Gamma_R^{(1)}}$, has to be observed. In other words, the nuclear fusion reaction in the molecule concerned is considerably enhanced.

Note in a conclusion that the formulae (53) and (54) may be used for a practical estimation of the width $\Gamma_R^{(m)}$. Here, a crucial role belongs to the values "$\varphi(0)$" (cf. the Jackson formula [21]) of the molecular function φ_2 at small (nuclear) distances where the strong interaction v_1 is localized in configuration space. Surely, such estimations for concrete molecules require numerical computations.

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V. EXPONENTIAL DECAY OF THE MOLECULAR STATE

In Section IV, we have accepted a description of the nuclear subsystem of a molecule by a (realistic) effective Hamiltonian (33). Let us suppose now that an initial state of the molecule corresponds exactly to the pure "molecular" wave function φ_2, $(h_2 - \lambda_2)\varphi_2 = 0$, $\|\varphi_2\| = 1$. Then, a consequent evolution (in time t) of the nuclear subsystem is described by a solution $\Psi(t)$ of the Cauchy problem

$$i\frac{d\Psi}{dt} = H\Psi, \qquad \Psi\big|_{t=0} = \varphi_2.$$

Probability $P_{\text{mol}}(t)$ at a time moment t to find the subsystem still in the molecular state φ_2 is given by

$$P_{\text{mol}}(t) = |\langle \Psi(t), \varphi_2 \rangle|^2.$$

Since $\lambda_2 < E_0$ and, thereby, the continuous spectrum channel of the "molecular" Hamiltonian h_2 is closed down, the remainder $1 - P_{\text{mol}}(t)$ determines a decay probability of the state φ_2 into open channels (branches) of continuous spectrum of the nuclear Hamiltonian h_1. The latter correspond to all possible variants of synthesis of the nuclear constituents or/and their rearrangement at energies below E_0.

It is easy to check that

$$\Psi(t) = U_1^{(1)}(t) + U_1^{(2)}(t) + \varphi_2 \cdot u_2(t)$$

where $U_1^{(1)} \in \mathcal{H}_1$, $U_1^{(2)} \in Q_2\mathcal{H}_2$ and $u_2 \in \mathbb{C}$ stand for components of solution $U = \begin{pmatrix} U_1^{(1)} \\ U_1^{(2)} \\ u_2 \end{pmatrix}$, $U \in \tilde{\mathcal{H}}$, of the evolutionary problem

$$i\frac{dU}{dt} = H'_F U,$$
$$U_1^{(1)}\big|_{t=0} = U_1^{(2)}\big|_{t=0} = 0, \quad u_2\big|_{t=0} = 1 \tag{56}$$

corresponding to the Faddeev operator H'_F. Therefore, to estimate the product

$$\langle \Psi(t), \varphi_2 \rangle = \langle U_1^{(1)}(t), \varphi_2 \rangle + u_2(t),$$

determining the probability $P_{\text{mol}}(t)$, we use the standard integral representation of function of operator via its resolvent. In the case considered we represent the evolution operator for the problem (56) in terms of the resolvent $(H'_F - z)^{-1}$,

$$\exp\{-iH'_F t\} = \frac{1}{2\pi i} \oint_\gamma dz\, e^{-izt}(H'_F - z)^{-1}. \tag{57}$$

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Integration in (57) is provided along a contour γ going clockwise in the physical sheet around spectrum of the Faddeev operator $\tilde{H}'_F$. Remember, this spectrum is real, being a union of the Hamiltonians h_0 and H spectra. With account of (37) and (57) one finds

$$\langle \Psi(t), \varphi_2 \rangle = \frac{1}{2\pi i} \oint_\gamma dz\, e^{-izt}\, \frac{1 - \langle g_1(z)b_{12}, \varphi_2 \rangle}{\lambda_2 - z - \langle g_1(z)b_{12}, b_{21} \rangle}. \tag{58}$$

In the physical sheet, norm of the generalized resolvent $g_1(z)$ allows the estimate $\|g_1(z)\| \leq \mathrm{dist}^{-1}(z, \sigma(\tilde{H}_F))$ where $\sigma(\tilde{H}_F)$ stands for spectrum of $\tilde{H}_F$. Consequently, at $t = 0$, the integrand in (58) behaves like z^{-1} as $|\mathrm{Im}\,z| \to \infty$. One checks immediately due to this fact that $\langle \Psi(0), \varphi_2 \rangle = 1$.

Concerning properties of $\langle \Psi(t), \varphi_2 \rangle$ for $t > 0$, the following important statements take place.

1. Behavior of the integral (58) for $t > 0$, in the conditions of Section IV, is described by the formula

$$\langle \Psi(t), \varphi_2 \rangle = \exp\{-iz_{\mathrm{mol}}t\} + \varepsilon(t) \tag{59}$$

where term $\varepsilon(t) = O(\|b_{12}\|)$ for all $t > 0$ is small, $|\varepsilon(t)| \ll 1$.

2. If, additionally, the nuclear resonance z_1 is "extremely" narrow, i. e. $\Gamma_R^{(1)} \ll E_0 - \lambda_2$, then a more detailed representation takes place,

$$
\begin{aligned}
\langle \Psi(t), \varphi_2 \rangle = {} & \exp\{-iz_{\mathrm{mol}}t\} \left[1 - \frac{4a}{\left(\Gamma_R^{(1)}\right)^2} + i\frac{2a_0}{\Gamma_R^{(1)}} + O(\|b_{12}\|) \right] + \\
& + \exp\{-iz_{\mathrm{nucl}}t\} \left[\frac{4a}{\left(\Gamma_R^{(1)}\right)^2} - i\frac{2a_0}{\Gamma_R^{(1)}} + O(\|b_{12}\|) \right] + \tilde{\varepsilon}(t)
\end{aligned}
\tag{60}
$$

with $a_0 \equiv A\, \langle \varphi_1^{\mathrm{res}}, \varphi_2 \rangle \langle b_{12}, \tilde{\varphi}_1^{\mathrm{res}} \rangle = A\, \langle \varphi_1^{\mathrm{res}}, \varphi_2 \rangle \langle v_1\varphi_2, \tilde{\varphi}_1^{\mathrm{res}} \rangle$. As in (59), a background term $\tilde{\varepsilon}(t) = O(\|b_{12}\|)$ is small, $|\tilde{\varepsilon}(t)| \ll 1$, for all $t > 0$.

Proof of the formula (59) is carried out via estimating a contribution to the integral (58) from the resonance pole z_{mol} only. The formula (60) explicitly includes also a contribution from the pole z_{nucl}, because, with the condition $\Gamma_R^{(1)} \ll E_0 - \lambda_2$, one finds the background summands are of a more high order of smallness as compared to the contribution above from z_{nucl}. The estimation of the contributions from z_{mol} and z_{nucl} is realized as a result of deforming the contour γ fragments situated in a vicinity of the molecular energy λ_2. A part of γ situated initially in upper rim of the cut, is pulled into the domain $\mathcal{D}$ (see Section IV) of a neighboring unphysical sheet. Having done such a deformation one finds explicitly the residues at $z = z_{\mathrm{mol}}$ and $z = z_{\mathrm{nucl}}$ of the integrand in (58). An analogous deformation of a part of γ, situated initially in the lower rim, is realized in a domain $\mathrm{Im}\,z < 0$ of the physical sheet. In such

a way one shows, for $t > 0$, that the conjugate resonances $\bar{z}_{mol}$ and $\bar{z}_{nucl}$ give to the integral (58) only a very small contribution which is then included into the background terms $\varepsilon(t)$ and $\tilde{\varepsilon}(t)$. At the same time, the summands $\varepsilon(t)$ and $\tilde{\varepsilon}(t)$ include also a contribution to (58) from the discrete spectrum of H (with ignorance of factors oscillating when t changes, a value of this contribution stays practically the same for all t) as well as a contribution (decreasing non-exponentially as $t \to \infty$) from the rest part of the Hamiltonian H continuous spectrum.

The formulae (59) and (60) show explicitly, that, *in a large time interval* $0 \le t < T$, $T \sim \dfrac{2}{\Gamma_R^{(m)}}|\ln\max|\varepsilon(t)||$, *decay of the "molecular" state* φ_2 *in a presence of the narrow pre-threshold nuclear resonance do has an exponential character*[††]. *A rate of this decay is determined mainly by the width* $\Gamma_R^{(m)}$ *of the "molecular" resonance* z_{mol}, *i. e. by a concrete value of the ratio* $|\operatorname{Re}a|/\Gamma_R^{(1)}$:

$$P_{\text{mol}}(t) \cong \exp\{-\Gamma_R^{(m)}t\} \cong \exp\left\{-\frac{4|\operatorname{Re}a|}{\Gamma_R^{(1)}}\,t\right\}. \tag{61}$$

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[††]Surely, a similar statement takes place as well in the case of the model Hamiltonians (1) and (22), generally more simple than Hamiltonian (33). In particular, the two-channel model (22) gives us for $P_{\text{mol}}(t)$ the following value:

$P_{\text{mol}}(t) = \left|\dfrac{1}{2\pi i}\oint_\gamma dz\, e^{-izt}\left[\lambda_2 - z - \langle r_1(z)b, b\rangle\right]^{-1}\right|^2$. Here, the contour γ goes clockwise around spectrum of the operator (22). The function $P_{\text{mol}}(t)$ represents a probability for a time moment t to find a system in the initial "molecular" state described in the model (22) as $\varphi = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The integral included in the expression above for $P_{\text{mol}}(t)$, is quite analogous to (58). One can show in conditions of Section III that all the dependence of the integral on t is described exactly by the formula (59) or by a more detail formula like (60).

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Возмущёние собственного значения, погруженного
в непрерывный спектр, близколежащим резонансом

Рассматриваются квантово-механические системы (в том числе электронные молекулы), гамильтонианы которых позволяют, например, с помощью метода Фаддеева отделять слабосвязанный канал. Ширина (т.е. мнимая часть) резонанса, порождаемого точкой дискретного спектра отделенного канала, исследуется в случае, когда основная компонента гамильтониана также порождает резонанс. Показывается, что если вещественные части этих резонансов совпадают, а связь между каналами достаточно мала, то ширина резонанса, отвечающего выделенному (молекулярному) каналу, обратно пропорциональна ширине резонанса в основном (ядерном) канале. Имея универсальный характер, этот эффект может играть важную роль в увеличении вероятности «холодного синтеза» в молекулах, ядерные подсистемы которых обладают узкими предпороговыми резонансами.

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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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