Curve crossing in linear potential grids: the quasidegeneracy approximation

V. A. Yurovsky and A. Ben-Reuven
School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel
(November 8, 2018)

I. INTRODUCTION

The concept of curve crossing has many applications in the study of atomic collisions [1, 2], excitations of atoms and molecules by nonstationary fields [3–11], Bose-Einstein condensates [12, 13], and solid state physics [14–16]. Typical curve crossing problems are generally divided into two classes, R-dependent and t-dependent ones. The description of inelastic collisions, for example, involves crossings of coordinate-dependent potentials, and can therefore be treated as an R-dependent problem, described by a set of coupled second-order stationary Schrödinger equations. By the use of a common-trajectory approximation [1], R-dependent problems can be reduced to t-dependent ones. The latter class also naturally appears in the description of transitions due to non-stationary fields. Typical t-dependent problems involve the crossing of time-varying potentials, and their description requires a set of coupled first-order non-stationary Schrödinger equations.

Curve crossing problems are usually solved by using semiclassical approximations. Two-state crossing is described by the Landau-Zener (LZ) formula [17, 18] (or one of its various modifications [19, 20]), while multistate crossing is treated as a sequence of independent two-state crossings. Although semiclassical approaches are satisfactory for many applications (see, e.g., [21]), they fail to describe certain effects found recently in experiments, numerical calculations, and analytically-soluble potential models [22, 23].

The LZ formula forms an exact solution of the problem involving the crossing of two linear potentials infinitely diverging on both asymptotes. It gives good results even when local perturbations in the vicinity of the crossing are taken into account [24]. However, if the potentials retain a finite potential gap on an asymptote [25], have singularities [26, 27], or are truncated [28], the transition probabilities deviate essentially from the LZ formula. Some interesting effects appear also in state crossing involving Bose-Einstein condensates, described by the nonlinear Gross-Pitaevskii equations (see [29]), instead of the linear Schrödinger equations.

The treatment of multistate curve crossing as a sequence of independent two-state crossings, commonly used in semiclassical approaches, fails to describe “counterintuitive” transitions (see [30, 31]), in which the second crossing precedes the first one. In the case of a t-dependent linear grid (see [14, 15, 24, 25]) consisting of two sets of mutually parallel potentials (see Fig. 1), counterintuitive transitions are exactly forbidden if the problem is defined on the infinite time interval \( (t' \to \infty, t'' \to -\infty) \), as has been shown in Ref. [21]. However, the potentials in the grid infinitely diverge on both asymptotes, which is unphysical. We consider here a truncated linear grid, defined on a finite time interval \([-t', t'']\). Such a truncation is relevant for application to transitions in time-dependent fields (e.g., single electrons [14, 15]), since the field variation is actually finite.

The problem is studied here with the help of the “quasidegeneracy” approximation, introduced in [12] for the case when one of the sets consists of only one potential. This approximation treats a non-degenerate system with small potential gaps as a perturbed degenerate system (see [21]). A special form of the quasidegeneracy approximation was used also in Ref. [14]. This form is applicable to a linear grid consisting of two potentials in each set, with equal couplings between all states belonging to different sets, while only one of the sets is quasidegenerate. The method of Ref. [14] is actually a simplified form of the method of Ref. [12]. A linear grid in which one set of parallel potentials is exactly degenerate was considered also in Ref. [14], by using a method different from the quasidegeneracy approximation.

The quasidegeneracy approximation is generalized here to the case of a truncated linear grid with arbitrary number of potentials in both sets. In Sec. [3] we introduce a “decoupling” transformation, which approximately transforms the problem to a set of parallel two-state crossings. The transition amplitudes are calculated in Sec. [4], and applicability criteria are presented in Sec. [5]. Results are shown and discussed in Sec. [5]. A few preliminary results of this work have been presented in...
II. DECOUPLING TRANSFORMATION

Let us consider two sets of mutually parallel linear potentials. This problem can be easily reduced by a gauge transformation to the case of a set of horizontal potentials $V_j$ ($j = 1, \ldots, n_1$) crossed by a set of slanted parallel linear potentials $V_{n_1+k}$ ($k = 1, \ldots, n_2$) (see Fig. [I]). The interactions between the states within each set of parallel potentials can be eliminated by a unitary transformation. Therefore, without loss of generality, we can describe the problem by the following system of coupled equations for the expansion coefficients $\varphi_j (t)$,

$$i \frac{\partial \varphi_j}{\partial t} = V_j \varphi_j + \sum_{k=1}^{n_2} g_{jk} \varphi_{n_1+k}, \quad 1 \leq j \leq n_1$$  \hspace{1cm} (1)

$$(V_{n_1+k} + \beta t) \varphi_{n_1+k} + \sum_{j=1}^{n_1} g_{jk} \varphi_j, \quad 1 \leq k \leq n_2$$

(1)

(using a system of units in which $\hbar = 1$). The only non-vanishing coupling coefficients $g_{jk}$ involve pairs of crossed potentials. The problem is defined here on the finite time-interval $-t' \leq t \leq t''$.

The special case of $n_2 = 1$ has been considered in [27], by using a quasidegeneracy approximation. In order to generalize this approximation, let us perform a singular value decomposition (SVD) for the coupling matrix $g_{jk}$, of the form

$$g_{jk} = \sum_{l=1}^{n} X_{lj} g_l Y_{lk}, \quad n \leq \min (n_1, n_2).$$  \hspace{1cm} (2)

This decomposition is well known in the theory of spline approximations (see, e.g., [25]). The two matrices with elements $X_{lj}$ and $Y_{lk}$ are unitary, and their rows are the eigenvectors of the quadratic matrices formed by products of the $g_{jk}$ and their hermitian conjugates:

$$\sum_{k,j} g_{jk}^* g_{kj} X_{lj} = |g_l|^2 X_{lj'}, \quad \sum_{k,j} g_{jk} g_{kj}^* Y_{lk} = |g_l|^2 Y_{lk'}.$$

A transformation of the expansion coefficients $\varphi_j (t)$ using the matrices $X_{lj}$ and $Y_{lk}$,

$$a_l (t) = \sum_{j=1}^{n_1} X_{lj} \varphi_j (t), \quad b_l (t) = \sum_{k=1}^{n_2} Y_{lk} \varphi_{n_1+k} (t),$$  \hspace{1cm} (3)

leads to a new system of coupled equations

$$i \frac{\partial a_l}{\partial t} = V_l^{(a)} a_l + g_l b_l + \sum_{l' \neq l} V_{ll'}^{(a)} a_{l'}, \quad 1 \leq l \leq n$$

$$i \frac{\partial b_l}{\partial t} = (V_l^{(b)} + \beta t) b_l + g_l a_l + \sum_{l' \neq l} V_{ll'}^{(b)} b_{l'}, \quad 1 \leq l \leq n$$

$$i \frac{\partial a_{l+n_1}}{\partial t} = V_{l+n_1}^{(a)} a_{l+n_1} + \sum_{l' \neq l+n_1} V_{ll'}^{(a)} a_{l'}, \quad 1 \leq l \leq n_1$$

$$i \frac{\partial b_{l+n_1}}{\partial t} = (V_{l+n_1}^{(b)} + \beta t) b_{l+n_1} + \sum_{l' \neq l+n_1} V_{ll'}^{(b)} b_{l'}, \quad 1 \leq l \leq n_1$$

(4)

in which

$$V_l^{(a)} = \sum_{j=1}^{n_1} X_{lj} V_j, \quad V_l^{(b)} = \sum_{k=1}^{n_2} Y_{lk} V_{n_1+k}.$$  \hspace{1cm} (5)

Given a matrix $g_{jk}$, its SVD is not unique, and may be chosen in such a way that its singular values $g_l$ are real and non-negative, and the non-diagonal potential elements $V_{ll'}^{(a)}$ and $V_{ll'}^{(b)}$ vanish when $l > n$ and $l' > n$.

When both parallel sets of potentials are degenerate, the matrices $V_{ll'}^{(a)}$ and $V_{ll'}^{(b)}$ are diagonal, and the system (4) reduces to a set of $n$ independent pairs of crossing potentials, $n_1 - n$ separate horizontal potentials (not coupled to other channels), and $n_2 - n$ separate slanted potentials. Since the transformation (5) partially eliminates the coupling between the states, hereafter it is called the “decoupling transformation”. The channels described by coefficients $a$ and $b$ will be called the “decoupled channels”.

In the non-degenerate case the non-diagonal elements of $V_{ll'}^{(a)}$ and $V_{ll'}^{(b)}$ lead to transitions between the decoupled channels. However, the magnitudes of these non-diagonal elements are bounded by the inequalities

$$\sum_{l \neq l'} |V_{ll'}^{(a)}|^2 = \sum_{j=1}^{n_1} V_j^2 - \sum_{l=1}^{n_1} (V_l^{(a)})^2 \leq \frac{1}{4} n_1 \Delta V_1^2,$$

$$\sum_{l \neq l'} |V_{ll'}^{(b)}|^2 = \sum_{k=1}^{n_2} V_{n_1+k}^2 - \sum_{l=1}^{n_2} (V_l^{(b)})^2 \leq \frac{1}{4} n_2 \Delta V_2^2,$$

(6)

where the bandwidths of the potential sets are defined as

$$\Delta V_1 = V_{n_1} - V_1, \quad \Delta V_2 = V_{n_1+n_2} - V_{n_1+1}.$$  \hspace{1cm} (7)

Therefore, these transitions are negligible if the bandwidths of the two potential sets are small enough. (Appropriate applicability criteria are presented in Sec. [V] below.) Neglecting the non-diagonal elements of $V_{ll'}^{(a)}$ and $V_{ll'}^{(b)}$, we obtain a zero-order-approximation system of equations for $a_l (t)$ and $b_l (t)$,

$$i \frac{\partial a_l^{(0)}}{\partial t} = V_l^{(a)} a_l^{(0)} + g_l b_l^{(0)}, \quad 1 \leq l \leq n$$

$$i \frac{\partial b_{l+n_1}^{(0)}}{\partial t} = (V_{l+n_1}^{(b)} + \beta t) b_{l+n_1}^{(0)} + \sum_{l' \neq l+n_1} V_{ll'}^{(b)} b_{l'}^{(0)}, \quad 1 \leq l \leq n_1$$

(8a)
which describes the same set of decoupled channels as

and the other rows are orthogonal to the first one. The

analytical form. Nevertheless, analytical expressions can

be obtained in the specific case of a separable matrix

where the same set of coupled potentials as the one that prevails in the case of degenerate potentials.

Given an arbitrary matrix $g_{jk}$, the transformation matrices $X_{ij}$ and $Y_{ik}$ cannot be generally expressed analytically. Nevertheless, analytical expressions can be obtained in the specific case of a separable matrix $g_{jk} = \xi_j^* \eta_k$. In this case, one of the rows (the first, for definiteness) has the form

$$X_{1j} = \left( \sum_{j'=1}^{n_1} |\xi_{j'}|^2 \right)^{-1/2} \xi_j, \quad Y_{ik} = \left( \sum_{k'=1}^{n_2} |\eta_{k'}|^2 \right)^{-1/2} \eta_k,$$

and the other rows are orthogonal to the first one. The singular values can then be written as

$$g_l = \left( \sum_{j'=1}^{n_1} |\xi_{j'}|^2 \sum_{k'=1}^{n_2} |\eta_{k'}|^2 \right)^{1/2} \delta_{l1}.$$

In this case, $n = 1$ and the transformed system consists of one pair of coupled potentials, together with $n_1 - 1$ horizontal, and $n_2 - 1$ slanted, separate potentials.

In the case of equal couplings $g_{jk} = g$ (independent of $j$ and $k$), $X_{1j} = n_1^{-1/2}$, $Y_{1j} = n_2^{-1/2}$, and $g_l = (n_1 n_2)^{1/2} g \delta_{l1}$. The opposite situation (in which $g_l$ is independent of $l$) takes place in the case in which the coupling matrix $g_{jk}$ is proportional to a unitary matrix.

### III. TRANSITION AMPLITUDES

The zero-order equations (8d) and (8d) representing separate channels have the simple analytical solutions

$$a_l^{(0)}(t') = a_l^{(0)}(t') \exp \left( -i V_{ll}^{(a)}(t' + t') \right),$$

$$b_l^{(0)}(t') = b_l^{(0)}(t') \times \exp \left( -i V_{ll}^{(b)}(t' + t') - i \beta (t'^2 - t^2) / 2 \right).$$

The remaining equations (8d) and (8d) represent a set of $n$ two-state linear curve-crossing problems. In the limit $t' \to \infty$, $t'' \to \infty$ the transition amplitude in each of these systems is given by the LZ formula. However, the solution of this problem converges to the asymptotic limit very slowly. We shall therefore use the exact solution of the linear two-state curve crossing problem, known since the pioneering work of Zener [17]. The two independent solutions $A_{ml}(t)$, $B_{ml}(t)$, with $m = 1, 2$, can be expressed in terms of the confluent hypergeometric function $1F_1$ (see [29]) as

$$A_{1l}(t) = 1F_1 \left( -\frac{i}{2} \lambda_l, 1; \frac{i}{2} \beta (t - t_l) \right) \exp \left( -i V_{ll}^{(a)}(t) \right),$$

$$A_{2l}(t) = (t - t_l) 1F_1 \left( \frac{1}{2} \lambda_l, 1; \frac{3}{2}, \frac{i}{2} \beta (t - t_l) \right) \times \exp \left( -i V_{ll}^{(a)}(t) \right),$$

$$B_{ml}(t) = \frac{i}{g_l} \frac{\partial A_{ml}(t)}{\partial t} - \frac{V_{ll}^{(a)}}{g_l} A_{ml}(t),$$

where

$$\lambda_l = g_l^2 / \beta, \quad t_l = \left( V_{ll}^{(a)} - V_{ll}^{(b)} \right) / \beta$$

are, respectively, the LZ exponent for the two-state crossing and the position of the crossing point on the time scale.

The transition matrix $S^{(l)}$, connecting the coefficients $a_l^{(0)}$, $b_l^{(0)}$ at the boundaries $t'$ and $-t'$ as

$$a_l^{(0)}(t') = S_{aa}^{(l)} a_l^{(0)}(-t') + S_{ab}^{(l)} b_l^{(0)}(-t'),$$

$$b_l^{(0)}(t') = S_{ba}^{(l)} a_l^{(0)}(-t') + S_{bb}^{(l)} b_l^{(0)}(-t'),$$

can be expressed in terms of the fundamental solutions [13] in the form

$$S_{aa}^{(l)} = (A_{11}(t') B_{2l}(-t') - A_{2l}(t') B_{1l}(-t')) / D_l,$$

$$S_{ab}^{(l)} = (-A_{11}(t') A_{2l}(-t') + A_{2l}(t') A_{1l}(-t')) / D_l,$$

$$S_{ba}^{(l)} = (B_{11}(t') B_{2l}(-t') - B_{2l}(t') B_{1l}(-t')) / D_l,$$

$$S_{bb}^{(l)} = (-B_{11}(t') A_{2l}(-t') - B_{2l}(t') A_{1l}(-t')) / D_l,$$

where

$$D_l = A_{11}(t') B_{2l}(-t') - A_{2l}(t') B_{1l}(-t').$$

In our numerical calculations we expressed the confluent hypergeometric functions in terms of cylindrical wavefunctions, using the algorithm of [30] for their evaluation.

When the original representation [9] is recovered by application of the transformation [9] one obtains the transition matrix $S$, defined by

$$\varphi_j(t'') = \sum_{j'=1}^{n_1 + n_2} S_{jj'} \varphi_{j'}(-t'), \quad 1 \leq j \leq n_1 + n_2,$$

in the zero-order approximation, as
where the bandwidths of the potential sets \( \Delta V \) give constraints on \( t \)'s, as can be shown by the use of \( 4 \)-tuples and analogous expressions for \( \Delta X \) as small contributions to the transition amplitudes. Thus, the quasidegeneracy approximation described in Sec. III is applicable when the terms neglected in Eqs. (8) yield sufficiently small contributions to the transition amplitudes. First-order perturbation theory estimates these contributions as

\[
\Delta S_{l,l'}^{(a)} = \int_{-t'}^{t'} \frac{V_{il}^{(a)}(t)}{1 + i \lambda_l} \left[ a_{l'}^{(0)*}(t) a_{l}^{(0)}(t) \right] dt,
\]

and analogous expressions for \( \Delta S_{l,l'}^{(b)} \), obtained by replacing \( a \) with \( b \) everywhere in Eq. (13).

An overestimate for these amplitudes can be obtained by substituting \( a_{l}^{(0)}(t) = b_{l}^{(0)}(t) = 1 \), resulting in the criteria

\[
(t' + t'') \Delta V_{1,2} \ll 1,
\]

where the bandwidths of the potential sets \( \Delta V \) are defined by Eq. (14). However, in certain situations less stringent criteria may exist, as can be shown by the use of approximate expressions for the unperturbed wavefunctions [solutions of Eqs. (8)].

Such approximate expressions can be obtained in two limiting cases. The first one is the asymptotic case, in which the bounds \(-t' \) and \( t'' \) lie far outside the two-state transition ranges \( g_l/\beta \), i.e.,

\[
t' + t' \gg g_l/\beta, \quad t'' - t' \gg g_l/\beta \quad \text{for all } l.
\]

In this case, an asymptotic expansion of the confluent hypergeometric function (see Eq. (22)) on the left-hand asymptote \( t' + t' \gg t - t' \gg g_l/\beta \) yields

\[
a_{l}^{(0)}(t) \approx a_{l}^{(0)}(t') (t'/t')^{\lambda_l} \exp \left( -i V_{il}^{(a)}(t + t) \right),
\]

\[
b_{l}^{(0)}(t) \approx b_{l}^{(0)}(t') (t'/t')^{-\lambda_l}
\times \exp \left( -i V_{il}^{(a)}(t + t') - i \beta (t^2 - t'^2)/2 \right),
\]

and on the right-hand asymptote \( g_l/\beta < t - t' < t'' - t' \) it yields

\[
a_{l}^{(0)}(t) \approx a_{l}^{(0)}(t'') (t'/t'')^{\lambda_l} \exp \left( -i V_{il}^{(a)}(t - t'') \right),
\]

\[
b_{l}^{(0)}(t) \approx b_{l}^{(0)}(t'') (t'/t'')^{-\lambda_l}
\times \exp \left( -i V_{il}^{(a)}(t - t'') - i \beta (t^2 - t'^2)/2 \right).
\]

Whenever \( l > n \), Eqs. (22) and (23) become exact [see Eqs. (14)]. Hereafter one should set \( \lambda_l = 0 \) if \( l > n \).

The first-order corrections to the amplitudes (19) can be therefore estimated as

\[
\Delta S_{l,l'}^{(a)} \approx \frac{V_{il}^{(a)}}{1 + i \lambda_l} \left[ (t') a_{l'}^{(0)*} \left( t' \right) a_{l}^{(0)} \left( t' \right)
+ (t'') a_{l'}^{(0)*} \left( t'' \right) a_{l}^{(0)} \left( t'' \right) \right],
\]

for the horizontal set, and a similar expression, with \( b \) replacing \( a \), for the slanted set.

Finally, using Eq. (14) one can write the applicability criteria in the form

\[
(t' + t'') \Delta V_{1,2} \ll |1 + i \lambda_{l'} - i \lambda_l|.
\]

Let us consider now the second limiting case, in which both boundaries \(-t' \) and \( t'' \) lie far inside the two-state transition ranges \( g_l/\beta \), i. e.,

\[
t' + t' \ll g_l/\beta, \quad t'' - t' \ll g_l/\beta \quad \text{for all } l.
\]

In addition, let \( \lambda_l \gg 1 \), in order to obtain an adiabatic evolution. Within the range defined by Eq. (24), the adiabatic energies are approximately \( V_{il}^{(a)} \pm g_l \), and

\[
\left( \begin{array}{c}
\frac{a_{l}^{(0)}(t)}{b_{l}^{(0)}(t)}
\end{array} \right)
\approx
\frac{a_{l}^{(0)}(t') + b_{l}^{(0)}(t')}{2}
\times \exp \left( -i \left( V_{il}^{(a)} + g_l \right) (t' + t') \right)
\pm
\frac{a_{l}^{(0)}(t') - b_{l}^{(0)}(t')}{2}
\times \exp \left( -i \left( V_{il}^{(a)} - g_l \right) (t' + t') \right).
\]
Substitution of Eqs. (27) in Eq. (19), taking into account Eq. (18), gives the applicability criteria
\[(t' + t'') \Delta V_{1,2} \ll 1 + |g_1 - g_V| (t' + t'').\] (28)

Criteria combining the cases (20), (25), and (28) can be written with the help of Eq. (13) as the single expression
\[(t' + t'') \Delta V_{1,2} \ll 1 + |g_1 - g_V| \min(t' + t'', (g_1 + g_V) / \beta).\] (29)

These criteria allow for an interpretation that stems from the viewpoint of the uncertainty principle. Equation (29) means that the potentials become indistinguishable within a limited time interval. The second term in the right-hand side of Eq. (29) describes a broadening of the allowed uncertainty as the coupling increases.

V. RESULTS AND DISCUSSION

In the limiting case of a linear grid defined on the infinite time interval $-\infty < t < \infty$, some transitions become forbidden (see 24). An example of such transitions is shown in Fig. 1, in which two time-independent potentials are shown crossed by three parallel time-slanted potentials. The forbidden transitions, such as $2 \rightarrow 1$, $3 \rightarrow 4$, $3 \rightarrow 5$, and $4 \rightarrow 5$, are called counterintuitive, since in order to treat them as a sequence of independent two-state crossings, one has to assume a motion backwards in time.

Counterintuitive transitions can nonetheless occur, as has been proven in numerical calculations involving crossings of nonlinear potentials 5, and in uses of the quasidegeneracy approximation for truncated and piecewise linear problems, involving a set of horizontal potentials, crossed by one slanted potential 4. Such transitions are present in truncated linear grids as well, since the transformations 3 connect the initial and final states to all the decoupled channels.

Hereafter we shall demonstrate the application of the quasidegeneracy approximation to a particular example. Consider the model of a linear grid with $n_1 = n_2 = 2$, $V_1 = V_3 = -\Delta V/2$, and $V_2 = V_4 = \Delta V/2$ (recalling that $V_3$ and $V_4$ are the time-independent parts of the slanted potentials). Let the coupling matrix have one of the two special forms, either
\[g_{jk} = g_0 \begin{pmatrix} 1/1.2 & 1/1.2 \\ 1 & 1.2 \exp(\im \pi/4) \end{pmatrix},\] (30)

with integer values of $m$, or the equal-coupling form, with
\[g_{11} = g_{12} = g_{21} = g_{22} = g_0.\] (31)

All the following calculations are performed for the slope $\beta = 1$. The results can be readily expanded to other $\beta$ values by the substitutions $g/\sqrt{\beta} \rightarrow g$, $\Delta V/\sqrt{\beta} \rightarrow \Delta V$, and $t/\sqrt{\beta} \rightarrow t$.

Figure 2 presents the dependence of counterintuitive transition probabilities on the coupling strength $g_0$ for two cases: an exactly degenerate one ($\Delta V = 0$), and a one in which $\Delta V (t' + t'') = 0.5$, on the verge of the validity criteria (29). At low values of $g_0$ the amplitudes $S_{1a}^{(l)}$ and $S_{1b}^{(l)}$ in the decoupled representation Eq. (15) are close to unity and practically independent of $l$, and therefore all transitions (including counterintuitive ones) within each of the two sets of parallel potentials in the original representation have small probabilities [see discussion following Eqs. (15)]. In cases in which the singular values are quite similar, the probabilities of such transitions become small at high coupling strengths, since $S_{1a}^{(l)}$ and $S_{1b}^{(l)}$ are small for all $l$ (see, for example, the plots for $m = 3$ in Fig. 3, where $g_1 = 1.73g_0$ and $g_2 = 1.07g_0$).

However, if the singular values of the coupling matrix are significantly different, the counterintuitive transitions remain significant over a wide range of coupling strengths as some of the amplitudes $S_{1a}^{(l)}$ (or $S_{1b}^{(l)}$) are large, and some are small (see the plots for $m = 1$ in Fig. 2, where $g_1 = 2g_0$ and $g_2 = 0.38g_0$). In the case of a separable matrix (see the plot for $m = 0$ in Fig. 2, where $g_1 = 2.03g_0$ and $g_2 = 0$), such transitions persist even in the limit of high coupling strength. It is worth noting that even a change of the phase of one element of the coupling matrix transforms a separable matrix to a non-separable one, and therefore changes the behavior of the transition probability at high values of the coupling strengths.

Counterintuitive transitions persist at finite values of the potential gap $\Delta V$ as well (see Figs. 2b and 3). As one can see, the higher is the coupling strength, the better are the results of the quasidegeneracy approximation [in agreement with the criteria Eq. (29)]. At low coupling strengths the predictions of the quasidegeneracy approximation are correct as long as $(t' + t'') \Delta V < 0.2$ (see 2b), while at high coupling strengths they are correct as long as $(t' + t'') \Delta V < 0.2\Lambda$ (see 3b).

Probabilities of counterintuitive transitions (see Fig. 3b) and other transitions (see Fig. 4) demonstrate an oscillating pattern in their dependence on the potential gap. The nature of these oscillations is different from the well-known St"{u}ckelberg oscillations (see Ref. 4), which may be present only in transitions including two or more interfering “intuitive” paths. (Such paths exist in the transitions from 1 or 4 to 2 or 3 in the case presented in Figs. 2b and 4.) The period of the St"{u}ckelberg oscillations is $\Delta V/\beta$; i.e., it is dependent on the potential gap $\Delta V$ but independent of the time interval $t' + t''$. These properties, as well as the magnitude of the St"{u}ckelberg oscillation period, are not in agreement with the behavior of the oscillations presented in Figs. 2b and 4.

The quasidegeneracy approximation relates the oscillations reported here to the interference of the terms in Eqs. (15), corresponding to different decoupled channels. The dependence on $\Delta V$ is due to exponent in Eqs. (12) and in the second sum of each of the two equations (18a) and (18b). The oscillation period in $\Delta V$ is $2\pi p/(t' + t'')$, where
where $\rho = \Delta V / \left( V_{22}^{(a)} - V_{11}^{(a)} \right) = \Delta V / \left( V_{22}^{(b)} - V_{11}^{(b)} \right)$ is the ratio of the potential gaps in the original and decoupled representations. For the coupling matrix (30) we have $\rho = 5.6, 5.3, 4.0,$ and 2.5 for $m = 0, 1, 2,$ and 3, respectively, which explains the variation of the oscillation period with $m$ in Fig. 3. It is worth noting that in Fig. 4 these oscillations are absent just for the transitions for which one would expect St"uckelberg oscillations (4 → 2 and 1 → 3). The reason for not seeing St"uckelberg oscillations in our model is the $\Delta V$ variation (between Figs. 3, 4b, and 4c), leading to an incomplete population transfer. This effect is similar to the effect of incomplete optical shielding in ultracold atom collisions [5,6]. The effect is also similar to the effect of incomplete population transfer between the sets. This property was used in a recent proposal of single-electronics devices, based on transitions between quantum dots (Refs. [12, 13]). The effect is similar to the effect of incomplete population transfer between the sets. This property was used in a recent proposal of single-electronics devices, based on transitions between quantum dots (Refs. [12, 13]).

VI. CONCLUSIONS

Equations (22) describe the transition amplitudes in a truncated linear potential grid, whenever the applicability criteria (23) are observed. The results can be applied also to a more general case, in which the grid may be broken into well-separated groups of quasidegenerate crossings. In this case the transition amplitudes can be represented as products of the transition amplitudes given by Eqs. (22) for the quasidegenerate groups. Thus the approximation can be used in a wide variety of physical problems in which a multistate curve crossing occurs.

[1] E. E. Nikitin and S. Ya. Umanskii, Theory of Slow Atomic Collisions (Springer-Verlag, Berlin, 1984).
[2] E. E. Nikitin, Annu. Rev. Phys. Chem. 50, 1 (1999).
[3] M. S. Child, Molecular Collisions Theory (Academic Press, London and New York, 1974).
[4] M. S. Child, Semiclassical Mechanics with Molecular Applications (Clarendon Press, Oxford, 1991).
[5] R. Napolitano, J. Weiner, and P. S. Julienne, Phys. Rev. A 55, 1191 (1997).
[6] V. A. Yurovsky and A. Ben-Reuven, Phys. Rev. A 55, 3772 (1997).
[7] I. I. Fabricant and M. I. Chibisov, Phys. Rev. A 61, 022718 (2000).
[8] B. W. Shore, The Theory of Coherent Atomic Excitation (Wiley, New York, 1990).
[9] N. V. Vitanov and K.-A. Suominen, Phys. Rev. A 59, 4580 (1999).
[10] V. M. Akulin, Zh. Eksp. Teor. Fiz. 87, 1182 (1984) [Sov. Phys. JETP 60, 676 (1984)].
[11] D. A. Harmin and P. N. Price, Phys. Rev. A 49, 1933 (1994); D. A. Harmin, Phys. Rev. A 56, 232 (1997).
[12] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne and C. J. Williams, Phys. Rev. A 60, R765 (1999); Phys. Rev A (to be published).
[13] F. H. Mies, P. S. Julienne, and E. Tiesinga, Phys. Rev. A 61, 022721 (2000).
[14] T. Usuki, Phys. Rev. B 56, 13360 (1997).
[15] T. Usuki, Phys. Rev. B 57, 7124 (1998); Microel. Eng. 47, 269 (1999).
[16] L. D. Landau, Phys. Z. Sowjetunion 2, 46 (1932).
[17] C. Zener, Proc. R. Soc. London Ser. A 137, 696 (1932).
[18] H. Nakamura and C. Zhu, Comments At. Mol. Phys. 32, 249 (1996).
[19] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne, and Y. B. Band, J. Phys. B 32, 1845 (1999).
[20] E. E. Nikitin, Opt. i Spektrosk. 13, 761 (1962) [Opt. and Spectrosc. (USSR) 13, 431 (1962)]; E. E. Nikitin, Discuss. Faraday Soc. 33, 14 (1962); E. E. Nikitin, Izv. Akad. Nauk SSSR 27, 996 (1963).
[21] A. D. Bandrauk, Molec. Phys. 24, 661 (1972).
[22] V. A. Yurovsky and A. Ben-Reuven, Phys. Rev. A 60, 4561 (1999).
[23] N. V. Vitanov and B. M. Garraway, Phys. Rev. A 53, 4288 (1996).
[24] S. Brundobler and V. Elser, J. Phys. A 26, 1211 (1993);
[25] Yu. N. Demkov and V. N. Ostrovsky, J. Phys. B 28, 1589 (1995); Yu. N. Demkov, P. B. Kurasov, and V. N. Ostrovsky, J. Phys. A 28, 4361 (1995); V. N. Ostrovsky and H. Nakamura, Phys. Rev. A 58, 429 (1998).
[26] V. A. Yurovsky and A. Ben-Reuven, J. Phys. B 31, 1 (1998).
[27] V. A. Yurovsky and A. Ben-Reuven, in 32nd EGAS. Abstracts, edited by Z. Rudzikas (TFAI, Vilnius, 2000), p. 44; in 15th International Conference on Spectral Line Shapes. Program and Abstracts (PTB, Berlin, 2000), p.
[28] C. L. Lowson and R. J. Hanson, *Solving Least Squares Problems* (Prentice-Hall, Englewood Cliffs, 1974); G. E. Forsythe, M. A. Malcolm, and C. B. Moler, *Computer methods for mathematical computations* (Prentice-Hall, Englewood Cliffs, 1977).

[29] *Handbook of Mathematical Functions*, edited by M. Abramovitz and I. E. Stegun (NBS, Washington, 1964).

[30] I. J. Thompson and A. R. Barnett, Comp. Phys. Comm. **36**, 363 (1985).

![FIG. 1. Schematic illustration of a truncated linear grid, involving \( n_1 = 2 \) horizontal potentials and \( n_2 = 3 \) slanted potentials. The broken dotted arrow shows a counterintuitive transition. The numbers denote the states to which the potentials correspond.](image1)

![FIG. 2. Counterintuitive transition probabilities vs. the coupling strength \( g_0 \) [see Eq. (30)] for a truncated linear grid with the bounds \( t' = t'' = 100 \) (on a scale in which the potential slopes \( \beta = 1 \)) and the potential gaps (a) \( \Delta V = 0 \), and (b) \( \Delta V = 2.5 \times 10^{-3} \). The numbers denote the values of the phase parameter \( m \) in Eq. (30). The results of numerical integration of the coupled equations (1) are presented by solid lines. The dashed-line plots in part (b) are calculated with the quasi-degeneracy approximation using Eqs. (18).](image2)
FIG. 3. Counterintuitive transition probabilities vs. the potential gap $\Delta V$, calculated for (a) $t' = t'' = 100$, $g_0 = 0.5$, or (b) $t' = t'' = 20$, $g_0 = 5$. Other notations as in Fig. 2.

FIG. 4. Probabilities of specified state-to-state transitions vs. the potential gap $\Delta V$ for a truncated linear grid with $t' = t'' = 50$ and $g_0 = 5$. Parts (a) and (b) correspond to the coupling matrix (30) with $m = 4$ and $m = 0$, respectively, while part (c) corresponds to the case of equal couplings (see Eq. (31)). Other notations as in Fig. 2.