EXACTLY SOLVABLE MULTISTATE COULOMB MODEL FOR NON-ADIABATIC TRANSITIONS

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Solving Schrödinger equation in a finite basis of states is of importance in various applications of quantum mechanics, and, in particular, in atomic collisions. If an exact analytical solution is achieved, then one is capable to describe transitions between several closely coupled states (channels) with a full account for non-adiabatic effects. The number of exactly solvable *multistate* models is very limited. Apparently the most known one is Demkov-Osherov [1] model which provides multistate generalisation of two-state Landau-Zener model.

In this study we obtain exact solution of non-stationary Schrödinger equation with an arbitrary number of states N and arbitrary number of parameters. The model Hamiltonian matrix corresponds to a single diabatic potential curve with Coulomb dependence on time, $\sim 1/t$. An arbitrary number of other diabatic potential curves are horizontal, i.e. time-independent and with arbitrary energies. The horizontal states are coupled by constant interactions to the Coulomb state.

The wave function $|\Psi\rangle$ is presented as expansion over basis of *diabatic* channel states $|\alpha\rangle$ ($\alpha = 0, 1, 2, \ldots N-1$)

$$|\Psi(t)\rangle = \sum_{\alpha} \psi_\alpha(t)\, |\alpha\rangle \ .$$

The non-stationary Schrödinger equation provides set of coupled differential equations for expansion coefficients $\psi_\alpha(t)$:

$$\begin{aligned} \left(-i\,\frac{d}{dt} - \frac{Z}{vt} + D_0\right)\psi_0(t) + \sum_j V_j\,\psi_j(t) &= 0\ , \\ \left(-i\,\frac{d}{dt} + D_j\right)\psi_j(t) + V_j^*\,\psi_0(t) &= 0\ , \end{aligned}$$

where V_j is t-independent coupling between 0-th and j-th channels, v is velocity parameter, parameter Z is interpreted as charge. The parameter D_j is *diabatic* 'dissociation limit' for α-th channel. Note that the adiabatic dissociation limits differ from D_j.

The set of equations is solved by the method of contour integral. The feasibility of such a solution was indicated by Demkov and Osherov [1] long ago but was never actually implemented, probably because of the difficulty to physically interpret the $1/t$ singularity in the Hamiltonian. We notice that the situation of interest for physics corresponds to initial (at instant of time $t \to +0$) population of the Coulomb potential curve. In this approach the singularity lies at the edge of time interval and does not create problems. We obtain in a simple analytical form the probabilities of transitions as $t \to \infty$ to any other state. The result applies both to the case when a horizontal diabatic potential curve is crossed by the Coulomb one ($D_j < D_0$), and to the 'non-crossing' situation ($D_j > D_0$). In the limit of weak coupling the results are interpreted in terms of pairwise Landau-Zener-type transitions; the probabilities of 'non-crossing' transitions are exponentially small. Our multistate model incorporates the two-state model treated recently in Ref. [2]. Much earlier Child [3] and Bandrauk [4] considered two-state Coulomb model in a different formulation. The coupling between diabatic states was presumed to be not a constant, but time-dependent, namely $\sim 1/t$.

Mapping of the Coulomb model onto a new exponential multistate model is established; in the special two-state case the well-known Nikitin model is recovered.

References

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