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# Model system with periodicity both in energy and time: an unconventional type of zone structure

V N Ostrovsky

Insitute of Physics, University of St Petersburg, 198904 St Petersburg, Russia

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**Abstract.** Two infinite bands of equidistant potential curves cross each other forming patterns which are periodic both in time and in energy. The dependence of the quasi-energy on the quasi-momentum (related to the translations along the energy axis) manifests zone structure analogous to that known in solid state physics. The properties of the zones are analysed.

Recently a quantum model problem was considered with the crossing of two bands of potential curves [1–3]. Mathematically it implies the solution of the time-dependent Schrödinger equation in matrix form. The original (*diabatic*) basis vector states are subdivided in two groups, each of them being infinitely dimensional. The Hamiltonian matrix $H$ within each of these subspaces is diagonal with the diagonal elements respectively

$$H_{nn}(t) = \omega n + \beta t \tag{1}$$

and

$$H_{nn}(t) = \omega n - \beta t. \tag{2}$$

These matrix elements are named *diabatic potential curves* bearing in mind their dependence on time $t$. The parameter $\omega$ is the level spacing within each of two bands (1) or (2); $\beta$ is the slope of potential curves which differs in sign for the first and the second bands. Hence we have two *parallel and equidistant* bands of *linear* diabatic potential curves crossing each other. All the matrix elements of the Hamiltonian between the basis vectors belonging to *different subspaces* are assumed to be the same and equal to the *interaction (or coupling)* parameter $V$ which is time independent.

The eigenvalues of the Hamiltonian $H(t)$ calculated for the fixed time $t$ are generally named *adiabatic potential curves* (as functions of time $t$). For the model under consideration they were obtained [1] as

$$E_{N\pm}(t) = \pm\frac{\omega}{2\pi}\cos^{-1}\left(\frac{\omega^2 - \pi^2V^2}{\omega^2 + \pi^2V^2}\cos\frac{2\pi\beta t}{\omega}\right) + N\omega. \tag{3}$$

Each adiabatic curve is labelled by the double subscript $\pm$ and $N$, where $N$ is an integer ($N = 0, \pm1, \pm2, \ldots$). It is convenient [2] to characterize the coupling by the parameter $s$ ($0 \leqslant s \leqslant \frac{1}{2}$) instead of $V$:

$$\tan\pi s \equiv \frac{\pi V}{\omega}. \tag{4}$$

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Then (3) is rewritten as

$$E_{N\pm}(t) = \pm\frac{\omega}{2\pi}\cos^{-1}\left(\cos 2\pi s \cos\frac{2\pi\beta t}{\omega}\right) + N\omega. \tag{5}$$

We will use the shortened notation $E_0(t) \equiv E_{0+}(t)$.

There are numerous physical realizations of the model† as already discussed [1, 3]. Therefore the properties of the model seem to deserve study. Some of them are the subject of the present communication.

The *adiabatic eigenstates* corresponding to the eigenvalues (3) or (5) were found by Demkov and Ostrovsky ([1], see formulae (2.1), (2.3) and (2.6)) and presented in a more compact form by Demkov *et al* ([2], see formula (16)), where they were denoted as $\tilde{\psi}^{\pm,N}(t)$.

An arbitrary time-dependent solution of the Schrödinger equation can be expanded over the adiabatic basis

$$\Psi(t) = \sum_N [c^{+,N}(t)\tilde{\psi}^{+,N}(t) + c^{-,N}(t)\tilde{\psi}^{-,N}(t)] \tag{6}$$

where the coefficients obey the system of equations

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}c^{+,N}}{\mathrm{d}t} &= E_{N+}(t)c^{+,N} + \sum_M \langle\tilde{\psi}^{+,N}|\tilde{H}(t)|\tilde{\psi}^{-,M}\rangle c^{-,M} \\ \mathrm{i}\frac{\mathrm{d}c^{-,N}}{\mathrm{d}t} &= E_{N-}(t)c^{-,N} + \sum_M \langle\tilde{\psi}^{-,N}|\tilde{H}(t)|\tilde{\psi}^{+,M}\rangle c^{+,M}. \end{aligned} \tag{7}$$

The right-hand side of these equations contains some matrix elements which can be considered as the matrix elements of the effective Hamiltonian in the adiabatic basis. They were obtained by Harmin [3] in the simple explicit form

$$\begin{aligned} \langle\tilde{\psi}^{-,N}|\tilde{H}(t)|\tilde{\psi}^{+,M}\rangle &= -\langle\tilde{\psi}^{-,M}|\tilde{H}(t)|\tilde{\psi}^{+,N}\rangle \\ &= \mathrm{i}\frac{\pi\beta}{\omega}\sin(2\pi s)\frac{(-1)^{N-M-1}}{[2\pi E_0(t)/\omega - \pi(N-M)]^2}. \end{aligned} \tag{8}$$

Note that the direct coupling inside the subspaces of adiabatic $\tilde{\psi}^{+,N}$ or $\tilde{\psi}^{-,N}$ states is absent, i.e.

$$\langle\tilde{\psi}^{+,N} \mid \tilde{H}(t)|\tilde{\psi}^{+,M}\rangle = \langle\tilde{\psi}^{-,N}|\tilde{H}(t)|\tilde{\psi}^{-,M}\rangle = 0. \tag{9}$$

An advantage of the adiabatic representation is that the adiabatic potential curves (5) and the matrix elements (8) are explicitly periodic in time $t$ with the period $T_1 = \omega/\beta$. In addition, the system retains the specific property which it also has in the diabatic basis [1]. Namely, equations (7) are invariant under 'translation in the indices': $\{N, M\} \Rightarrow \{N + J, M + J\}$ for an arbitrary integer $J$. In the adiabatic basis this follows from the fact that the coupling (8) depends only on the difference of indices $N - M$. This transformation can also be considered as a *translation along the energy axis*. Invariance under such a transformation is a unique property of the model under consideration.

In order to fully account for this translational invariance, we look for the solution of (7) in the form, which is analogous to the Bloch wavefunctions for the electron in the space-periodic lattice:

$$c^{\pm,N}(t) = \exp[\mathrm{i}N(\kappa + \omega t)]C^{\pm}(t). \tag{10}$$

† Here we add only that the recent paper by Zobay and Alber [4] treats the wave packets of electronic states in Rydberg atoms under laser field and presents the plot of energies for the dressed Rydberg states (figures 9(a) and (b)) which essentially coincides with the plots of adiabatic curves (3) shown in figure 1 of [1].

Here $\kappa$ is the analogue of quasi-momentum introduced in the solid state physics. It can be checked easily using (5), (7) and (8) that $C^+(t)$ and $C^-(t)$ do not depend on the index $N$. These functions obey a system of two equations:

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}C^+(t) &= E_0(t)C^+(t) - \mathrm{i}G(\kappa,t)C^-(t) \\ \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}C^-(t) &= -E_0(t)C^-(t) + \mathrm{i}G(\kappa,t)C^+(t) \end{aligned} \tag{11}$$

where

$$\begin{aligned} G(\kappa,t) &= \frac{\pi\beta}{\omega}\sin(2\pi s)\sum_{m=-\infty}^{\infty}\frac{\exp[-\mathrm{i}m(\kappa+\omega t)+\mathrm{i}\pi m]}{[2\pi E_0(t)/\omega-\pi m]^2} \\ &= \frac{2\pi\beta}{\omega}\sin(2\pi s)\sum_{m=0}^{\infty}\frac{(-1)^m\cos[m(\kappa+\omega t)]}{[2\pi E_0(t)/\omega-\pi m]^2}. \end{aligned} \tag{12}$$

In the latter representation the function $G(\kappa,t)$ is explicitly real. Note that $C^+$ and $C^-$ depend parametrically on $\kappa$, although this dependence is suppressed in the notations.

At this stage we can note that the periodicity issue for the problem under consideration is not that simple. In order to discuss it we introduce the function

$$G(\kappa,t_1,t_2) = \frac{2\pi\beta}{\omega}\sin(2\pi s)\sum_{m=0}^{\infty}\frac{(-1)^m\cos[m(\kappa+\omega t_2)]}{[2\pi E_0(t_1)/\omega-\pi m]^2}. \tag{13}$$

For $t_1 = t_2 = t$ it coincides with the function (12). We see that the function (13) has the period $T_1 = \omega/\beta$ in the 'time' variable $t_1$ and the period $T_2 = 2\pi/\omega$ in the 'time' variable $t_2$. The second period $T_2$ is the period for the revival of an arbitrary wave packet in the system with equidistant energy levels. Generally the periods $T_1$ and $T_2$ are incommesurable. Thus, in fact, we have a doubly-periodic problem which is somewhat hidden in the other representations.

Furthermore, we consider the special case with equal periods: $T_1 = T_2 \equiv T$ which imposes a restriction on the system parameters, $\omega^2 = 2\pi\beta$.

The non-stationary systems, periodic in time, are conventionally described using the quasi-energy (or Floquet-state) formulation (see, for instance, [5]). Namely, one looks for the solutions $\psi_\epsilon(t)$ with the definite quasi-energy $\epsilon$. Such states have to satisfy the condition $\psi_\epsilon(t+T) = \exp(\mathrm{i}\epsilon T)\psi_\epsilon(t)$, where $T$ is the period.

In our case we take some fixed value of the quasi-momentum $\kappa$ and look for the quasi-energetic solutions of (11). Thus the quasi-energy is obtained as some function of the quasi-momentum $\epsilon(\kappa)$. In solid state physics the dependence of energy on the quasi-momentum manifests universally known zone structure. It is interesting to construct its analogue in the present quite unconventional situation.

We did not succeed in the analytical solution of this problem (even the closed expression for the coupling function $G(\kappa,t)$ (12) cannot be obtained for arbitrary values of the arguments). However, the numerical treatment does not pose any problem. The equations (11) were solved numerically on the interval $0 \leqslant t \leqslant T$ and the propagation matrix was diagonalized; its eigenvalues are expressed via the quasi-energies as $\exp(\mathrm{i}\epsilon T)$. There are two values of the quasi-energy differing by sign; below we will refer to the positive one (see figure 1). Note that the function $\epsilon(\kappa)$ depends parametrically on the coupling $V$ (or $s$).

Some general properties of the function $\epsilon(\kappa)$ can be established.

(1) The function $\epsilon(\kappa)$ is even and periodic with period $2\pi$ like the function $G(\kappa,t)$. Thus the interval $[0, 2\pi]$ is 'the unit cell' on the $\kappa$ axis, i.e. analogue of the Brillouin zones considered in solid state physics.

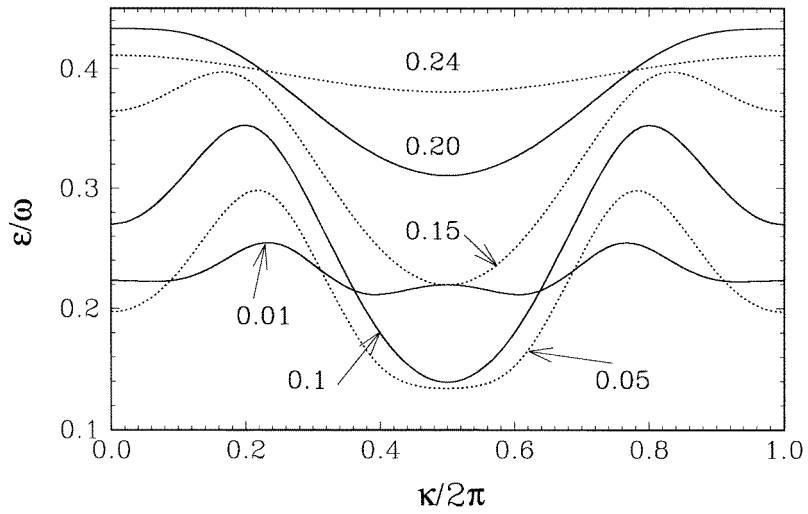


**Figure 1.** Zone structure: reduced quasi-energy $\epsilon/\omega$ as a function of the reduced quasi-momentum $\kappa/(2\pi)$ for various values of the coupling parameter $s$ indicated in the figure.

(2) The function $G(\kappa, t)$ does not change under the transformation $\{\kappa \Rightarrow 2\pi - \kappa, t \Rightarrow T - t\}$. Therefore $\epsilon(\kappa)$ is symmetric with respect to the point $\kappa = \pi$.

(3) There is a less evident relation between the functions $\epsilon(\kappa)$ for various values of the coupling parameter. Namely, the transformation $\{s \Rightarrow \frac{1}{2} - s, \kappa \Rightarrow \kappa + \pi, t \Rightarrow t + \frac{1}{2}T\}$ does not change the functions $E_0(t)$ and $G(\kappa, t)$. Hence we have the relation $\epsilon(\kappa, s) = \epsilon(\kappa + \pi, \frac{1}{2} - s)$. Therefore it is sufficient to consider the domain $0 \leqslant s \leqslant \frac{1}{4}$.

(4) If the coupling is absent ($s = 0$), then the quasi-energy does not depend on $\kappa$ and can easily be evaluated as the adiabatic energy $E_0(t)$ averaged over the period: $\epsilon = \frac{1}{4}\omega$. Note that even for weak coupling quite strong deviations appear from this value (figure 1).

(5) There is another less trivial case when the zone is completely flat. Namely, for $s = \frac{1}{4}$ the adiabatic potential curves become constant [1]: $E_0(t) = \frac{1}{4}\omega$. In this case the function $G(\kappa, t)$ depends only on the linear combination of its arguments, $\kappa + \omega t$. Clearly this leads to some constant value for the function $\epsilon(\kappa)$. The latter is obtained from the numerical calculations as $0.3965\omega$.

As a summary, we have considered a unique problem with periodicity both in energy and time and have found an unconventional zone structure for this system in the quasi-energy as a function of the quasi-momentum.

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