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QUANTUM DYNAMICAL SYSTEMS WITH SOME DEGREES OF FREEDOM

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The topological nature of the space of complex systems, characterized by the interaction of fast (intrinsic) degrees of freedom with slow (collective) degrees of freedom, gives rise to monopole gauge potentials and, as consequences, to such interesting phenomena as nonintegrable geometric phase [1, 3] discovered by Berry [1], the molecular Aharonov-Bohm effect [4] and chaos for the collective dynamics [5]. The conditions for the existence of such phenomena very often occur if real or avoided level crossings take place. Here we investigate the role of the level crossing for collective motion in the presence of fast dynamics of separate particles in a system in the framework of the adiabatic representation method. It enables one to take into account the mutual influence of slowly varying collective fields and rapidly varying intrinsic fields.

In the adiabatic approach, solution of the whole scattering problem is reduced to two effective scattering problems in the spaces of a lower dimension, then the original one $\mathcal{M} = \mathsf{B} \times \hat{\mathsf{M}}$. The N–dimensional inverse scattering problem in the adiabatic representation is formulated on the basis of consistent formulation of the both multichannel inverse problem for the gauge system of equations describing "slow" dynamics of the complex system and the parametric problem for "fast" dynamics [6] – [9]. Based on the multichannel and one-channel technique of Bargmann potentials for a system of coupled equations and the parametrically dependent equation, the method of analytic modeling of effective interactions in complicated quantum systems with some degrees of freedom and finding appropriate solutions has been developed in [7] – [9].

Suppose that the state $|\Psi(t)>$ of the system evolves according to the Schrödinger equation

$$i\hbar\frac{d|\Psi(t)>}{dt} = H(t)|\Psi(t)> . \qquad (1)$$

If $\phi_n(x(t); y)$ are solutions to the equation

$$H(\mathbf{x}(t))|\phi_n(\mathbf{x}(t); y) >= \mathcal{E}_n(\mathbf{x}(t))|\phi_n(\mathbf{x}(t); y) > \qquad (2)$$

and form a complete orthonormal set $\{|\phi_n(\mathbf{x}(t), y) >\}$, with elements depending on $x = x(t)$ parametrically, then Ψ can be given [10] by the expansion

$$|\Psi(t, \mathbf{x}(t), \mathbf{y}) >= \sum_n c_n(t) exp(-\frac{i}{\hbar}\int_0^t \mathcal{E}_n(\mathbf{x}(t'))dt')|\phi_n(\mathbf{x}(t); \mathbf{y}) > . \qquad (3)$$

Upon substituting this expansion (3) into the equation (1) with an account of orthogonality $< n|m >= \delta_{nm} \; \forall \, \mathbf{x}$ of the eigenfunctions $|\phi_n(t) > \equiv |n(t) >$ of H we arrive at the following system of linear differential equations for the expansion coefficients $c_n(t)$

$$i\hbar \frac{dc_n(t)}{dt} = -\mathcal{E}_n(t)c_n(t) + \Big\{ -i\hbar \sum_m < m|\dot{n} > c_m(t) + \sum_m < m|H|n > c_m(t) \Big\} exp[-\frac{i}{\hbar}\int_0^t (\mathcal{E}_n(t') - \mathcal{E}_m(t'))dt']. \quad (4)$$

With an account of (2) the system of equations for $c_n(t)$ may be written in the form

$$\dot{c}_n(t) = \sum_m B_{nm}(\mathbf{x}(t)) exp[-\frac{i}{\hbar}\int_0^t (\mathcal{E}_n(t') - \mathcal{E}_m(t'))dt'] c_m(t). \quad (5)$$

Here, the matrix elements of exchange interaction

$$B_{nm}(\mathbf{x}(t)) =< n|\dot{m} >= A_{nm}(\mathbf{x}) \cdot \dot{\mathbf{x}}(t),$$

are generated by basis functions $|n >$ of "instantaneous" Hamiltonian (2) where

$$A_{nm}(\mathbf{x}) =< n(\mathbf{x})| \nabla_{\mathbf{x}} |m(\mathbf{x}) > . \quad (6)$$

Differentiating eq.(2) with respect to t for $n \neq m$ one can find

$$< m|\dot{n} >=< m|\dot{H}|n > /(\mathcal{E}_n - \mathcal{E}_m).$$

In the adiabatic approximation, when the admixture of other states to a given state n is small, evaluation of nondiagonal elements of the relation (5) leads to the following condition

$$\frac{< m|\dot{H}|n >}{(\mathcal{E}_n - \mathcal{E}_m)^2} \ll 1. \quad (7)$$

Then the relation (5) yields

$$c_n(t) = c_n(0) exp[-\int_0^t < n|\dot{n} > dt'].$$

Berry [1] showed, for a cyclic adiabatic evolution, the phase

$$\delta = -i\int_0^T < n|\dot{n} > dt'$$

is independent on the choice of the state $|n(t) >$ and therefore it reflects a geometrical property of the parameter space of which $H(\mathbf{x}(t))$ is function.

In the vicinity of level crossings, as can be easily seen, the adiabatic approximation (7) is invalid. In these cases one usually assumes diabatic Landau–Zener dynamics. In papers [5],[11] the mutual influence of collective and intrinsic degrees of freedom is investigated and it is shown that the transition region between the diabatic and adiabatic pictures of the interaction exists and it is impossible to pass smoothly between adiabatic and diabatic dynamics.

We study the problem of the level crossing on the basic of exactly solvable models within the adiabatic approach. Using the results of [7] – [9] we shall write down an algebraic scheme of the solution of the parametric inverse problem in the adiabatic representation and construct a lot of potentials $V(x, y)$ for which solutions$|\phi(x; y) >$ to the parametric Schrödinger Eq.(2) in a closed analytic form can be found. Thereafter, for a given functional dependence of spectral characteristics $\{\mathcal{E}_n(x), \mathcal{S}(x, k)\}$ on dynamic variables x, we can trace the behavior of matrix elements of the operator of induced connection (6) when the levels move towards the crossing in both approaches: the consistent adiabatic one and in the case of the system evolving according to (1), (2).

In the consistent adiabatic approach, the parametric dependence of potential curves $\mathcal{E}_i(x)$ on "slow" variables should be determined by solving the inverse problem for a system of gauge equations

$$[-(\nabla \otimes I - iA(\mathbf{x}))^2 + V(\mathbf{x}) \otimes I - P^2]F(\mathbf{x}) = 0, P = diag(p_n), \quad (8)$$

generated by the procedure of adiabatic expansion of the wave function

$$|\psi(\mathbf{X}) >= |n >< n|\psi >= \sum_n \int \phi_n(\mathbf{x}; \mathbf{y}) F_n(\mathbf{x}) \quad (9)$$

of the total Hamiltonian H over eigen states of the self-adjoint parametric Hamiltonian h^f

$$h^f(\mathbf{x})|\phi_n(\mathbf{x}; \mathbf{y}) >= \mathcal{E}_n(\mathbf{x})|\phi_n(\mathbf{x}; \mathbf{y}) >, \quad h^f(\mathbf{x}) = -\Delta_{\mathbf{y}} + V(\mathbf{x}, \mathbf{y}). \quad (10)$$

The matrix elements

$$A_{nm}(\mathbf{x}) =< \phi_n(\mathbf{x}; .)|i\nabla_{\mathbf{x}}|\phi_m(\mathbf{x}; .) >, \quad (11)$$

are components of the connection operator A on the Hilbert fibre bundle $\mathcal{H}(\mathsf{B}, \mathcal{F}_x, \pi)$ realizing the coupling between channels in contrast with the ordinary coupled channel method. The matrix components

$$V_{nm}(\mathbf{x}) =< \phi_n(\mathbf{x};.)|h^f(\mathbf{x})|\phi_m(\mathbf{x};.) >= \mathcal{E}_n(\mathbf{x})\delta_{nm} \tag{12}$$

are the diagonal elements of effective scalar potential coinciding with the energetic levels $\mathcal{E}_n(x)$ of the "fast" Hamiltonian (2) or (10). The connection operator A represents an effective gauge field in the "slow" system of equations and generates the unitary bilocal operator $\mathcal{U}(\mathbf{x},\mathbf{x}_o) = P\exp i\int_{\mathbf{x}} A(\mathbf{x}')d\mathbf{x}'$ acting from $\mathcal{F}_{\mathbf{x}_o}$ to $\mathcal{F}_{\mathbf{x}}$. Upon such gauge transformation, the effective scalar and vector potentials $V(\mathbf{x})$ and $A(\mathbf{x})$ are transformed as

$$V'(\mathbf{x}) = \mathcal{U}(\mathbf{x})V(\mathbf{x})\mathcal{U}^{-1}(\mathbf{x}), \quad A'(\mathbf{x}) = \mathcal{U}(\mathbf{x})A(\mathbf{x})\mathcal{U}^{-1}(\mathbf{x}) - i\mathcal{U}^{-1}(\mathbf{x})\nabla_{\mathbf{x}}\mathcal{U}.$$

Now, using the unitary gauge transformation, one can annihilate A and reduce the system of equations (8) to the system of ordinary equations for the new coefficients $F' = \mathcal{U}F$ coupled by means of the effective potential matrix $V'(\mathbf{x})$

$$[-\nabla^2 + V'(\mathbf{x}) - P^2]F'(\mathbf{x},P) = 0. \tag{13}$$

Now one can apply the methods of the ordinary multichannel inverse scattering problem because the completeness is valid for the physical and regular solutions of the system (13).

At the beginning we reconstruct the potential matrix $V'(x)$ and find the solutions F' from the set of scattering data $S(P); \{E_n, \gamma_n^2\}$ corresponding to the system (13), using the multichannel Gel'fand–Levitan–Marchenko equations. Now in order to find energy terms (12) $\mathcal{E}(x)$ and the matrix of diagonalization $\mathcal{U}(x)$ it is necessary to solve the algebraic eigenvalue problem

$$V'(x)\mathcal{U}(x) = \mathcal{U}(x)\mathcal{E}(x). \tag{14}$$

In this method the potential curves $\mathcal{E}(x)\forall x \in$ B are found from the solution of the inverse scattering problem for the system of equations, instead of the solution of the direct eigenvalue problem for the reference equation with the parametric Hamiltonian (10).

With the help of the technique of degenerate kernels we will present an example of a two-dimensional exactly solvable model via generalizing the Bargmann-potential technique to the parametric family of the inverse problems and the system of coupled equations. Let us reconstruct

reflectionless potential matrices with respect to slow variables. At the reconstruction of such potentials in the kernel $Q(x,x')$ only the sum over bound states remains

$$Q_{ij}(x,x') = \sum_{\lambda}^{N} \exp(-\kappa_i^\lambda x)\gamma_i^\lambda\gamma_j^\lambda \exp(-\kappa_j^\lambda x). \tag{15}$$

From the matrix analog of the inversion main equations

$$K(x,x') + Q(x;x') + \int_x^\infty K(x,x'')Q(x'',x')dx'' = 0, \tag{16}$$

$$V(x) = \overset{\circ}{V}(x) - 2\frac{d}{dx}K(x,x), \tag{17}$$

$$\phi(k,x) = \overset{\circ}{\phi}(k,x) + \int_x^\infty K(x,x')\overset{\circ}{\phi}(k,x')dx', \tag{18}$$

it is easily obtained the explicit form for the elements of the potential matrix and the solutions [12]

$$V'_{ij}(x) = 2\frac{d}{dx}\sum_{\nu\lambda} \exp(-\kappa_i^\nu x)\gamma_i^\nu P_{\nu\lambda}^{-1}(x)\gamma_j^\lambda \exp(-\kappa_j^\lambda x), \tag{19}$$

$$F'^{\pm}_{jj'}(k,x) = \exp(\pm ik_jX)\delta_{jj'} - \frac{\gamma_j\gamma_{j'}\exp(-\kappa_j x)\int_x^\infty \exp(-(\kappa_{j'} \pm ik_{j'})x')dx'}{1 + \sum_i^m(\gamma_i^2/2\kappa_i)\exp(-2\kappa_i x)} \tag{20}$$

where

$$P_{\nu\lambda} = \delta_{\nu\lambda} + \sum_{j'}^{m} \frac{\gamma_{j'}^\nu\gamma_{j'}^\lambda}{\kappa_{j'}^\nu + \kappa_{j'}^\lambda}\exp(-(\kappa_{j'}^\nu + \kappa_{j'}^\lambda)x).$$

Now one can obtain $\mathcal{E}(x)$, $\mathcal{U}(x)$, and $\delta(x)$ from diagonalizing procedure (14) of the potential matrix V'. Let us consider two channel exactly solvable model: the channel indices take only two values $i,j = 1,2$. The diagonalization matrix $\mathcal{U}(x)$ is

$$\mathcal{U}(x) = \begin{pmatrix} cos\ \delta(x)/2 & sin\ \delta(x)/2 \\ -sin\ \delta(x)/2 & cos\ \delta(x)/2 \end{pmatrix}. \tag{21}$$

Here

$$\delta(x)/2 = \int_x A_{12}(x')dx'.$$

From the relation (14) follow

$$\begin{pmatrix} \mathcal{E}_1 cos^2\,\delta/2 + \mathcal{E}_2 sin^2\,\delta/2 & (\mathcal{E}_1 - \mathcal{E}_2) cos\,\delta/2\; sin\,\delta/2 \\ (\mathcal{E}_1 - \mathcal{E}_2) cos\,\delta/2\; sin\,\delta/2 & \mathcal{E}_1 sin^2\,\delta/2 + \mathcal{E}_2 cos^2\,\delta/2 \end{pmatrix} = \begin{pmatrix} V'_{11} & V'_{12} \\ V'_{21} & V'_{22} \end{pmatrix}.$$

As a result, we obtain

$$tg\;\delta(x) = \frac{2V'_{21}(x)}{V'_{11}(x) - V'_{22}(x)} \quad or \quad sin\;\delta(x) = \frac{2V'_{21}(x)}{\mathcal{E}_1(x) - \mathcal{E}_2(x)}, \tag{22}$$

$$\mathcal{E}_{1,2}(x) = \frac{1}{2}[V'_{11}(x) + V'_{22}(x) \pm \frac{V'_{12}(x)}{sin\;\delta(x)}]. \tag{23}$$

This is the simple and fruitful model for investigating the level crossing problem using analytical expressions (19) and (21).

Really, let us consider the transparent potential matrix with one bound state $\nu = 1$ and one threshold; $E_1 = -\kappa_j^2 + \epsilon_j, j = 1, 2, E_1 = -0.5$, $\epsilon_1 = 0, \epsilon_2 = 0.25, \gamma_1^1 = 1, \gamma_2^1 = 0.001$. The elements of the potential matrix V'_{ij} and the corresponding terms $\mathcal{E}_j(x)$ are presented in Fig.1, Fig.2. The vector potential elements $A_{12} = -A_{21}$ and argument $\delta(x)$ are shown in Fig. 3,4, accordingly. One can see that the matrix elements A are singular at the points of the level crossing.

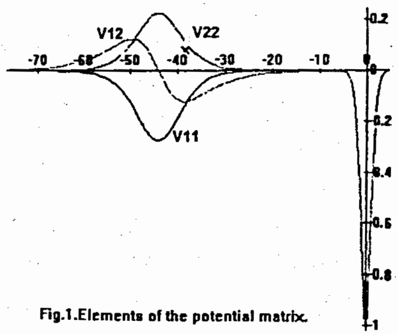

Fig.1.Elements of the potential matrix.

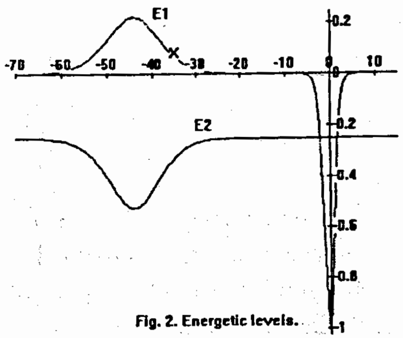

Fig. 2. Energetic levels.

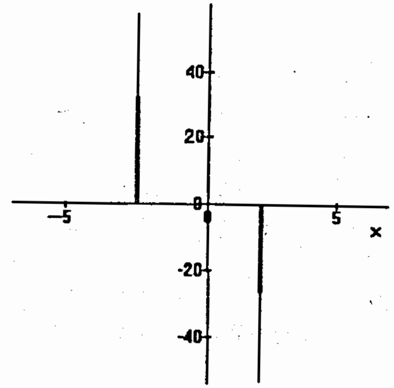

Fig. 3. Components of the vector potential.

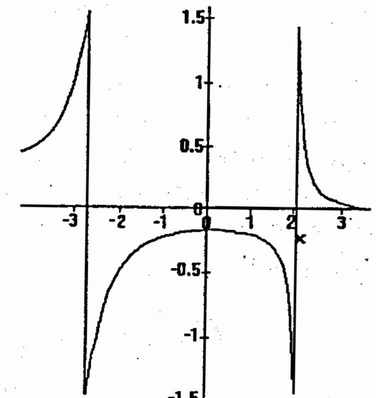

Fig. 4. The argument of the transformation U.

The behaivior of $\delta(x)$ is very interesting. By the first level crossing $\delta(x_2) - \delta(x_1)$ changes 2π and the function changes its sign

$$\begin{pmatrix} F_1(x_2) \\ F_2(x_2) \end{pmatrix} = - \begin{pmatrix} F_1(x_1) \\ F_2(x_1) \end{pmatrix}. \tag{24}$$

The change of the function sign is topological effect, arising in the simple case of the two-channel system in the one-dimensional space of slow variables $x \in \mathsf{B}$. As a result of the second crossing, 2π is once more added to δ and the function sign is reconstructed. Therefore in spite of the evident appearance of topological phase at the level crossings it is not detected in our closed physical system.

The multidimensional potential $V(\mathbf{x})$ can be reconstructed and functions of the moving vector $\phi(x, y)$ found by means of the parametric inverse problem for (10) in Marchenko or Gelfand–Levitan approaches with the scattering data $\{s(x, k), \gamma_n^2(x), \mathcal{E}_n(x)\}$ or spectral data $\{\rho(x, k), N^2(X), \mathcal{E}(x)\}$. The peculiarity of the nonstandard parametric inverse problem is that the spectral data, on which potentials are restored, are dependent on "slow" coordinate variables x. The rational Jost functions

$$f(x;k) = \overset{\circ}{f}(k) \prod \frac{k - i\alpha(x)}{k + i\beta(x)} \tag{25}$$

will be reply the Bargmann type potentials (for details see [9]).

Reflectionless (transparent) potentials along the fast variable are described by the one-dimensional inverse problem along the whole axis with the zero-th reflection coefficient, $\mathcal{S}^{ref} = 0$. The transmission coefficient $\mathcal{S}^{tr}$ with the absolute value equal to unity is a rational function. Then $Q(x;y,y')$

$$\begin{aligned} Q(x;y,y') &= \frac{1}{2\pi}\int_{-\infty}^{\infty} s^{ref}(x;k)\exp[ik(y+y')]dk \\ &+ \sum_n^m \gamma_n^2(x)\exp[-\kappa_n(x)(y+y')], \end{aligned} \tag{26}$$

will contain only the contribution of states of the discrete spectrum

$$Q(x;y,y') = \sum_n^m \gamma_n^2(x)\exp[-\kappa_n(x)(y+y')]. \tag{27}$$

Analogously, for $K(x;y,y')$ we have

$$K(x;y,y') = -\sum_n^m \gamma_n^2(x) f(i\kappa_n(x),y)\exp[-\kappa_n(x)y']. \tag{28}$$

Symmetrical transparent potentials and according wave functions are completely defined by the energetic levels [13] due to the fact that the normalized functions can be determined by the energetic levels

$$\gamma_n^2(x) = iRes\mathcal{S}^{tr}(k)_{/k=i\kappa_n(x)} = 2\kappa_n(x)\prod_{m\neq n}\left|\frac{\kappa_m(x)+\kappa_n(x)}{\kappa_m(x)-\kappa_n(x)}\right|. \tag{29}$$

The normalizations, in more general case of nonsymmetrical transparent potential, are defined by the ordinary normalizations M_n^2 and the matrix of transformation $\mathcal{U}(x)$

$$\gamma_n^{-2}(x) = \int_0^\infty |f(i\kappa_n(x),y)|^2 dy = \sum_j^m \mathcal{U}_{nj}(x)M_j^{-2}\mathcal{U}_{jn}(x). \tag{29a}$$

For the Jost solutions at $k = i\kappa_n(x)$ we get from the main equations of the parametric inverse problem the following system of the algebraic equations

$$\phi(i\kappa_n(x),y) = \sum_j \exp(-\kappa_j(x)y)P_{jn}^{-1}(x;y) \tag{30}$$

with the matrix of the coefficients $P_{jn}(x;y)$ parametrically depending on x:

$$P_{nj}(x;y) = \delta_{nj} + \frac{\gamma_n^2(x)\exp[-(\kappa_n(x)+\kappa_j(x))y]}{\kappa_n(x)+\kappa_j(x)}.$$

Upon substituting $f(i\kappa_n(x),y)$ into $K(x;y,y')$ (28) and using relations of the inverse problem [9], we get

$$V(x;y) = -2\frac{d^2}{dy^2}\ln\det||P_{nj}(x;y)||, \tag{31}$$

$$\begin{aligned} f_\pm(x;k,y) &= \exp(\pm iky) \\ &+ \sum_{nj}\gamma_n^2(x)\exp[-\kappa_n(x)y]P_{nj}^{-1}(x;y)\frac{\exp[(-\kappa_j(x)\pm ik)y]}{\kappa_j(x)\mp ik}. \end{aligned} \tag{32}$$

Now using the potential curves and their normalizations determined upon solving the inverse problem (16) – (18) for the slow system of equations and diagonalization procedure (14) we can reproduce the model multidimensional potential in an explicit form and get the corresponding solutions. In particular, in the considered case of two potential curves we substitute relations (23) and (29) into (31) and (32) and obtain two-dimensional exact models in the closed analytic form.

The matrix elements (6) or (11) of the induced connection A can be computed in terms of the analytical eigenfunctions of Eqs.(2) or (10) for a given functional dependence of scattering data $\{\mathcal{E}_n(x),\ \gamma_n^2(x),\ \mathcal{S}(x,k)\}$ on the slow coordinate variables x. After that the transition amplitudes $c(t)$ can be defined from (4). Consider the case of two crossing terms defined as follows $\mathcal{E}_1 = 2/ch^2(x/2), \mathcal{E}_2 = 1/ch^2(x/3)$. The behavior of matrix elements $A_{12} = -A_{21}$ is pictured on the fig.6. They are singular in the points of level crossing. For the comparison we present situation without level crossing (fig.5): $\mathcal{E}_1 = 2/ch^2(x/2), \mathcal{E}_2 = 1/ch^2(x/3) + 0.5$.

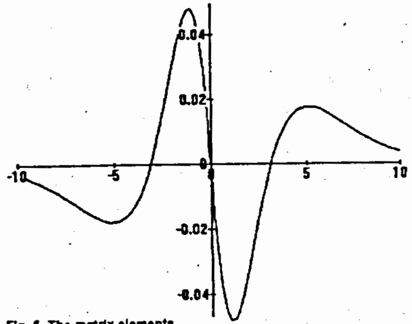

Fig. 5. The matrix elements of the induced connection A without level crossing.

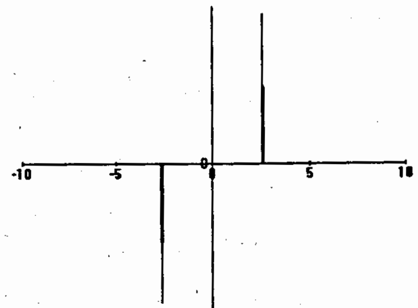

Fig.6. The matrix elements of the induced connection A with level crossing.

The method of investigating the level crossing problem with the use of analytical expressions in the framework of the adiabatic approach is suggested. Level crossings induce nontrivial connections and, consequently, monopole gauge potentials, which can produce an important effect on the behavior of physical systems. By the analyzing of the simple two-channel exactly solvable models it was shown that the system acquires the topological phases at level crossings which take place even in the one-dimensional slow moving cases but it is not manifested at two level crossigs.

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