

PERTURBATION OF A LATTICE SPECTRAL BAND BY A NEARBY RESONANCE

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ABSTRACT. A soluble model of weakly coupled “molecular” and “nuclear” Hamiltonians is studied in order to exhibit explicitly the mechanism leading to the enhancement of fusion probability in case of a narrow near-threshold nuclear resonance. We, further, consider molecular cells of this type being arranged in lattice structures. It is shown that if the real part of the narrow nuclear resonance lies within the molecular band generated by the intercellular interaction, an enhancement, proportional to the inverse width of the nuclear resonance, is to be expected.

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1. INTRODUCTION

Molecules are usually treated as purely Coulombic systems, while the strong interaction between their nuclear constituents is assumed to play a negligible role. However, at least in principle, any Coulombic molecular level lying above the lower threshold of the nuclear subsystem, is embedded in the continuous spectrum of the nuclear sub-Hamiltonian. The coupling between the molecular and nuclear channels, hence, turns this level into a resonance (see, e. g., Refs. [1, 2, 3, 4, 5] and references cited therein). Of course, due to the wide Coulombic barrier between the nuclei and the short-range character of the nuclear interaction, this coupling, and thus the width of the resonance, which determines the fusion probability of the nuclear constituents of the molecule, is in general extremely small.

However, as pointed out in [6, 7], the situation is rather different if the nuclear subsystem of a molecule has a sufficiently narrow near-threshold resonance. Examples of such nuclear systems may be read off from the data presented in [8]. Among them are even customary systems like $pp^{16}\text{O}$ and $p^{17}\text{O}$ [9, 10], i. e., the nuclear constituents of the water molecule H_2O or the hydroxyl ion OH^- with O being the isotope ^{17}O . For LiD and H_2O the influence of near-threshold nuclear resonances on the molecular properties has been studied in [11, 12, 13] by estimating the overlap integrals between the corresponding molecular and nuclear wave functions. The best known example of such phenomena is the muon catalyzed fusion of deuteron and triton in the $dt\mu$ molecule, where the near-threshold nuclear resonance $^5\text{He}(3/2^+)$ plays a decisive role [14].

Being motivated by the above special cases, we deal in this paper with a rather general model Hamiltonian related to the ones considered by Friedrichs in [15]. This Hamiltonian consists of a “nuclear” part, a “molecular” part with eigenvalues embedded in the continuous spectrum of the nuclear part, and a weak coupling term which turns these unperturbed eigenvalues into “molecular” resonances. Since the model is explicitly solvable, the mechanism of formation of the resonances becomes clearly visible.

The following property pointed out in [6, 7] appears, in particular, as a general feature: if the “nuclear” channel itself has a narrow resonance with a position close to the “molecular” energy, then the width (the imaginary part) of the resulting “molecular” resonance is found to be inversely proportional to the “nuclear” width. In other words, a large increase of the decay rate of the “molecular” state, i. e. of the fusion probability, is observed in this case. Such a coincidence of nuclear and molecular energies is, of course, a rather rare phenomenon in nature.

A further goal of the present work is to show that the decay rate may be considerably enhanced when arranging molecular clusters of this type within a crystalline structure. The reason is that in such a configuration the original discrete molecular energy turns into a band, i. e., into a whole interval of the continuous spectrum. (Note that in the models under consideration, the spectral band generated by the “molecular” level is shifted finally, after switching on the coupling between the “nuclear” and “molecular” channels, into the unphysical sheet.) That is, even if the position of the “nuclear” resonance differs from the original “molecular” level, it can get into this band. This allows for a fine tuning by exciting the crystalline structure to energies as close as possible to the energy of the “nuclear” resonance. We show that the lattice states, which correspond to such an initial choice of their quasimomentum distribution, decay exponentially with a rate which is again inversely proportional to the width of the “nuclear” resonance.

Concluding this introduction, we would like to mention the papers [16] and [17] which develop approaches of the direct spectral modelling resembling the one employed in the present work. Paper [16] is devoted, in particular, to the study of a one-electron model of a solid having a cubic crystalline lattice (see Sec. 3.2 in [16]). This model exhibits a mechanism of the formation of gaps in the absolutely continuous spectrum of the total Hamiltonian due to the resonance coupling between the electron and lattice sub-Hamiltonians, while the absolutely continuous spectra of the sub-Hamiltonians do not have the corresponding gaps. The recent e-print [17] discusses a similar effect of formation of gaps in the absolutely continuous spectrum of a self-adjoint operator defined in a Hilbert space associated with a periodically “decorated” periodic graph. The gaps are produced by the resonance interaction between the basic graph and the attached (“decorating”) graphs.

Notice that the phenomena we discuss in the present paper also arise partly due to the resonance coupling between the sub-Hamiltonians. In particular, some resonances and resonance bands are formed of an eigenvalue or spectral band of one of the sub-Hamiltonians embedded into the absolutely continuous spectrum of another sub-Hamiltonian. We refer, however, not to details of the structure of the resulting (real) spectrum of the total Hamiltonian like the spectral gaps of [16, 17], but study an interplay between the arising resonances (or resonance bands) and the resonances which occurred before coupling.

The paper is organized as follows.

In Sec. 2 we introduce the explicitly soluble model designed to demonstrate the interplay of the molecular and nuclear resonance widths. It is also shown that in a wide time interval the decay of the “molecular” state is indeed of the standard exponential character [19]. This transition will take place primarily into the open nuclear channels and its rate is determined by the inverse width of the nuclear resonance. In Sec. 3 we consider the case where molecular Hamiltonians of the type considered in Sec. 2 are arranged in form of an infinite one-dimensional lattice. Sec. 4 is devoted to the generalization to multi-dimensional lattices. In both these sections, the time evolution of originally pure molecular states, extended to a spectral band within a lattice, is studied. It is shown that if the real part of the “nuclear”

resonance lies within such a spectral band, then there exist molecular states which decay exponentially, with a rate inversely proportional to the “nuclear” width.

2. TWO-CHANNEL MOLECULAR RESONANCE MODEL

2.1. Description of the model Hamiltonian. Let us consider a two-channel Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ consisting of a “nuclear” Hilbert space \mathcal{H}_1 (channel 1) and a one-dimensional “molecular” space $\mathcal{H}_2 = \mathbb{C}$ (channel 2). The elements of \mathcal{H} are represented as vectors $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ where $u_1 \in \mathcal{H}_1$ and $u_2 \in \mathcal{H}_2$, with u_2 being a complex number. The inner product $\langle u, v \rangle_{\mathcal{H}} = \langle u_1, v_1 \rangle + u_2 \bar{v}_2$ in \mathcal{H} is naturally defined via the inner products $\langle u_1, v_1 \rangle$ in \mathcal{H}_1 and $u_2 \bar{v}_2$ in \mathcal{H}_2 .

As a Hamiltonian in \mathcal{H} we consider the 2×2 operator matrix

$$A = \begin{pmatrix} h_1 & b \\ \langle \cdot, b \rangle & \lambda_2 \end{pmatrix} \quad (2.1)$$

where h_1 is the (selfadjoint) “nuclear Hamiltonian” in \mathcal{H}_1 , and $\lambda_2 \in \mathbb{R}$ a trial “molecular” energy. A vector $b \in \mathcal{H}_1$ provides the coupling between the channels. It should be mentioned that the Hamiltonian (2.1) resembles one of the well known Friedrichs models [15] (for a discussion of the other Friedrichs-type models see, e. g., Ref. [18] and the references cited therein).

If there is no coupling between the channels, i. e. for $b = 0$, the spectrum of A consists of the spectrum of h_1 and the additional discrete eigenvalue λ_2 . We assume that the continuous spectrum $\sigma_c(h_1)$ of the Hamiltonian h_1 is not empty and that the eigenvalue λ_2 is embedded in $\sigma_c(h_1)$. It is also assumed that λ_2 is not a threshold point of $\sigma_c(h_1)$, and that this spectrum is absolutely continuous in a sufficiently wide neighborhood of λ_2 .

A nontrivial coupling ($b \neq 0$) between the channels will, in general, shift the eigenvalue λ_2 into an unphysical sheet of the energy plane. The resulting perturbed energy appears as a resonance, i. e., as a pole of the analytic (or, more precisely, meromorphic) continuation of the resolvent $r(z) = (A - z)^{-1}$ taken between suitable states (see, e. g., [5]). In the present paper we assume that such a continuation through the absolutely continuous spectrum of h_1 in some neighborhood of λ_2 is possible at least for the matrix element $\langle r_1(z)b, b \rangle$ of the resolvent $r_1(z) = (h_1 - z)^{-1}$. Then one infers a meromorphic continuability at least for the compressed resolvent $P_2(A - z)^{-1}|_{\mathcal{H}_2}$ where P_2 denotes the orthogonal projection onto the space \mathcal{H}_2 . Indeed, the explicit representation for the resolvent $r(z)$ is easily seen to be

$$r(z) = \begin{pmatrix} r_1(z) + \frac{r_1(z)b\langle \cdot, b \rangle r_1(z)}{M_2(z)} & -\frac{r_1(z)b}{M_2(z)} \\ -\frac{\langle \cdot, b \rangle r_1(z)}{M_2(z)} & \frac{1}{M_2(z)} \end{pmatrix}. \quad (2.2)$$

where the transfer function $M_2(z)$ reads $M_2(z) = \lambda_2 - z - \beta(z)$ with $\beta(z) = \langle r_1(z)b, b \rangle$. Thus, if $\beta(z)$ admits a meromorphic continuation through an interval of the absolutely continuous spectrum of the “nuclear” Hamiltonian h_1 , then the function $P_2(A - z)^{-1}|_{\mathcal{H}_2} = M_2^{-1}(z)$ admits such a continuation, too.

Evidently the poles of $r(z)$ on the physical sheet are either due to zeros of the function $M_2(z)$ or due to poles of the resolvent $r_1(z)$. The latter correspond to the discrete spectrum of the operator h_1 which may determine part of the point spectrum of A . This is true, in

particular, for the multiple eigenvalues of h_1 . In any case it is obvious that the perturbation of the eigenvalue λ_2 only corresponds to solutions of the equation $M_2(z) = 0$, i. e., of

$$z = \lambda_2 - \beta(z). \quad (2.3)$$

This equation has no roots z with $\text{Im } z \neq 0$ on the physical sheet. For, being eigenvalues of the selfadjoint operator A , they have, of course, to be real. Thus, Eq. (2.3) may have solutions only on the real axis and in the unphysical sheet(s) of the Riemann surface of the resolvent $r_1(z)$.

We start with a brief discussion of the case where the “nuclear” channel Hamiltonian h_1 generates no resonances close to λ_2 in a domain \mathcal{D} of the unphysical sheet which adjoins the physical sheet from below the cut. This assumption implies that for a wide set of unit vectors $\widehat{b} = b/\|b\|$ the quadratic form $\beta(z) = \|b\|^2 \langle r_1(z)\widehat{b}, \widehat{b} \rangle$ can be analytically continued in \mathcal{D} . Moreover, under certain smallness conditions for $\|b\|$, Eq. (2.3) is uniquely solvable [22] in \mathcal{D} providing in first order perturbation theory (see, e. g., [20, 21])

$$z_2 \underset{\|b\| \rightarrow 0}{=} \lambda_2 - \langle r_1(\lambda_2 + i0)b, b \rangle + o(\|b\|^2). \quad (2.4)$$

The real and imaginary parts of the resonance $z_2 = E_R^{(2)} - i\frac{\Gamma_R^{(2)}}{2}$, thus, are given by

$$\begin{aligned} E_R^{(2)} &= \lambda_2 - \text{Re} \langle r_1(\lambda_2 + i0)b, b \rangle + o(\|b\|^2), \\ \Gamma_R^{(2)} &= 2 \text{Im} \langle r_1(\lambda_2 + i0)b, b \rangle + o(\|b\|^2). \end{aligned} \quad (2.5)$$

2.2. Perturbation of the “molecular” resonance by a nearby “nuclear” resonance.

Our main interest concerns the opposite case of a “nuclear” resonance $z_1 = E_R^{(1)} - i\frac{\Gamma_R^{(1)}}{2}$, $\Gamma_R^{(1)} > 0$, with a real part $E_R^{(1)}$ close to λ_2 . For the sake of simplicity we assume the corresponding pole of $r_1(z)$ to be of first order. Let the element $b \in \mathcal{H}_1$ be such that the function $\beta(z)$ admits an analytic continuation into a domain \mathcal{D} which contains both points λ_2 and z_1 . This domain, moreover, is assumed to belong to the unphysical sheet which adjoins the physical sheet along the upper rim of the cut. In \mathcal{D} the function $\beta(z)$, thus, can be written as

$$\beta(z) = \frac{a}{z_1 - z} + \beta^{\text{reg}}(z) \quad (2.6)$$

with $\beta^{\text{reg}}(z)$ being a holomorphic function. For a fixed “structure function” $\widehat{b} = b/\|b\|$ we have $|a| = C_a \|b\|^2$ with a constant C_a determined by the residue of $r_1(z)$ at $z = z_1$. Note that this residue is usually expressed in terms of resonance (Gamow) functions (see for example [23]). In fact, we assume that the resonance corresponds to an “almost eigenstate” of h_1 . That is, in principle a limiting procedure $\Gamma_R^{(1)} \rightarrow 0$ is possible so that the resonance turns into a usual eigenvalue with an eigenvector $\psi_1 \in \mathcal{H}_1$. More precisely, we assume

$$C_a = C_a^{(0)} + o(1) \quad \text{as} \quad \Gamma_R^{(1)} \rightarrow 0 \quad (2.7)$$

with $C_a^{(0)} \equiv \langle \widehat{b}, \psi_1 \rangle \langle \psi_1, \widehat{b} \rangle \neq 0$. This can be achieved, e. g., if the Hamiltonian h_1 itself has a matrix representation of the form (2.1) and the resonance z_1 is generated by a separated one-dimensional channel. In such a case, according to (2.2) and (2.4), we would have $C_a^{(0)} = 1$ (for details see Ref. [7], Sec. II).

Let

$$\text{Re } a > 0 \quad \text{and} \quad \text{Im } a \ll \text{Re } a \quad (2.8)$$

and, for $z \in \mathcal{D}$,

$$|\operatorname{Im} \beta^{\text{reg}}(z)| \geq c_{\mathcal{D}} \|b\|^2 \quad \text{and} \quad |\beta^{\text{reg}}(z)| \leq C_{\mathcal{D}} \|b\|^2.$$

with constants $c_{\mathcal{D}} > 0$ and $C_{\mathcal{D}} > 0$. Furthermore, the coupling between the channels in the Hamiltonian (2.1) is assumed to be so weak that

$$|\beta^{\text{reg}}(z)| \leq C_{\mathcal{D}} \|b\|^2 \ll \Gamma_R^{(1)} \quad \text{while} \quad |a| = C_a \|b\|^2 \ll \left(\Gamma_R^{(1)}\right)^2. \quad (2.9)$$

It can be expected that these conditions are fulfilled in specific molecular systems even under the supposition that the “nuclear” width $\Gamma_R^{(1)}$ itself is very small.

After inserting (2.6) for $\beta(z)$, Eq. (2.3) turns into the “quadratic” equation

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

which can be “solved”, i. e., can be rewritten in form of two equations

$$z = \frac{\lambda_2 + z_1 - \beta^{\text{reg}}(z)}{2} \pm \sqrt{\left(\frac{\lambda_2 - z_1 - \beta^{\text{reg}}(z)}{2}\right)^2 + a}. \quad (2.10)$$

Under conditions (2.9) the existence of solutions of (2.10), and thus of Eq. (2.3), is guaranteed, analogously to the proof in [22], by Banach’s Fixed Point Theorem. Each of the equations (2.10) has only one solution in the domain \mathcal{D} . In case of the sign “−” we denote the root of (2.10) by z_{nucl} , in case of the sign “+” by z_{mol} .

The inequalities (2.9) imply

$$\frac{|a|}{\left|\lambda_2 - z_1 - \beta^{\text{reg}}(z)\right|_{z \in \mathcal{D}}^2} \approx \frac{|a|}{\left|\lambda_2 - E_R^{(1)}\right|^2 + \left(\frac{\Gamma_R^{(1)}}{2}\right)^2} \leq \frac{4C_a \|b\|^2}{\left(\Gamma_R^{(1)}\right)^2} \ll 1. \quad (2.11)$$

For $z \in \mathcal{D}$ the value of

$$\varepsilon(z) = \frac{4a}{[\lambda_2 - z_1 - \beta^{\text{reg}}(z)]^2} \quad (2.12)$$

is very small, $|\varepsilon(z)| \ll 1$. Thus, to separate the main terms of the solutions of Eqs. (2.10), one can apply the asymptotic relation $\sqrt{1 + \varepsilon} = 1 + \varepsilon/2 + O(\varepsilon^2)$. As a result we find

$$z = \frac{\lambda_2 + z_1 - \beta^{\text{reg}}(z)}{2} \pm \frac{\lambda_2 - z_1 - \beta^{\text{reg}}(z)}{2} \left(1 + \frac{2a}{(\lambda_2 - z_1 - \beta^{\text{reg}}(z))^2} + O(\varepsilon^2)\right). \quad (2.13)$$

In other words, the roots z_{nucl} and z_{mol} of (2.10) are essentially given by

$$z_{\text{nucl}} \cong z_1 - \frac{a}{\lambda_2 - z_1 - \beta^{\text{reg}}(z_1)} \cong z_1 - \frac{a}{\lambda_2 - z_1}, \quad (2.14)$$

$$z_{\text{mol}} \cong \lambda_2 - \beta^{\text{reg}}(\lambda_2 + i0) + \frac{a}{\lambda_2 - z_1 - \beta^{\text{reg}}(\lambda_2 + i0)} \cong \lambda_2 + \frac{a}{\lambda_2 - z_1}. \quad (2.15)$$

From the second condition (2.9) follows $\left|\frac{a}{\lambda_2 - z_1}\right| \ll \Gamma_R^{(1)}$. Consequently, this term provides

in z_{nucl} a very small perturbation of the initial “nuclear” resonance z_1 . As compared to $\Gamma_R^{(1)}$ it represents also in z_{mol} a very weak perturbation of the “molecular” energy λ_2 . However, as compared to the result (2.4), valid in case of a missing nearby “nuclear” resonance, it can

be rather large. In particular, if the “molecular” energy λ_2 coincides with the real part $E_R^{(1)}$ of the “nuclear” resonance z_1 , then $z_{\text{mol}} = E_R^{(m)} - i\frac{\Gamma_R^{(m)}}{2}$ with

$$E_R^{(m)} \cong \lambda_2 - 2\frac{\text{Im } a}{\Gamma_R^{(1)}} \quad \text{and} \quad \Gamma_R^{(m)} \cong 4\frac{\text{Re } a}{\Gamma_R^{(1)}}. \quad (2.16)$$

The width of the “molecular” resonance z_{mol} in the presence of a nearby “nuclear” resonance z_1 , thus, turns out to be inversely proportional to the “nuclear” width $\Gamma_R^{(1)}$.

Let us contrast the results (2.4) and (2.16) in some more detail. Since such a comparison is necessarily of a qualitative character, we simulate the situation of a missing nearby nuclear resonance simply by dropping the pole term in the representation (2.6) of $\beta(z)$. After this removal we get $\beta(z) \equiv \beta^{\text{reg}}(z)$ and for $\text{Im } z \leq 0$ the eigenvalue λ_2 generates the resonance (2.4) having the width $\Gamma_R^{(2)} \approx 2\text{Im } \beta^{\text{reg}}(\lambda_2 + i0)$. The latter satisfies the inequalities $c_{\mathcal{D}}\|b\|^2 \leq \Gamma_R^{(2)}/2 \leq C_{\mathcal{D}}\|b\|^2$. Substituting $|\text{Re } a| \sim C_a\|b\|^2 \sim \frac{C_a}{c_{\mathcal{D}}}\Gamma_R^{(2)}$ in (2.16) we find the following approximate estimate of $\Gamma_R^{(m)}$ relative to $\Gamma_R^{(2)}$:

$$\Gamma_R^{(m)} \sim \Gamma_R^{(2)} \cdot \frac{C_a/c_{\mathcal{D}}}{\Gamma_R^{(1)}}. \quad (2.17)$$

The second inequality (2.9), chosen as a condition for $\|b\|$ reflects the fact that the “usual” molecular width $\Gamma_R^{(2)}$ is much smaller than the width of a usual “nuclear” resonance $\Gamma_R^{(1)}$,

$$C_a\Gamma_R^{(2)} \ll c_{\mathcal{D}} \left(\Gamma_R^{(1)}\right)^2. \quad (2.18)$$

This can practically always be assumed for concrete molecules.

Under condition (2.7) the value of $C_a = |a|/\|b\|^2$ differs from zero, $C_a \geq C > 0$, as $\Gamma_R^{(1)} \rightarrow 0$. Therefore the estimates (2.16) and (2.17) imply that in the presence of a narrow ($\Gamma_R^{(1)} \ll C_a/c_{\mathcal{D}}$) “nuclear” resonance close to λ_2 the “molecular” width $\Gamma_R^{(m)}$ is much larger than the “molecular” width $\Gamma_R^{(2)}$ observed in absence of such a resonance. In fact, according to (2.17) this ratio is determined by the large quotient $\frac{C_a/c_{\mathcal{D}}}{\Gamma_R^{(1)}}$.

Finally we note that if the conditions (2.9), and hence the condition (2.18) are not fulfilled, i. e., if the coupling between the channels in the Hamiltonian (2.1) is not small compared with the “nuclear” width, then it follows from (2.10) that the molecular width $\Gamma_R^{(m)}$ achieves itself an order of $\Gamma_R^{(1)}$. We do not discuss this case since such a situation can hardly be assumed to exist.

2.3. Exponential decay of the “molecular” state. Let us suppose that an initial state of the system described by the Hamiltonian A corresponds exactly to the pure “molecular” wave function $\varphi = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Then, the time evolution of the system is described by the solution $\psi(t)$ of the Cauchy problem

$$i\frac{d\psi}{dt} = A\psi, \quad \psi|_{t=0} = \varphi. \quad (2.19)$$

The probability of finding the system at the time t still in the molecular state φ is given by

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

The remainder $1 - P_{\text{mol}}(t)$, hence, determines the probability for the state φ to decay into open channels of the continuous spectrum of the “nuclear” sub-Hamiltonian h_1 .

To estimate the probability $P_{\text{mol}}(t)$, we use the standard integral representation of a function of an operator via its resolvent. In the case considered this means

$$\exp\{-iAt\} = -\frac{1}{2\pi i} \oint_{\gamma} dz e^{-izt} (A - z)^{-1}. \quad (2.20)$$

The integration in (2.20) is performed in the physical sheet along a contour γ going counter-clockwise around the spectrum of the matrix A . Recall that, due to the selfadjointness of the operator A , this spectrum is real. Taking into account the representations (2.2) and (2.20) one finds

$$\langle \psi(t), \varphi \rangle = -\frac{1}{2\pi i} \oint_{\gamma} dz \frac{\exp(-izt)}{\lambda_2 - z - \beta(z)} \quad (2.21)$$

This leads to the following important result. Under the conditions of Subsection 2.2 the behavior of the integral (2.21) for $t > 0$ is described by the formula

$$\begin{aligned} \langle \psi(t), \varphi \rangle &= \exp\{-iz_{\text{mol}}t\} \left[1 - \frac{a}{\left(\lambda_2 - z_1 - \beta^{\text{reg}}(\lambda_2 + i0)\right)^2} + O\left(\varepsilon^4(\lambda_2 + i0)\right) \right] \\ &+ \exp\{-iz_{\text{nucl}}t\} \left[\frac{a}{\left(\lambda_2 - z_1 - \beta^{\text{reg}}(z_1)\right)^2} + O\left(\varepsilon^4(z_1)\right) \right] + \tilde{\varepsilon}(t) \end{aligned} \quad (2.22)$$

where the value of $\varepsilon(z)$ is given by Eq. (2.12). The background term $\tilde{\varepsilon}(t) = O(\|b\|^2)$ is small, $|\tilde{\varepsilon}(t)| \ll 1$, for all $t > 0$. In particular, if $E_R^{(1)} = \lambda_2$ we have

$$\langle \psi(t), \varphi \rangle \approx \exp\{-iz_{\text{mol}}t\} \left[1 + \frac{4a}{\left(\Gamma_R^{(1)}\right)^2} + \dots \right] + \exp\{-iz_{\text{nucl}}t\} \left[-\frac{4a}{\left(\Gamma_R^{(1)}\right)^2} + \dots \right] \quad (2.23)$$

The proof of the asymptotic relation (2.22) is carried out by estimating the contribution of the resonance poles z_{mol} and z_{nucl} to the integral (2.21). This is done by deforming parts of the contour γ situated in a neighborhood of the molecular energy λ_2 (see Figure 1). A part γ^+ of γ , situated initially on the upper rim of the cut, is shifted into the neighboring unphysical sheet. Having done such a deformation one finds explicitly the residues of the integrand in (2.21) at $z = z_{\text{mol}}$ and $z = z_{\text{nucl}}$. An analogous deformation of a part γ^- of γ , situated initially on the lower rim, is performed in a domain $\text{Im } z < 0$ of the physical sheet. It is assumed that, though the parts γ^+ and γ^- belong to different energy sheets, their positions on these sheets coincide. It is also assumed that for any $z \in \gamma^{\pm}$ the estimate

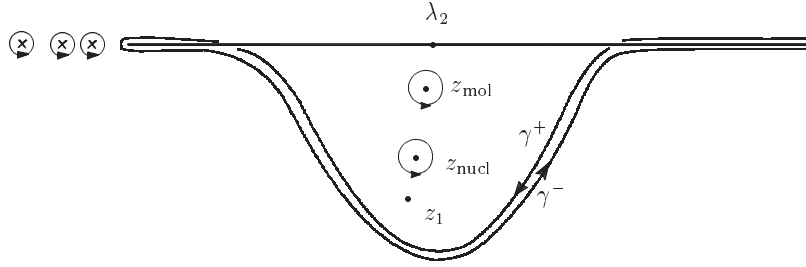


FIGURE 1. A scheme showing the deformation of the integration path γ . The part γ^+ of the resulting contour belongs to the unphysical sheet, part γ^- to the physical sheet. The crosses “ \times ” denote the discrete eigenvalues of the Hamiltonian A while the solid line corresponds to the continuous spectrum.

$|\beta^\pm(z)| \ll |\lambda_2 - z|$ holds. Thus, the integration in (2.21) around the continuous spectrum of A , except the residues at $z = z_{\text{mol}}$ and $z = z_{\text{nucl}}$, gives

$$\begin{aligned} & -\frac{1}{2\pi i} \int_{\gamma^+} dz \exp(-izt) \left(\frac{1}{\lambda_2 - z - \beta^+(z)} - \frac{1}{\lambda_2 - z - \beta^-(z)} \right) \\ &= -\frac{1}{2\pi i} \int_{\gamma^+} dz \exp(-izt) \frac{\beta^+(z) - \beta^-(z)}{[\lambda_2 - z - \beta^+(z)][\lambda_2 - z - \beta^-(z)]}. \end{aligned} \quad (2.24)$$

Here we have used the specific notation $\beta^+(z)$ for the values of the function $\beta(z)$ at points z belonging to the curve γ^+ (i. e., lying in the unphysical sheet), and $\beta^-(z)$ for the values of $\beta(z)$ at the same points of the curve γ^- (i. e., lying in the physical sheet). Both $\beta^-(z)$ and $\beta^+(z)$ are of the order of $O(\|b\|^2)$, and $|\beta^\pm(z)| \ll |\lambda_2 - z|$, while the exponential $\exp(-izt)$ at $\text{Im } z < 0$ is decreasing for $t > 0$. The value of the function (2.24), thus, is always small, having an order of $O(\|b\|^2)$, and is even decreasing (in general nonexponentially) with increasing t . We include the contribution of this function in the background term $\tilde{\varepsilon}(t)$. The summand $\tilde{\varepsilon}(t)$ also includes a contribution to (2.21) from the residues at the discrete eigenvalues of A . Apart from factors oscillating when t changes, the value of this contribution remains practically the same for all $t \geq 0$.

The formulae (2.22) and (2.23) show explicitly that in a large time interval $0 \leq t < T$, $T \sim \frac{2}{\Gamma_R^{(m)}} \left| \ln \max |\tilde{\varepsilon}(t)| \right|$, the decay of a “molecular” state φ in the presence of a narrow “nuclear” resonance is indeed of exponential character. The rate of this decay is determined mainly by the width $\Gamma_R^{(m)}$ of the “molecular” resonance z_{mol} , i. e., by the ratio $|\text{Re } a|/\Gamma_R^{(1)}$,

$$P_{\text{mol}}(t) \cong \exp\{-\Gamma_R^{(m)} t\} \cong \exp\left\{-\frac{4|\text{Re } a|}{\Gamma_R^{(1)}} t\right\}. \quad (2.25)$$

3. “MOLECULAR” RESONANCES IN A ONE-DIMENSIONAL LATTICE

Let us assume that the “molecules” described by the Hamiltonian (2.1) are arranged in form of an infinite one-dimensional (linear) crystalline structure. To describe such a crystal we introduce the lattice Hilbert space

$$\mathcal{G} = \bigoplus_{i=-\infty}^{+\infty} \mathcal{H}^{(i)}$$

representing an orthogonal sum of the Hilbert spaces associated with the individual cells

$$\mathcal{H}^{(i)} = \mathcal{H}_1^{(i)} \oplus \mathcal{H}_2^{(i)}. \quad (3.1)$$

Here the subspaces $\mathcal{H}_1^{(i)} \equiv \mathcal{H}_1$ and $\mathcal{H}_2^{(i)} \equiv \mathcal{H}_2 \equiv \mathbb{C}$ are exactly the same ones as in Sec. 2 and, thus, $\mathcal{H}^{(i)} \equiv \mathcal{H}$. The elements of the total Hilbert space \mathcal{G} are represented by the sequences

$$u = (\dots, u^{(-2)}, u^{(-1)}, u^{(0)}, u^{(1)}, u^{(2)}, \dots) \text{ with components } u^{(i)} = \begin{pmatrix} u_1^{(i)} \\ u_2^{(i)} \end{pmatrix} \text{ where } u_1^{(i)} \in \mathcal{H}_1$$

and $u_2^{(i)} \in \mathcal{H}_2 = \mathbb{C}$. The inner product in \mathcal{H} is defined by $\langle u, v \rangle_{\mathcal{H}} = \sum_{i=-\infty}^{+\infty} \langle u^{(i)}, v^{(i)} \rangle_{\mathcal{H}^{(i)}}$. The

subspaces $\mathcal{G}_1 = \bigoplus_{i=-\infty}^{+\infty} \mathcal{H}_1^{(i)}$ and $\mathcal{G}_2 = \bigoplus_{i=-\infty}^{+\infty} \mathcal{H}_2^{(i)}$, with $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$, are called pure nuclear and pure molecular channels, respectively.

In the present section we deal with the Hamiltonian H acting in \mathcal{H} according to

$$(Hu)^{(i)} = Wu^{(i-1)} + Au^{(i)} + Wu^{(i+1)} \quad (3.2)$$

where only the interaction between neighboring cells is taken into account and the interaction operator W is chosen in the simplest form

$$W = \begin{pmatrix} 0 & 0 \\ 0 & w \end{pmatrix} \quad (3.3)$$

with w being a positive number. Such a choice of the interaction corresponds to the natural assumption that the cells interact between each other via the molecular states, while the direct interaction between nuclear constituents belonging to different cells is negligible. We assume that the closed interval $[\lambda_2 - 2w, \lambda_2 + 2w]$ is totally embedded in the continuous spectrum $\sigma_c(h_0)$ of h_0 and, moreover, that no thresholds of $\sigma_c(h_0)$ belong to this interval. For the sake of simplicity we also assume that the interval belongs to the domain \mathcal{D} introduced in Sec. 2 and that for any $\mu \in [\lambda_2 - 2w, \lambda_2 + 2w]$

$$\text{Im} \langle r_0(\mu \pm i0) \widehat{b}, \widehat{b} \rangle \neq 0. \quad (3.4)$$

Obviously, the Hamiltonian (3.2) represents a special case of the infinite Jacobi operator matrix (regarding the properties of some infinite scalar Jacobi matrices see, e. g., [24, 25] and Refs. cited therein). It is a selfadjoint operator on the domain $\mathcal{D}(H) = \bigoplus_{i=-\infty}^{+\infty} \mathcal{D}^{(i)}$ with $\mathcal{D}^{(i)} = \mathcal{D}(h_1) \oplus \mathbb{C}$.

The resolvent $R(z) = (H - z)^{-1}$ of H possesses a natural block structure, $R(z) = \{R(j, k; z)\}$, $j, k = 0, \pm 1, \pm 2, \dots, \pm \infty$. The blocks $R(j, k; z)$, providing the mapping $\mathcal{H}^{(k)} \rightarrow \mathcal{H}^{(j)}$, satisfy the equations

$$WR(j-1, k; z) + (A - z)R(j, k; z) + WR(j+1, k; z) = \delta_{jk}I \quad (3.5)$$

where δ_{jk} stands for the Kronecker delta and I for the identity operator in the Hilbert space \mathcal{H} of cells. Hereafter we assume $\text{Im } z \neq 0$ so that the value of z automatically belongs to the resolvent set of the operator H . The blocks $R(j, k; z)$ themselves possess a 2×2 matrix structure, $R(j, k; z) = \{R_{mn}(j, k; z)\}$, $m, n = 1, 2$, corresponding to the decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$.

The Fourier transform

$$(Fu)(p) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{+\infty} u^{(j)} \exp(ipj) \quad (3.6)$$

in \mathcal{G} reduces Eq. (3.5) to

$$(A - z)R(p, p'; z) + 2 \cos p W R(p, p'; z) = \delta(p - p') I \quad (3.7)$$

where the quasi-momentum p runs through the interval $[-\pi, \pi]$ and the function $R(p, p'; z)$ represents the kernel of the resolvent $R(z)$ in this representation. From (3.7) follows immediately

$$R(p, p'; z) = G(p; z) \delta(p - p') \quad (3.8)$$

where

$$G(p; z) = \begin{pmatrix} r_1(z) + \frac{r_1(z)b \langle \cdot, b \rangle r_1(z)}{\widetilde{M}_2(p; z)} & -\frac{r_1(z)b}{\widetilde{M}_2(p; z)} \\ -\frac{\langle \cdot, b \rangle r_1(z)}{\widetilde{M}_2(p; z)} & \frac{1}{\widetilde{M}_2(p; z)} \end{pmatrix}. \quad (3.9)$$

This corresponds to the representation (2.2) of the resolvent of the cell Hamiltonian A , the only difference being that the transfer function $M_2(z)$ is replaced by the expression

$$\widetilde{M}_2(p; z) = \lambda_2 - z + 2w \cos p - \beta(z). \quad (3.10)$$

The factorization (3.8) implies

$$R(j, k; z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp e^{-ip(j-k)} G(p; z)$$

and with the representation (3.9) we, thus, obtain

$$R(j, k; z) = \begin{pmatrix} \delta_{jk} r_1(z) + r_1(z)b R_{22}(j, k; z) \langle \cdot, b \rangle r_1(z) & -r_1(z)b R_{22}(j, k; z) \\ -R_{22}(j, k; z) \langle \cdot, b \rangle r_1(z) & R_{22}(j, k; z) \end{pmatrix} \quad (3.11)$$

where

$$R_{22}(j, k; z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \frac{e^{-ip(j-k)}}{\lambda_2 - z + 2w \cos p - \beta(z)}. \quad (3.12)$$

Introducing the new variable $\zeta = e^{-ip}$, this integral is reduced to

$$R_{22}(j, k; z) = \frac{1}{2\pi i} \oint_{\gamma} d\zeta \frac{\zeta^{j-k}}{w\zeta^2 + M_2(z)\zeta + w}.$$

Here, γ stands for the unit circle centered at the origin, the integration over γ being performed in the counterclockwise sense. Further, applying the Residue Theorem and taking into account the sign of the difference $j - k$ one finds

$$R_{22}(j, k; z) = \frac{\left\{ \frac{1}{2w} \left[\sqrt{[M_2(z) - 2w][M_2(z) + 2w]} - M_2(z) \right] \right\}^{|j-k|}}{\sqrt{[M_2(z) - 2w][M_2(z) + 2w]}}. \quad (3.13)$$

It is assumed here that the branch $\sqrt{(\xi - 2w)(\xi + 2w)}$ of the function $\left((\xi - 2w)(\xi + 2w)\right)^{1/2}$ is defined in the plane of the complex parameter ξ , cut along the interval $[-2w, 2w]$, and that $\text{Im } \xi > 0$ implies

$$\text{Im } \sqrt{(\xi - 2w)(\xi + 2w)} > 0,$$

while $\text{Im } \xi < 0$ implies

$$\text{Im } \sqrt{(\xi - 2w)(\xi + 2w)} < 0.$$

From Eqs. (3.11) and (3.13) it follows that all the nontrivial singularities of the resolvent $R(z)$, differing from those of the cell “nuclear” channel resolvent $r_1(z)$, are determined by the properties of the function

$$D(z) = \sqrt{[M_2(z) - 2w][M_2(z) + 2w]}.$$

First, we note that if $\|b\| = 0$, and thus $M_2(z) = \lambda_2 - z$, then the “molecular” and “nuclear” channels in the Hamiltonian H decouple. In this case the eigenvalue λ_2 generates for H an additional branch of the absolutely continuous spectrum which occupies the interval $[\lambda_2 - 2w, \lambda_2 + 2w]$. Second, even if $\|b\| \neq 0$ then the function $D(z)$ cannot have roots z with $\text{Im } z \neq 0$ in the physical sheet. Otherwise such roots would generate for H a complex spectrum. But this is impossible because of the selfadjointness of H . Also, under the condition (3.4) this function cannot have real roots within the interval $[\lambda_2 - 2w, \lambda_2 + 2w]$ since for $\lambda_2 - 2w \leq \mu \leq \lambda_2 + 2w$ the imaginary part

$$\text{Im}[M_2(\mu \pm i0) - 2w] = \text{Im}[M_2(\mu \pm i0) + 2w] = -\|b\|^2 \text{Im}\langle r_1(\mu \pm i0)\widehat{b}, \widehat{b} \rangle$$

is nonzero by the assumption (3.4). Thus, in a close neighborhood of the interval $[\lambda_2 - 2w, \lambda_2 + 2w]$ the equation $D(z) = 0$ may only have roots in the unphysical sheet. In fact, assuming the conditions (2.9) and repeating literally the considerations which led to (2.13), one can rewrite this equation in form of the four equations,

$$z = \frac{\lambda_2 - 2w + z_1 - \beta^{\text{reg}}(z)}{2} \pm \frac{\lambda_2 - 2w - z_1 - \beta^{\text{reg}}(z)}{2} \left[1 + \frac{2a}{(\lambda_2 - 2w - z_1 - \beta^{\text{reg}}(z))^2} + O(\varepsilon_-^2) \right], \quad (3.14)$$

$$z = \frac{\lambda_2 + 2w + z_1 - \beta^{\text{reg}}(z)}{2} \pm \frac{\lambda_2 + 2w - z_1 - \beta^{\text{reg}}(z)}{2} \left[1 + \frac{2a}{(\lambda_2 + 2w - z_1 - \beta^{\text{reg}}(z))^2} + O(\varepsilon_+^2) \right], \quad (3.15)$$

where $\varepsilon_{\pm} = 4a/(\lambda_2 \pm 2w - z_1 - \beta^{\text{reg}}(z))$. In that part of the domain \mathcal{D} which belongs to the unphysical sheet, equation $D(z) = 0$ has four solutions being given essentially by

$$z_{\text{nucl}}^{(\pm)} \cong z_1 - \frac{a}{\lambda_2 \pm 2w - z_1 - \beta^{\text{reg}}(z_1)} \cong z_1 - \frac{a}{\lambda_2 \pm 2w - z_1}, \quad (3.16)$$

$$z_{\text{mol}}^{(\pm)} \cong \lambda_2 \pm 2w - \beta^{\text{reg}}(\lambda_2 \pm 2w + i0) + \frac{a}{\lambda_2 \pm 2w - z_1 - \beta^{\text{reg}}(\lambda_2 \pm 2w + i0)} \quad (3.17)$$

$$\cong \lambda_2 \pm 2w + \frac{a}{\lambda_2 \pm 2w - z_1}.$$

Obviously, each of the roots $z_{\text{nucl}}^{(\pm)}$ and $z_{\text{mol}}^{(\pm)}$ represents an additional square-root branching point of the Riemann surface of the functions $R_{22}(j, k; z)$. Consequently, these roots are

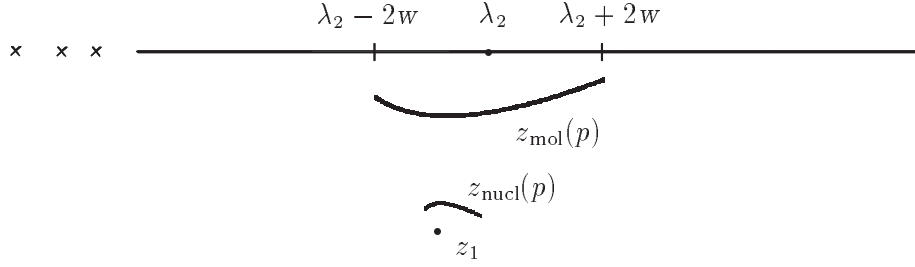


FIGURE 2. A scheme showing the position of the resonance bands generated in the unphysical sheet by the “molecular” eigenvalue λ_2 and the “nuclear” resonance z_1 . These bands are generated respectively by the points $z_{\text{mol}}(p)$ and $z_{\text{nucl}}(p)$ with the quasimomentum p running through the interval $[-\pi, \pi]$.

also the branching points of the Riemann surface of the total resolvent $R(z)$. Thus, one has to introduce the “resonance” cuts in the unphysical sheet considered. The cuts can be made, say, between $z_{\text{nucl}}^{(-)}$ to $z_{\text{nucl}}^{(+)}$ and between $z_{\text{mol}}^{(-)}$ and $z_{\text{mol}}^{(+)}$. Evidently, these cuts are to be interpreted as the resonance spectral bands generated by the initial “molecular” level λ_2 and the “nuclear” resonance z_1 (see Figure 2).

Consider now the time evolution of the system described by the Hamiltonian H starting from a pure molecular state $\varphi = \varphi_1 \oplus \varphi_2$, $\|\varphi_n\| \in \mathcal{G}_n$, $n = 1, 2$, with $\varphi_1 = 0$ and $\|\varphi\| = \|\varphi_2\| = 1$. The probability to find the system at a time $t \geq 0$ in the molecular channel is given by

$$P_{\text{mol}}(\varphi, t) = \|\mathbf{P}_2 e^{-iHt} \varphi\|^2 \quad (3.18)$$

where \mathbf{P}_2 is the orthogonal projection in \mathcal{G} on the pure molecular subspace \mathcal{G}_2 .

As in (2.20) we represent the time evolution operator $\exp(-iHt)$ in terms of the resolvent $R(z) = (H - z)^{-1}$,

$$\exp\{-iHt\} = -\frac{1}{2\pi i} \oint_{\gamma} dz e^{-izt} (H - z)^{-1} \quad (3.19)$$

where the integration is performed along a counterclockwise contour γ in the physical sheet encircling the spectrum of the Hamiltonian H . Recall that this spectrum is real since H is a selfadjoint operator.

According to Eqs. (3.8) and (3.10) the operator $\mathbf{P}_2 R(z)|_{\mathcal{G}_2}$ acts in quasi-momentum representation as the multiplication operator

$$G_{22}(p, z) = [\widetilde{M}_2(p; z)]^{-1} \quad (3.20)$$

and, thus,

$$\left(\mathbf{P}_2 R(z) \varphi \right)(p) = \frac{1}{\widetilde{M}_2(p; z)} \varphi_2(p), \quad p \in [-\pi, \pi].$$

Here $\varphi_2(p)$ stands for the values of the Fourier transform (3.6) of the vector

$$\varphi_2 = (\dots, \varphi_2^{(-2)}, \varphi_2^{(-1)}, \varphi_2^{(0)}, \varphi_2^{(1)}, \varphi_2^{(2)}, \dots),$$

which means

$$\left(\mathbf{P}_2 e^{-iHt} \varphi \right)(p) = -\frac{1}{2\pi i} \varphi_2(p) J(p, t) \quad (3.21)$$

with

$$J(p, t) = \oint_{\gamma} dz \frac{\exp(-izt)}{\tilde{\lambda}_2(p) - z - \beta(z)}. \quad (3.22)$$

This expression has exactly the same form as the integral (2.21). The only difference consists in the replacement of λ_2 by the sum

$$\tilde{\lambda}_2(p) = \lambda_2 + 2w \cos p. \quad (3.23)$$

Thus, to estimate the function $J(p, t)$ one can immediately use the relation (2.22) in order to find

$$\begin{aligned} J(p, t) = & \exp\{-iz_{\text{mol}}(p)t\} \left[1 - \frac{a}{\left(\tilde{\lambda}_2(p) - z_1 - \beta^{\text{reg}}(\tilde{\lambda}_2(p) + i0)\right)^2} + O\left(\varepsilon^4(p, \tilde{\lambda}_2(p) + i0)\right) \right] \\ & + \exp\{-iz_{\text{nucl}}(p)t\} \left[\frac{a}{\left(\tilde{\lambda}_2(p) - z_1 - \beta^{\text{reg}}(z_1)\right)^2} + O\left(\varepsilon^4(p, z_1)\right) \right] + \tilde{\varepsilon}(p, t), \end{aligned} \quad (3.24)$$

where

$$\varepsilon(p, z) = \frac{a}{[\tilde{\lambda}_2(p) - z_1 - \beta^{\text{reg}}(z)]^2}. \quad (3.25)$$

The function $\tilde{\varepsilon}(p, t) = O(\|b\|^2)$ is always small, $|\tilde{\varepsilon}(p, t)| \ll 1$. In accordance with Eqs. (2.14) and (2.15) we, hence, obtain for the positions of the poles

$$z_{\text{nucl}}(p) \cong z_1 - \frac{a}{\lambda_2 + 2w \cos p - z_1}, \quad (3.26)$$

$$z_{\text{mol}}(p) \cong \lambda_2 + 2w \cos p + \frac{a}{\lambda_2 + 2w \cos p - z_1}. \quad (3.27)$$

The resonance bands representing the ranges of the functions $z_{\text{nucl}}(p)$ and $z_{\text{mol}}(p)$, with p running through the interval $[-\pi, \pi]$, are schematically depicted in Figure 2.

The asymptotics (3.24) implies

$$P_{\text{mol}}(\varphi, t) = \int_{-\pi}^{\pi} dp |J(p, t)|^2 |\varphi_2(p)|^2 = \int_{-\pi}^{\pi} dp \exp\{-\Gamma_R^{(m)}(p)t\} |\varphi_2(p)|^2 + \tilde{\varepsilon}(t) \quad (3.28)$$

where

$$\Gamma_R^{(m)}(p) = -2 \operatorname{Im} z_{\text{mol}}(p) \cong -2 \operatorname{Im} \frac{a}{\lambda_2 + 2w \cos p - z_1}. \quad (3.29)$$

The background term $\tilde{\varepsilon}(t)$ in (3.28) is small for any $t \geq 0$, $\tilde{\varepsilon}(t) = O(\|b\|^2)$ and $|\tilde{\varepsilon}(t)| \ll 1$.

Further, let us assume that the real part $E_R^{(1)}$ of the “nuclear” resonance z_1 belongs to the interval $[\lambda_2 - 2w, \lambda_2 + 2w]$, that is $|E_R^{(1)} - \lambda_2| \leq 2w$. Then, one can always prepare an initial “molecular” state φ which decays via the “nuclear” channel with a rate as close as possible to the desired maximal value. Under the assumption (2.8), this maximum is given by

$$\max_{-\pi \leq p \leq \pi} \Gamma_R^{(m)}(p) \cong 4 \frac{\operatorname{Re} a}{\Gamma_R^{(1)}}$$

(cf. formula (2.16)). The correspondingly prepared “molecular” state φ has an almost monochromatic component $\varphi_2(p)$ being localized in a close neighborhood of the quasi-momenta

$$p = \pm \arccos \frac{E_R^{(1)} - \lambda_2}{2w}.$$

For example, if the function $\varphi_2(p)$ is nonzero only for quasimomenta p restricted by

$$\left| \cos p - \frac{E_R^{(1)} - \lambda_2}{2w} \right| \leq \delta \frac{\Gamma_R^{(1)}}{4w}$$

with some small $\delta > 0$, then the width $\Gamma_R^{(m)}$ given by the relation (3.29) varies in an interval lying approximately between $\frac{1}{1 + \delta^2} \frac{4 \operatorname{Re} a}{\Gamma_R^{(1)}}$ and $\frac{4 \operatorname{Re} a}{\Gamma_R^{(1)}}$.

4. “MOLECULAR” RESONANCES IN A MULTI-DIMENSIONAL LATTICE

In this section we consider the case where the “molecules” described by the Hamiltonians (2.1) form an infinite N -dimensional crystalline structure. To label the cells of the respective lattice we use the multi-index $i \in \mathbb{Z}^N$, i. e., $i = (i_1, i_2, \dots, i_N)$ with $i_k = \dots, -2, -1, 0, 1, 2, \dots, k = 1, 2, \dots, N$. The Hilbert space of the system considered is in this case $\mathcal{G} = \bigoplus_{i \in \mathbb{Z}^N} \mathcal{H}^{(i)}$, where the individual cell spaces are given by (3.1), with $\mathcal{H}_1^{(i)} \equiv \mathcal{H}_1$ and

$\mathcal{H}_2^{(i)} \equiv \mathcal{H}_2 \equiv \mathbb{C}$ being the spaces introduced in Sec. 2. For the components $u^{(i)} \in \mathcal{H}^{(i)}$ of the elements u of the total Hilbert space \mathcal{G} we again use the column representation

$$u^{(i)} = \begin{pmatrix} u_1^{(i)} \\ u_2^{(i)} \end{pmatrix} \text{ with } u_1^{(i)} \in \mathcal{H}_1 \text{ and } u_2^{(i)} \in \mathcal{H}_2 = \mathbb{C}. \text{ The inner product in } \mathcal{H} \text{ is defined}$$

as $\langle u, v \rangle_{\mathcal{H}} = \sum_{i \in \mathbb{Z}^N} \langle u^{(i)}, v^{(i)} \rangle_{\mathcal{H}^{(i)}}$. The subspaces $\mathcal{G}_1 = \bigoplus_{i \in \mathbb{Z}^N} \mathcal{H}_1^{(i)}$ and $\mathcal{G}_2 = \bigoplus_{i \in \mathbb{Z}^N} \mathcal{H}_2^{(i)}$, with $\mathcal{G}_1 \oplus \mathcal{G}_2 = \mathcal{G}$, represent pure nuclear and pure molecular channels, respectively.

The Hamiltonian is defined in \mathcal{G} by the expression

$$(Hu)^{(i)} = Au^{(i)} + \sum_{j \in \mathbb{Z}^N, j \neq i} W(i, j)u^{(j)} \quad (4.1)$$

where the interaction matrices

$$W(i, j) = \begin{pmatrix} w_{11}(i, j) & w_{12}(i, j) \\ w_{21}(i, j) & w_{22}(i, j) \end{pmatrix}$$

consist of the block components $w_{mn}(i, j)$ providing the mappings $\mathcal{H}_n \rightarrow \mathcal{H}_m$, $m, n = 1, 2$. These components describe the direct interaction between the m -th and n -th channels of the different cells i and j , respectively. The matrices $W(i, j)$ are assumed to be bounded operators in \mathcal{H} which depend only on the difference $i - j = (i_1 - j_1, i_2 - j_2, \dots, i_N - j_N)$, i. e. $W(i, j) = W(i - j)$ and, thus, the same holds for the block components,

$$w_{mn}(i, j) = w_{mn}(i - j).$$

Moreover, the series of $W(j)$ is assumed to be convergent with respect to the operator norm topology, i. e.

$$\sum_{j \in \mathbb{Z}^N, j \neq 0} \|W(j)\| < +\infty \quad (4.2)$$

and the property

$$W(j-i) = [W(i-j)]^* \quad (4.3)$$

is assumed. With such $W(i, j)$ the Hamiltonian (4.1) is a selfadjoint operator on the domain $\mathcal{D}(H) = \bigoplus_{i \in \mathbb{Z}^N} \mathcal{D}^{(i)}$ with $\mathcal{D}^{(i)} = \mathcal{D}(h_1) \oplus \mathbb{C}$. Note that, since $\mathcal{H}_2 = \mathbb{C}$, the quantities $w_{22}(i-j)$ are complex numbers. The $w_{12}(i-j)$ are vectors in \mathcal{H}_1 , the $w_{21}(i-j)$ are continuous linear forms on \mathcal{H}_1 , and the $w_{11}(i-j)$ are bounded operators in \mathcal{H}_1 .

Let us denote by \mathbb{T}^N the Cartesian product $\mathbb{T}^N = \underbrace{\mathbb{T} \times \mathbb{T} \times \dots \times \mathbb{T}}_N$ of the N intervals

$\mathbb{T} = [-\pi, \pi]$ and by p the points of \mathbb{T}^N , $p = (p_1, p_2, \dots, p_N)$, $p_k \in \mathbb{T}$. The assumption (4.2) implies that the operator-valued function

$$\Omega(p) = \sum_{j \in \mathbb{Z}^n, j \neq 0} W(j) \exp(i\langle p, j \rangle), \quad \Omega(p) : \mathcal{H} \rightarrow \mathcal{H}, \quad p \in \mathbb{T}^N, \quad (4.4)$$

where $\langle p, j \rangle = \sum_{k=1}^N p_k j_k$ is continuous and bounded on \mathbb{T}^N . Due to Eq. (4.3), the values

$$\Omega(p) = \begin{pmatrix} \omega_{11}(p) & \omega_{12}(p) \\ \omega_{21}(p) & \omega_{22}(p) \end{pmatrix}$$

of this function represent selfadjoint operators in \mathcal{H} for any $p \in \mathbb{T}^N$, with

$$\omega_{mn}(p) : \mathcal{H}_n \rightarrow \mathcal{H}_m; \quad [\omega_{11}(p)]^* = \omega_{11}(p), \quad \omega_{22}(p) \in \mathbb{R} \quad \text{and} \quad [\omega_{21}(p)]^* = \omega_{12}(p).$$

The quantity $\tilde{b}(p) = \omega_{12}(p)$ can be considered as a vector of \mathcal{H}_1 while $\omega_{21}(p) = \langle \cdot, \tilde{b}(p) \rangle$ (cf. definition (2.1) of the Hamiltonian A).

The blocks $R(j, k; z)$, $R(j, k; z) : \mathcal{H}^{(k)} \rightarrow \mathcal{H}^{(j)}$, $j, k \in \mathbb{Z}^N$, of the resolvent $R(z) = (H - z)^{-1}$ satisfy the equation

$$(A - z)R(j, k; z) + \sum_{j' \in \mathbb{Z}^N, j' \neq j} W(j - j')R(j', k; z) = \delta_{jk}I. \quad (4.5)$$

After Fourier transformation in \mathcal{G} ,

$$(Fu)(p) = \frac{1}{(2\pi)^{N/2}} \sum_{j \in \mathbb{Z}^N} u^{(j)} \exp(i\langle p, j \rangle), \quad p \in \mathbb{T}^N,$$

the system (4.5) takes the form

$$(A - z)R(p, p'; z) + \Omega(p) R(p, p'; z) = \delta(p - p')I \quad (4.6)$$

where the quasi-momenta p, p' run through the set \mathbb{T}^N and $R(p, p'; z)$ stands for the transformed resolvent $R(z)$. Thus, the factorization (3.8) holds with

$$G(p; z) = [A + \Omega(p) - z]^{-1}. \quad (4.7)$$

First, let us consider the specific case where intercellular interactions $W(i-j)$ in the Hamiltonian (4.1) have the simple form

$$W(i-j) = \begin{pmatrix} 0 & 0 \\ 0 & w_{22}(i-j) \end{pmatrix}, \quad (4.8)$$

i. e., where the cells interact with each other only via the molecular channels. Obviously, in this case the factor $G(p; z)$ is still given by (3.9). As compared to this expression the only difference is that now $p \in \mathbb{T}^N$ and

$$\widetilde{M}_2(p; z) = \lambda_2 - z + \omega_{22}(p) - \beta(z). \quad (4.9)$$

Let $\omega_{22}^{\min} = \min_{p \in \mathbb{T}^N} \omega_{22}(p)$ and $\omega_{22}^{\max} = \max_{p \in \mathbb{T}^N} \omega_{22}(p)$. Similarly to the analogous assumption in Sec. 3 we assume that the closed interval $[\lambda_2 + \omega_{22}^{\min}, \lambda_2 + \omega_{22}^{\max}]$ is totally embedded in the absolutely continuous spectrum $\sigma_c(h_1)$ of h_1 , and no thresholds of this spectrum belong to $[\lambda_2 + \omega_{22}^{\min}, \lambda_2 + \omega_{22}^{\max}]$. We also assume that this interval belongs to the holomorphy domain \mathcal{D} of the function $\beta(z)$, and that for $\mu \in [\lambda_2 + \omega_{22}^{\min}, \lambda_2 + \omega_{22}^{\max}]$ the inequality (3.4) holds.

Let us consider the time evolution of the system described by the Hamiltonian (4.1) with the simple intercellular interactions (4.8) subject to the above conditions. We start again from a pure molecular state $\varphi = \varphi_1 \oplus \varphi_2$, $\|\varphi_n\| \in \mathcal{G}_n$, $n = 1, 2$, with $\varphi_1 = 0$ and $\|\varphi\| = \|\varphi_2\| = 1$. The probability $P_{\text{mol}}(\varphi, t)$ to find the system at a time $t \geq 0$ in the molecular channel is given by the analogue of (3.18). As in Sec. 3 one finds the quasi-momentum representation

$$\left(P_2 R(z) \varphi \right) (p) = G_{22}(p; z) \varphi_2(p) = \frac{1}{\widetilde{M}_2(p; z)} \varphi_2(p), \quad p \in \mathbb{T}^N,$$

and relations (3.21), (3.22) and (3.24) are still valid with the only difference that instead of (3.23) $\widetilde{\lambda}_2(p)$ is now of the form

$$\widetilde{\lambda}_2(p) = \lambda_2 + \omega_{22}(p), \quad p \in \mathbb{T}^N.$$

According to Eqs. (2.14) and (2.15) the main terms of the roots $z_{\text{nucl}}(p)$ and $z_{\text{mol}}(p)$ of the function (4.9) in the unphysical sheet read

$$z_{\text{nucl}}(p) \cong z_1 - \frac{a}{\lambda_2 + \omega_{22}(p) - z_1}, \quad (4.10)$$

$$z_{\text{mol}}(p) \cong \lambda_2 + \omega_{22}(p) + \frac{a}{\lambda_2 + \omega_{22}(p) - z_1}. \quad (4.11)$$

The asymptotic equation (3.24) now implies

$$P_{\text{mol}}(\varphi, t) = \int_{\mathbb{T}^N} dp |J(p, t)|^2 |\varphi_2(p)|^2 = \int_{\mathbb{T}^N} dp \exp\{-\Gamma_R^{(m)}(p) t\} |\varphi_2(p)|^2 + \widetilde{\varepsilon}(t) \quad (4.12)$$

with

$$\Gamma_R^{(m)}(p) = -2 \text{Im } z_{\text{mol}}(p) \cong -2 \text{Im} \frac{a}{\lambda_2 + \omega_{22}(p) - z_1}.$$

As in Sec. 3 the background term $\widetilde{\varepsilon}(t)$ is small for any $t \geq 0$, $\widetilde{\varepsilon}(t) = O(\|b\|^2)$ and $|\widetilde{\varepsilon}(t)| \ll 1$.

Thus, if the real part $E_R^{(1)}$ of the ‘‘nuclear’’ resonance z_1 belongs to the interval $[\lambda_2 + \omega_{22}^{\min}, \lambda_2 + \omega_{22}^{\max}]$ then there are ‘‘molecular’’ states φ which decay via the ‘‘nuclear’’ channel with a rate as close as possible to the maximal value (2.16). In this case the components $\varphi_2(p)$ are localized in a close neighborhood of the manifold

$$\lambda_2 + \omega_{22}(p) = E_R^{(1)} \quad (4.13)$$

in the quasi-momentum space \mathbb{T}^N . In particular, if the initial state φ is prepared such that the component $\varphi_2(p)$ is nonzero only for the quasi-momenta p lying in the domain $|\lambda_2 + \omega_{22}(p) - E_R^{(1)}| \leq \delta \Gamma_R^{(1)}/2$ with some small $\delta > 0$, then one should only integrate over this domain in the integral (4.12). In such a case, under the condition (2.8), a lower estimate for the decay rate $\Gamma_R^{(m)}$ is given, as in Sec. 3, by $\frac{1}{1 + \delta^2} \frac{4 \text{Re } a}{\Gamma_R^{(1)}}$. Thus, by varying δ one can get a rate as close as possible to the maximum (2.16).

Now, let us consider briefly the case of more general intercellular interactions $W(i-j)$ where all the components $\omega_{mn}(p)$, $m, n = 1, 2$, of the matrix $\Omega(p)$, $p \in \mathbb{T}^N$, can be nontrivial. In this case the component $G_{22}(p; z)$ of the factor (4.7) is given again by Eqs. (3.20) and (4.9). However, the function $\beta(z)$ in (4.9) is to be replaced by the modified function

$$\tilde{\beta}(p; z) = \langle [h_1 + \omega_{11}(p) - z]^{-1} [b + \tilde{b}(p)], [b + \tilde{b}(p)] \rangle$$

where $\tilde{b}(p) = \omega_{12}(p)$. We make the natural assumption that the direct intercellular interactions in nuclear channels $w_{11}(i-j)$ are so weak that the term $\omega_{11}(p)$ produces only a very small perturbation of the initial ‘‘nuclear’’ resonance z_1 generated by the Hamiltonian h_1 . More precisely, we assume that the resonance $\tilde{z}_1(p)$ generated by the perturbed Hamiltonian $h_1 + \omega_{11}(p)$ has the property

$$|\tilde{z}_1(p) - z_1| \ll \Gamma_R^{(1)} \quad \text{for any } p \in \mathbb{T}^N \quad (4.14)$$

and that no other resonances arise in the domain \mathcal{D} . Another natural assumption is that the strength of the interactions $w_{12}(i-j)$ and $w_{21}(i-j)$, $i \neq j$, between ‘‘nuclear’’ and ‘‘molecular’’ channels of different cells is much weaker than the one of a single cell. This is why we can assume $\|\tilde{b}(p)\|/\|b\| \lesssim 1$ and the following features. The elements $\tilde{b}(p) \in \mathcal{H}_1$ are such that for any $p \in \mathbb{T}^n$ the function $\tilde{\beta}(p; z)$ admits an analytic continuation into the domain \mathcal{D} of the unphysical sheet and in \mathcal{D} a representation of the type (2.6) holds for $\tilde{\beta}(p; z)$,

$$\tilde{\beta}(p; z) = \frac{\tilde{a}(p)}{\tilde{z}_1(p) - z} + \tilde{\beta}^{\text{reg}}(p; z), \quad (4.15)$$

with an explicitly separated pole term $\tilde{a}(p)/(\tilde{z}_1(p) - z)$ and a holomorphic remainder $\tilde{\beta}^{\text{reg}}(p; z)$. As in Sec. 2.2 we assume that $|\tilde{a}(p)| = C_a(p)\|b\|^2$, and that for any $p \in \mathbb{T}^N$ the limiting procedure (2.7) is possible for $C_a(p)$ while $\text{Im} \tilde{a}(p) \ll \text{Re} \tilde{a}(p)$. For the remainder $\tilde{\beta}^{\text{reg}}(p; z)$, $p \in \mathbb{T}^N$, $z \in \mathcal{D}$, the same statements are assumed to be valid as for the function $\beta^{\text{reg}}(z)$. Under these assumptions one can repeat almost literally the study of the probability $P_{\text{mol}}(\varphi, t)$ as performed above in case of the interactions (4.8). We find again that the asymptotics of $P_{\text{mol}}(\varphi, t)$ is given by (4.12) with

$$\Gamma_R^{(m)}(p) \cong -2 \text{Im} \frac{\tilde{a}(p)}{\lambda_2 + \omega_{22}(p) - \tilde{z}_1(p)}.$$

Let us denote by $(\text{Re} \tilde{a})_{\text{max}}$ the maximal value of the function $\text{Re} \tilde{a}(p)$ on the manifold (4.13). It is obvious that if one prepares the initial pure ‘‘molecular’’ state φ such that its component $\varphi_2(p)$ is localized in a close neighborhood of the subset of the manifold (4.13), where $\text{Re} \tilde{a}(p) = (\text{Re} \tilde{a})_{\text{max}}$, then for the probability $P_{\text{mol}}(\varphi, t)$ the main qualitative result remains practically the same as in case of the interactions (4.8). Namely, varying the support of the component $\varphi_2(p)$ in \mathbb{T}^N one can achieve a decay rate of the state φ as close as possible to the maximal value of the width $\Gamma_R^{(m)}(p)$ in (4.13). The main term $4(\text{Re} \tilde{a})_{\text{max}}/\Gamma_R^{(1)}$ of this value is again inversely proportional to the ‘‘nuclear’’ width $\Gamma_R^{(1)}$.

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