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PERTURBATION OF FINITE-LATTICE SPECTRAL LEVELS BY NEARBY NUCLEAR RESONANCES

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We consider finite linear or cyclic crystalline structures with molecular cells having narrow prethreshold nuclear resonance. We prove that, if the real part of such a nuclear resonance lies within the energy band (the convex hull of the energy levels) of the crystalline structure arising from a separated molecular level, then there exist molecular crystalline states that decay exponentially in time and the decay rate $\Gamma_R^{(m)}$ of these states in the main order is described by the formula $\Gamma_R^{(m)} \cong 4(\mathrm{Re}\,a/\Gamma_R^{(n)})$, where a is the value of the residue of the molecular channel transfer function at the nuclear resonance point and $\Gamma_R^{(n)}$ is the nuclear resonance width.

Мы исследуем конечные линейные и циклические кристаллические структуры, элементарные молекулярные ячейки которых обладают узким предпороговым резонансом. Мы доказываем, что если вещественная часть этого резонанса находится внутри выпуклой оболочки (полосы) уровней энергии кристалла, возникающих из некоторого выделенного молекулярного уровня, то существуют молекулярные состояния кристалла, скорость экспоненциального распада которых $\Gamma_R^{(m)}$ в старшем порядке описывается формулой $\Gamma_R^{(m)} \cong 4(\mathrm{Re}\,a/\Gamma_R^{(n)})$, где a — величина вычета трансфер-функции молекулярного канала в точке ядерного резонанса, а $\Gamma_R^{(n)}$ — ширина этого резонанса.

INTRODUCTION

Molecules are usually treated as purely Coulomb systems, while the strong interaction between their nuclear constituents is assumed to play a negligible role. However any Coulomb 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. [2,12,13,18,19] and references cited therein). Of course, due to the wide Coulomb 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 [3, 4], the situation may be 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 [10]. Among them are even customary systems like $pp\,^{16}\mathrm{O}$ and $p\,^{17}\mathrm{O}$ [1, 20], i.e., the nuclear constituents of the water molecule H_2O or the hydroxyl ion OH^- with O being the isotope $^{17}\mathrm{O}$. For LiD and H_2O the influence of near-threshold nuclear resonances on the molecular properties has been studied in [5,6,8] 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 $^5\mathrm{He}(3/2^+)$ plays a decisive role [9].

Being motivated by the above special cases, we deal in the present work, like in [3, 7], with a rather general model Hamiltonian related to the ones considered by Friedrichs in [11]. 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 [3, 4] 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 very rare phenomenon in nature.

Influence of the narrow pre-threshold resonances on the properties of infinite crystalline molecular structures was studied in [7]. In the present work we concentrate on more realistic finite crystals. A goal of this work is to show that the decay rate of a molecular state with the energy close to a near-threshold resonance may be considerably enhanced when arranging molecular clusters within a finite crystalline structure. The reason is that in such a configuration the original discrete molecular energy turns into a set of energy levels. That is, even if the position of the nuclear resonance differs from the original molecular level, it can get within this set. 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.

1. TWO-CHANNEL MOLECULAR RESONANCE MODEL

In this section we recall our main reasoning [3, 7] regarding an influence of a near-threshold nuclear resonance on the width of a molecular resonance in the case of a single molecule.

1.1. 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 $u_2 \in \mathcal{H}_2$ (u_2 is simply a complex number). The inner product $\langle u, v\rangle_{\mathcal{H}} = \langle u_1, v_1\rangle + u_2\overline{v}_2$ in $\mathcal{H}$ is naturally defined via the inner products $\langle u_1, v_1\rangle$ in $\mathcal{H}_1$ and $u_2\overline{v}_2$ in $\mathcal{H}_2$.

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

$$A = \begin{pmatrix} h_1 & b \\ \langle\,\cdot\,, b\rangle & \lambda_2 \end{pmatrix}, \tag{1}$$

where h_1 is the (self-adjoint) «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 (1) resembles one of the well-known Friedrichs models [11].

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 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 neighbourhood 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., [19]). In the present work we assume that such a continuation through the absolutely continuous spectrum of h_1 in some neighbourhood 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, from the explicit representation for the resolvent $r(z)$ [3, 7], one can easily see that the operator-valued function $P_2(A - z)^{-1}|_{\mathcal{H}_2}$ admits meromorphic continuation to the same neighbourhood, too.

The poles of $r(z)$ on the physical sheet are either due to zeros of the *transfer function* (see [15])

$$M_2(z) = \lambda_2 - z - \beta(z)$$

or due to poles of the resolvent $r_1(z)$ (see [3, 7]). 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

$$z = \lambda_2 - \beta(z). \tag{2}$$

This equation has no roots z with $\operatorname{Im} z \neq 0$ on the physical sheet. Therefore, being eigenvalues of the self-adjoint operator A, they have to be real. Thus, Eq. (2) 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) is uniquely solvable [15] in $\mathcal{D}$ providing in the main order (see, e. g., [14, 16])

$$z_2 \underset{\|b\|\to 0}{=} \lambda_2 - \langle r_1(\lambda_2 + i0)b, b\rangle + o(\|b\|^2). \tag{3}$$

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

$$\begin{aligned} E_R^{(2)} &= \lambda_2 - \operatorname{Re}\langle r_1(\lambda_2 + i0)b, b\rangle + o(\|b\|^2), \\ \Gamma_R^{(2)} &= 2\operatorname{Im}\langle r_1(\lambda_2 + i0)b, b\rangle + o(\|b\|^2). \end{aligned} \tag{4}$$

1.2. 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

$$\beta(z) = \frac{a}{z_1 - z} + \beta^{\mathrm{reg}}(z) \qquad (5)$$

with $\beta^{\mathrm{reg}}(z)$ 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, [17]). In fact, we assume that the resonance corresponds to an «almost eigenstate» of h_1. That is, in principle a limiting procedure $\Gamma_R^{(1)} \to 0$ is possible so that the resonance turns into a usual eigenvalue with an eigenvector $\psi_1 \in \mathcal{H}_1$. More precisely, we assume

$$C_a = C_a^{(0)} + o(1) \quad \text{as} \quad \Gamma_R^{(1)} \to 0 \qquad (6)$$

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 (1) and the resonance z_1 is generated by a separated one-dimensional channel. In such a case we would have $C_a^{(0)} = 1$ (for details see Ref. [4], Sec. II).

Let

$$\operatorname{Re} a > 0 \quad \text{and} \quad \operatorname{Im} a \ll \operatorname{Re} a \qquad (7)$$

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

$$|\operatorname{Im}\beta^{\mathrm{reg}}(z)| \geqslant c_{\mathcal{D}}\|b\|^2 \quad \text{and} \quad |\beta^{\mathrm{reg}}(z)| \leqslant C_{\mathcal{D}}\|b\|^2$$

with constants $c_{\mathcal{D}} > 0$ and $C_{\mathcal{D}} > 0$. Furthermore, the coupling between the channels in the Hamiltonian (1) is assumed to be so weak that

$$|\beta^{\mathrm{reg}}(z)| \leqslant C_{\mathcal{D}}\|b\|^2 \ll \Gamma_R^{(1)}, \quad \text{while} \quad |a| = C_a\|b\|^2 \ll \left(\Gamma_R^{(1)}\right)^2 \qquad (8)$$

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 (5) for $\beta(z)$, Eq. (2) turns into the «quadratic» equation

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

which can be «solved», i. e., can be rewritten in form of two equations

$$z = \frac{\lambda_2 + z_1 - \beta^{\mathrm{reg}}(z)}{2} \pm \sqrt{\left(\frac{\lambda_2 - z_1 - \beta^{\mathrm{reg}}(z)}{2}\right)^2 + a}. \qquad (9)$$

By Banach's Fixed Point Theorem, each of the equations (9) has only one solution in the domain $\mathcal{D}$. In case of the sign «$-$» we denote the root of (9) by z_{nucl}, in case of the sign «$+$» by z_{mol}.

According to [3] and [7], the roots z_{nucl} and z_{mol} of (9) are essentially given by

$$
\begin{aligned}
z_{\mathrm{nucl}} &\cong z_1 - \frac{a}{\lambda_2 - z_1 - \beta^{\mathrm{reg}}(z_1)} \cong z_1 - \frac{a}{\lambda_2 - z_1}, && (10)\\
z_{\mathrm{mol}} &\cong \lambda_2 - \beta^{\mathrm{reg}}(\lambda_2 + i0) + \frac{a}{\lambda_2 - z_1 - \beta^{\mathrm{reg}}(\lambda_2 + i0)} \cong \lambda_2 + \frac{a}{\lambda_2 - z_1}. && (11)
\end{aligned}
$$

From the second condition (8) 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 (3), 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 $z_{\mathrm{mol}} = E_R^{(m)} - i\frac{\Gamma_R^{(m)}}{2}$ with

$$
E_R^{(m)} \cong \lambda_2 - 2\frac{\operatorname{Im} a}{\Gamma_R^{(1)}} \quad \text{and} \quad \Gamma_R^{(m)} \cong 4\frac{\operatorname{Re} a}{\Gamma_R^{(1)}}. \tag{12}
$$

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* $\Gamma_R^{(1)}$.

The second inequality (8), 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 $\Gamma_R^{(1)}$,

$$
C_a \Gamma_R^{(2)} \ll c_{\mathcal{D}} \left(\Gamma_R^{(1)}\right)^2. \tag{13}
$$

This can practically always be assumed for concrete molecules.

Under condition (6) the value of $C_a = |a|/\|b\|^2$ differs from zero, $C_a \geqslant C > 0$, as $\Gamma_R^{(1)} \to 0$. Therefore, 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 the absence of such a resonance. In fact, this ratio is determined by the large quotient $\frac{C_a/c_{\mathcal{D}}}{\Gamma_R^{(1)}}$.

2. MOLECULAR RESONANCES IN A FINITE CRYSTALLINE LATTICE

Let us assume that the «molecules» described by the Hamiltonian (1) are arranged in form of a finite one-dimensional linear (chain) crystalline structure. To describe such a crystal we introduce the lattice Hilbert space

$$
\mathcal{G} = \bigoplus_{i=1}^{n} \mathcal{H}^{(i)} \tag{14}
$$

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

$$
\mathcal{H}^{(i)} = \mathcal{H}_1^{(i)} \oplus \mathcal{H}_2^{(i)}. \tag{15}
$$

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. 1 and, thus, $\mathcal{H}^{(i)} \equiv \mathcal{H}$. The elements of the total Hilbert space $\mathcal{G}$ are represented by the sequences $u = (u^{(1)}, u^{(2)}, \dots, u^{(n)})$ with components $u^{(i)} = \begin{pmatrix} u_1^{(i)} \\ u_2^{(i)} \end{pmatrix}$, 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 $\langle u, v\rangle_{\mathcal{H}} = \sum\limits_{i=1}^{n} \langle u^{(i)}, v^{(i)}\rangle_{\mathcal{H}^{(i)}}$. The subspaces $\mathcal{G}_1 = \bigoplus\limits_{i=1}^{n} \mathcal{H}_1^{(i)}$ and $\mathcal{G}_2 = \bigoplus\limits_{i=1}^{n} \mathcal{H}_2^{(i)}$, with $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$, represent respectively the pure nuclear and pure molecular channels.

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

$$\begin{aligned}
(Hu)^{(1)} &= Au^{(1)} + Wu^{(2)}, \\
(Hu)^{(i)} &= Wu^{(i-1)} + Au^{(i)} + Wu^{(i+1)}, \quad i = 2, \dots, n-1, \\
(Hu)^{(n)} &= Wu^{(n-1)} + Au^{(n)},
\end{aligned} \tag{16}$$

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

$$W = \begin{pmatrix} 0 & 0 \\ 0 & w \end{pmatrix}, \tag{17}$$

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 $\sigma_c(h_1)$ of h_1 and, moreover, that no thresholds of $\sigma_c(h_1)$ belong to this interval. For the sake of simplicity we also assume that the interval belongs to the domain $\mathcal{D}$ introduced in Sec. 1 and that for any $\mu \in [\lambda_2 - 2w, \lambda_2 + 2w]$

$$\operatorname{Im} \langle r_0(\mu \pm i0)\widehat{b}, \widehat{b}\rangle \neq 0. \tag{18}$$

Obviously, the Hamiltonian (16) is a self-adjoint operator on the domain $\operatorname{Dom}(H) = \bigoplus\limits_{i=1}^{n} D^{(i)}$ with $D^{(i)} = \operatorname{Dom}(h_1) \oplus \mathbb{C}$. The resolvent $R(z) = (H - z)^{-1}$ of H possesses a natural block structure, $R(z) = \{R(j,k;z)\}$, $j, k = 1, 2, \dots, n$. The blocks $R(j,k;z)$ satisfy the equations

$$WR(j-1,k;z) + (A - z)R(j,k;z) + WR(j+1,k;z) = \delta_{jk} I, \quad j, k = 1, 2, \dots, n, \tag{19}$$

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 $\operatorname{Im} z \neq 0$ 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 set of the sequences f_k, $k = 1, 2, \dots, n$, with the elements

$$f_k(j) = \sqrt{\frac{2}{n+1}} \sin(p_k j), \tag{20}$$

$$p_k = \frac{\pi k}{n+1}, \tag{21}$$

forms an orthonormal basis for the (n-dimensional) Hilbert space l_2^n of n-element sequences of the form $\{x_1, x_2, \ldots, x_n\}$, $x_j \in \mathbb{C}$, $j = 1, 2, \ldots, n$. The Fourier transform

$$(Fu)(p_k) = \sqrt{\frac{2}{n+1}} \sum_{j=1}^{n} u^{(j)} \sin(p_k j) \tag{22}$$

in $\mathcal{G}$ reduces Eq. (19) to

$$(A - z)R(p_k, p_{k'}; z) + 2\cos p_k \, W R(p_k, p_{k'}; z) = \delta_{kk'} \, I, \quad k, k' = 1, 2, \ldots, n, \tag{23}$$

and the numbers $R(p_k, p_{k'}; z)$ represent the matrix elements of the resolvent $R(z)$ in this representation. From (23) it immediately follows that

$$R(p_k, p_{k'}; z) = G(p_k; z)\delta_{kk'}, \tag{24}$$

where

$$G(p; z) = \begin{pmatrix} r_1(z) + \dfrac{r_1(z) b \langle \cdot, b \rangle r_1(z)}{\widetilde{M}_2(p; z)} & -\dfrac{r_1(z) b}{\widetilde{M}_2(p; z)} \\ -\dfrac{\langle \cdot, b \rangle r_1(z)}{\widetilde{M}_2(p; z)} & \dfrac{1}{\widetilde{M}_2(p; z)} \end{pmatrix} \tag{25}$$

Here, the scalar function $\widetilde{M}_2(p; z)$ reads

$$\widetilde{M}_2(p; z) = \lambda_2 - z + 2w\cos p - \beta(z). \tag{26}$$

The numbers p_k given by (21) represent the quasimomenta of the finite crystalline structure under consideration.

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

$$P_{\mathrm{mol}}(\varphi, t) = \|\mathsf{P}_2 \, \mathrm{e}^{-iHt} \varphi\|^2, \tag{27}$$

where P_2 is the orthogonal projection in $\mathcal{G}$ on the pure molecular subspace $\mathcal{G}_2$. Obviously, one can represent the time evolution operator $\exp(-iHt)$ in terms of the resolvent $R(z) = (H - z)^{-1}$,

$$\exp(-iHt) = -\frac{1}{2\pi i} \oint_{\gamma} dz \, \mathrm{e}^{-izt} (H - z)^{-1}, \tag{28}$$

where the integration is performed along a counterclockwise contour γ in the physical sheet encircling the spectrum of the Hamiltonian H.

According to Eqs. (24) and (26) the operator $\mathsf{P}_2(H - z)^{-1}|_{\mathcal{G}_2}$ acts in quasimomentum representation as the multiplication operator,

$$\Big(\mathsf{P}_2 R(z) \varphi\Big)(p_k) = \frac{1}{\widetilde{M}_2(p_k; z)} \varphi_2(p_k). \tag{29}$$

Here $\varphi_2(p_k)$ stands for the values of the Fourier transform (22) of the vector

$$\varphi_2 = (\varphi_2^{(1)}, \varphi_2^{(2)}, \ldots, \varphi_2^{(n)}).$$

Hence

$$\left(\mathsf{P}_2\, \mathrm{e}^{-iHt}\varphi\right)(p_k) = -\frac{1}{2\pi i}\, \varphi_2(p_k)\, J(p_k,t) \tag{30}$$

with

$$J(p_k,t) = \oint\limits_{\gamma} dz\, \frac{\exp(-izt)}{\widetilde{\lambda}_2(p_k) - z - \beta(z)}\,. \tag{31}$$

Repeating almost literally the analysis of Section III in [7], one finds that the asymptotics of the term $J(p_k,t)$ as $t \to \infty$ reads as follows:

$$\begin{aligned} J(p_k,t) = \\ = \exp\{-iz_{\rm mol}(p_k)t\}&\left[1 - \frac{a}{\left(\widetilde{\lambda}_2(p_k) - z_1 - \beta^{\rm reg}(\widetilde{\lambda}_2(p_k)+i0)\right)^2} + O\left(\varepsilon^4(p_k,\widetilde{\lambda}_2(p_k)+i0)\right)\right] + \\ + \exp\{-iz_{\rm nucl}(p)t\}&\left[\frac{a}{\left(\widetilde{\lambda}_2(p_k) - z_1 - \beta^{\rm reg}(z_1)\right)^2} + O\left(\varepsilon^4(p_k,z_1)\right)\right] + \widetilde{\varepsilon}(p_k,t)\,, \end{aligned} \tag{32}$$

where

$$\varepsilon(p_k,z) = \frac{a}{[\widetilde{\lambda}_2(p_k) - z_1 - \beta^{\rm reg}(z)]^2}\,. \tag{33}$$

The function $\widetilde{\varepsilon}(p,t) = O(\|b\|^2)$ is always small, $|\widetilde{\varepsilon}(p,t)| \ll 1$. By (10) and (11) for the positions of the resonance poles we then obtain

$$z_{\rm nucl}(p_k) \;\cong\; z_1 - \frac{a}{\lambda_2 + 2w\cos p_k - z_1}, \tag{34}$$

$$z_{\rm mol}(p_k) \;\cong\; \lambda_2 + 2w\cos p_k + \frac{a}{\lambda_2 + 2w\cos p_k - z_1}. \tag{35}$$

The asymptotics (32) implies

$$P_{\rm mol}(\varphi,t) = \sum_{k=1}^{n} |J(p_k,t)|^2\, |\varphi_2(p_k)|^2 = \sum_{k=1}^{n} \exp\{-\Gamma_R^{(m)}(p_k)\,t\}\, |\varphi_2(p_k)|^2 + \widetilde{\varepsilon}(t), \tag{36}$$

where

$$\Gamma_R^{(m)}(p_k) = -2\,\mathrm{Im}\, z_{\rm mol}(p_k) \cong -2\,\mathrm{Im}\, \frac{a}{\lambda_2 + 2w\cos p_k - z_1}. \tag{37}$$

The background term $\widetilde{\varepsilon}(t)$ in (36) is small for any $t \geqslant 0$, $\widetilde{\varepsilon}(t) = O(\|b\|^2)$ and $|\widetilde{\varepsilon}(t)| \ll 1$.

Let us next assume that the number n of cells in the lattice is large and the real part $E_R^{(1)}$ of the nuclear resonance z_1 belongs to the interval $[\lambda_2 - 2w, \lambda_2 + 2w]$, that is $|E_R^{(1)} - \lambda_2| \leqslant 2w$. Then, one can always prepare an initial molecular state φ which decays via the nuclear channel with a rate close to $4\frac{\mathrm{Re}\, a}{\Gamma_R^{(1)}}$ (cf. formula (12)). Indeed, under the assumption (7), this maximum is given by

$$\max_{0 \le p \le \pi} \Gamma_R^{(m)}(p) \cong 4\frac{\mathrm{Re}\, a}{\Gamma_R^{(1)}}.$$

The most appropriate is the monochromatic molecular state φ with the only nonzero component $\varphi_2(p_{k_0})$ associated with the quasimomentum p_{k_0} closest to

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

In particular, if the values of $\varphi_2(p_k)$ are nonzero only for quasimomenta p_k restricted by

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

with some small $\delta > 0$, then the width $\Gamma_R^{(m)}$ given by the relation (37) varies in an interval lying approximately between $\frac{1}{1+\delta^2}\frac{4\,\mathrm{Re}\, a}{\Gamma_R^{(1)}}$ and $\frac{4\,\mathrm{Re}\, a}{\Gamma_R^{(1)}}$.

In a similar way one also treats a one-dimensional cyclic crystalline structure. In this case the Hilbert space $\mathcal{G}$ is the same as in (14) but the operator H reads

$$\begin{aligned}
(Hu)^{(1)} &= Wu^{(n)} + Au^{(1)} + Wu^{(2)},\\
(Hu)^{(i)} &= Wu^{(i-1)} + Au^{(i)} + Wu^{(i+1)}, \quad i = 2, \dots, n-1,\\
(Hu)^{(n)} &= Wu^{(n-1)} + Au^{(n)} + Wu^{(1)}.
\end{aligned} \tag{38}$$

If the intercellular interaction is still given by (17), the only difference in the analysis will be the use of another complete orthonormal set in the space l_2^n. Instead of the sequences (20) one now employs the orthonormal sequences

$$f_k(j) = \frac{1}{\sqrt{n}}\exp(ip_k j), \quad j = 1, 2, \dots, n \tag{39}$$

with quasimomenta p_k given by

$$p_k = \frac{2\pi k}{n}, \quad k = 1, 2, \dots, n. \tag{40}$$

After the Fourier transform (22) with $\frac{1}{\sqrt{n}}\exp(ip_k j)$ the matrix elements of the resolvent $(H - z)^{-1}$ again acquire the form (24), (25) with the transfer function $\widetilde{M_2}(p; z)$ given by (26). Hence, one concludes with formulas like in (30)–(37) and then observes that if the number of cells is large enough it is possible to prepare pure molecular states that decay with the rate close to $4\frac{\mathrm{Re}\, a}{\Gamma_R^{(1)}}$.

In the same way one can also consider the finite two- and three-dimensional crystalline structures arranged of the molecular cells described by the Hamiltonian (1). If the cell has a sharp near-threshold nuclear resonance with energy embedded into the convex hull of the arising crystalline molecular levels, one again will find an enhancement of the decay rate for particular molecular states. As in the case of the one-dimensional lattices, these molecular states should decay with the rate close to $4\frac{\operatorname{Re} a}{\Gamma_R^{(1)}}$.

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