Curve crossing in linear potential grids: The quasidegeneracy approximation

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The quasidegeneracy approximation [V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne, and Y. B. Band, J. Phys. B **32**, 1845 (1999)] is used here to evaluate transition amplitudes for the problem of curve crossing in linear potential grids involving two sets of parallel potentials. The approximation describes phenomena, such as counterintuitive transitions and saturation (incomplete population transfer), not predictable by the assumption of independent crossings. Also, a new kind of oscillations due to quantum interference (different from the well-known Stückelberg oscillations) is disclosed, and its nature discussed. The approximation can find applications in many fields of physics, where multistate curve crossing problems occur.

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I. INTRODUCTION

The concept of curve crossing has many applications in the study of atomic collisions [1–7], excitations of atoms and molecules by nonstationary fields [8–11], Bose-Einstein condensates [12,13], and solid-state physics [14,15]. 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 nonstationary fields. Typical t-dependent problems involve the crossing of time-varying potentials, and their description requires a set of coupled first-order nonstationary Schrödinger equations.

Curve crossing problems are usually solved by using semiclassical approximations. Two-state crossing is described by the Landau-Zener (LZ) formula [16,17] (or one of its various modifications [18]), while multistate crossing is treated as a sequence of independent two-state crossings. Although semiclassical approaches are satisfactory for many applications (see, e.g. [6]), they fail to describe certain effects found recently in experiments, numerical calculations, and analytically soluble potential models [5,19–22].

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 [9]. However, if the potentials retain a finite potential gap on an asymptote [20], have singularities [21,22], or are truncated [23], the transition probabilities deviate essentially from the LZ formula. Some interesting effects also appear in state crossing involving Bose-Einstein condensates, described by the nonlinear Gross-Pitaevskii equations (see [12]), 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 [5,19]), in which the second crossing precedes the first one. A particular type of problem that has been studied by quantum approaches is that of a t-dependent linear grid consisting of two sets of mutually parallel potentials (see Fig. 1). This problem has a known exact solution [24] only in the case in which one of the two sets has only one potential, and the time interval is extended to infinity ($t' \to \infty, t'' \to -\infty$). Otherwise (see [11,14,15,25,26]) we have only numerical solutions, or a qualitative study of properties. We know, however, for certain (see [25]) that, for any pair of sets, counterintuitive transitions are exactly forbidden on the infinite time interval. 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 electronics [14,15]), since the field variation is actually finite.

The problem is studied here with the help of the ''quasidegeneracy'' approximation, introduced in [19] for the case when one of the sets consists of only one potential. This approximation treats a nondegenerate system with small potential gaps as a perturbed degenerate system (see [27]). 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

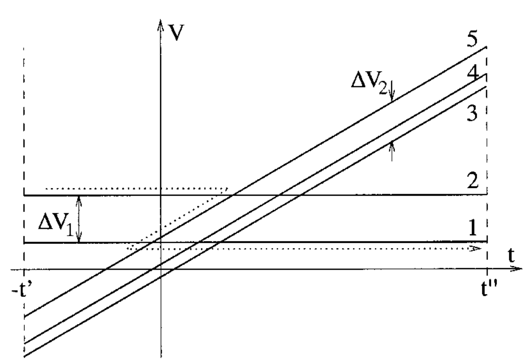

FIG. 1. Schematic illustration of a truncated linear grid, involving $n_1=2$ horizontal potentials and $n_2=3$ slanted potentials. The broken dotted arrow shows a counterintuitive transition. The numbers denote the states to which the potentials correspond.

of the sets is quasidegenerate. The method of Ref. [14] is actually a simplified form of the method of Ref. [19]. A linear grid in which one set of parallel potentials is exactly degenerate was also considered in Ref. [10], 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. II 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. III, and applicability criteria are presented in Sec. IV. Results are shown and discussed in Sec. V. A few preliminary results of this work have been presented in [28].

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 $V_{n_1+k}+\beta t$ ($k=1,\ldots,n_2$) (see Fig. 1). 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 $\varphi_j(t)$:

$$i\frac{\partial\varphi_j}{\partial t}=V_j\varphi_j+\sum_{k=1}^{n_2} g_{jk}\varphi_{n_1+k}, \quad 1\leqslant j\leqslant n_1,$$
$$i\frac{\partial\varphi_{n_1+k}}{\partial t}=(V_{n_1+k}+\beta t)\varphi_{n_1+k}+\sum_{j=1}^{n_1} g^*_{jk}\varphi_j, \quad 1\leqslant k\leqslant n_2 \tag{1}$$

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

The special case of $n_2=1$ has been considered in [19], 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

$$g_{jk}=\sum_{l=1}^{n} X^*_{lj}g_lY_{lk}, \quad n\leqslant\min(n_1,n_2). \tag{2}$$

This decomposition is well known in the theory of spline approximations (see, e.g., [29]). 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:

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

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

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

leads to a new system of coupled equations

$$i\frac{\partial a_l}{\partial t}=V^{(a)}_{ll}a_l+g_lb_l+\sum_{l'\neq l} V^{(a)}_{ll'}a_{l'}, \quad 1\leqslant l\leqslant n,$$
$$i\frac{\partial b_l}{\partial t}=(V^{(b)}_{ll}+\beta t)b_l+g_la_l+\sum_{l'\neq l} V^{(b)}_{ll'}b_{l'}, \quad 1\leqslant l\leqslant n,$$
$$i\frac{\partial a_l}{\partial t}=V^{(a)}_{ll}a_l+\sum_{l'\neq l} V^{(a)}_{ll'}a_{l'}, \quad n+1\leqslant l\leqslant n_1, \tag{4}$$
$$i\frac{\partial b_l}{\partial t}=(V^{(b)}_{ll}+\beta t)b_l+\sum_{l'\neq l} V^{(b)}_{ll'}b_{l'}, \quad n+1\leqslant l\leqslant n_2,$$

in which

$$V^{(a)}_{ll'}=\sum_{j=1}^{n_1} X_{lj}V_jX^*_{l'j}, \quad V^{(b)}_{ll'}=\sum_{k=1}^{n_2} Y_{lk}V_{n_1+k}Y^*_{l'k}. \tag{5}$$

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 nondiagonal potential elements $V^{(a)}_{ll'}$ and $V^{(b)}_{ll'}$ vanish when $l>n$ and $l'>n$.

When both parallel sets of potentials are degenerate, the matrices $V^{(a)}_{ll'}$ and $V^{(b)}_{ll'}$are diagonal, and the system Eq. (4) describes 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 Eq. (3) 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 nondegenerate case the nondiagonal elements of $V^{(a)}_{ll'}$ and $V^{(b)}_{ll'}$ lead to transitions between the decoupled channels. However, the magnitudes of these nondiagonal elements are bounded by the inequalities

$$\sum_{l\neq l'} |V^{(a)}_{ll'}|^2=\sum_{j=1}^{n_1} V_j^2-\sum_{l=1}^{n_1} (V^{(a)}_{ll})^2\leqslant\frac{1}{4}n_1\Delta V_1^2,$$
$$\sum_{l\neq l'} |V^{(b)}_{ll'}|^2=\sum_{k=1}^{n_2} V^2_{n_1+k}-\sum_{l=1}^{n_2} (V^{(b)}_{ll})^2\leqslant\frac{1}{4}n_2\Delta V_2^2, \tag{6}$$

where the bandwidths of the potential sets are defined as

$$\Delta V_1=V_{n_1}-V_1, \quad \Delta V_2=V_{n_1+n_2}-V_{n_1+1}. \tag{7}$$

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

$$i\frac{\partial a_l^{(0)}}{\partial t}=V_{ll}^{(a)}a_l^{(0)}+g_l b_l^{(0)}, \quad 1\leqslant l\leqslant n, \tag{8a}$$

$$i\frac{\partial b_l^{(0)}}{\partial t}=(V_{ll}^{(b)}+\beta t)b_l^{(0)}+g_l a_l^{(0)}, \quad 1\leqslant l\leqslant n, \tag{8b}$$

$$i\frac{\partial a_l^{(0)}}{\partial t}=V_{ll}^{(a)}a_l^{(0)}, \quad n+1\leqslant l\leqslant n_1, \tag{8c}$$

$$i\frac{\partial b_l^{(0)}}{\partial t}=(V_{ll}^{(b)}+\beta t)b_l^{(0)}, \quad n+1\leqslant l\leqslant n_2, \tag{8d}$$

which describes the same set of decoupled channels as the one that prevails in the case of degenerate potentials.

Given an arbitrary matrix g_{jk}, the transformation matrices X_{lj} and Y_{lk} cannot be generally expressed in an analytical form. 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

$$X_{1j}=\left(\sum_{j'=1}^{n_1}|\xi_{j'}|^2\right)^{-1/2}\xi_j, \quad Y_{1k}=\left(\sum_{k'=1}^{n_2}|\eta_{k'}|^2\right)^{-1/2}\eta_k, \tag{9}$$

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

$$g_l=\left(\sum_{j'=1}^{n_1}|\xi_{j'}|^2\sum_{k'=1}^{n_2}|\eta_{k'}|^2\right)^{1/2}\delta_{l1}. \tag{10}$$

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 (8c) and (8d) representing separate channels have the simple analytical solutions

$$a_l^{(0)}(t'')=a_l^{(0)}(-t')\exp[-iV_{ll}^{(a)}(t'+t'')],$$
$$b_l^{(0)}(t'')=b_l^{(0)}(-t')\exp[-iV_{ll}^{(b)}(t'+t'') -i\beta(t''^2-t'^2)/2]. \tag{11}$$

The remaining equations (8a) and (8b) 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 [30]) as

$$A_{1l}(t)={}_1F_1\left(-\frac{i}{2}\lambda_l,\frac{1}{2},-\frac{i}{2}\beta(t-t_l)^2\right)\exp(-iV_{ll}^{(a)}t),$$
$$A_{2l}(t)=(t-t_l){}_1F_1\left(\frac{1}{2}-\frac{i}{2}\lambda_l,\frac{3}{2},-\frac{i}{2}\beta(t-t_l)^2\right)\times\exp(-iV_{ll}^{(a)}t), \tag{12}$$
$$B_{ml}(t)=\frac{i}{g_l}\frac{\partial A_{ml}(t)}{\partial t}-\frac{V_{ll}^{(a)}}{g_l}A_{ml}(t),$$

where

$$\lambda_l=g_l^2/\beta, \quad t_l=(V_{ll}^{(a)}-V_{ll}^{(b)})/\beta \tag{13}$$

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

$$a_l^{(0)}(t'')=S_{aa}^{(l)}a_l^{(0)}(-t')+S_{ab}^{(l)}b_l^{(0)}(-t'),$$
$$b_l^{(0)}(t'')=S_{ba}^{(l)}a_l^{(0)}(-t')+S_{bb}^{(l)}b_l^{(0)}(-t'), \tag{14}$$

can be expressed in terms of the fundamental solutions Eq. (12) in the form

$$S_{aa}^{(lt)}=(A_{1l}(t'')B_{2l}(-t')-A_{2l}(t'')B_{1l}(-t'))/D_l,$$
$$S_{ab}^{(l)}=(-A_{1l}(t'')A_{2l}(-t')+A_{2l}(t'')A_{1l}(-t'))/D_l,$$
$$S_{ba}^{(l)}=(B_{1l}(t'')B_{2l}(-t')-B_{2l}(t'')B_{1l}(-t'))/D_l, \tag{15}$$
$$S_{bb}^{(l)}=(-B_{1l}(t'')A_{2l}(-t')+B_{2l}(t'')A_{1l}(-t'))/D_l,$$

where

$$D_l=A_{1l}(-t')B_{2l}(-t')-A_{2l}(-t')B_{1l}(-t'). \tag{16}$$

In our numerical calculations we expressed the confluent hypergeometric functions in terms of columbic wave functions, using the algorithm of [31] for their evaluation.

The elements of the transition matrix $S^{(l)}$ can be given a much simpler approximate form, expressing them in terms of LZ transition amplitudes

$$S_{aa}^{(l)}\approx\exp(-\pi\lambda_l-iV_{ll}^{(a)}(t'+t''))\left(\frac{t''-t_l}{t'+t_l}\right)^{i\lambda_l},$$

$$S_{ab}^{(l)}\approx-\sqrt{1-\exp(-2\pi\lambda_l)}$$
$$\times\exp\left(\frac{i}{2}\beta t'^2-i\chi_l-iV_{ll}^{(a)}t''-iV_{ll}^{(b)}t'\right),$$
$$S_{ba}^{(l)}\approx\sqrt{1-\exp(-2\pi\lambda_l)}$$
$$\times\exp\left(-\frac{i}{2}\beta t''^2+i\chi_l-iV_{ll}^{(a)}t'-iV_{ll}^{(b)}t''\right), \tag{17}$$

$$S_{bb}^{(l)}\approx\exp(-\pi\lambda_l+-iV_{ll}^{(b)}(t'+t'')-i\beta(t''^2-t'^2)/2)$$
$$\times\left(\frac{t''-t_l}{t'+t_l}\right)^{-i\lambda_l},$$

where

$$\chi_l=\frac{\pi}{4}+\arg\Gamma(i\lambda_l)-\lambda_l\ln[\beta(t'+t_l)(t''-t_l)]-\tfrac{1}{2}\beta t_l^2. \tag{18}$$

When the original representation Eq. (1) is recovered by application of the transformation Eq. (3) one obtains the transition matrix S, defined by

$$\varphi_j(t'')=\sum_{j'=1}^{n_1+n_2}S_{jj'}\varphi_{j'}(-t'),\quad 1\leqslant j\leqslant n_1+n_2, \tag{19}$$

in the zero-order approximation as

$$S_{jj'}=\sum_{l=1}^{n}X_{lj}^{*}S_{aa}^{(l)}X_{lj'}+\sum_{l=n+1}^{n_1}X_{lj}^{*}X_{lj'}\exp(-iV_{ll}^{(a)}(t'+t'')), \tag{20a}$$

$$S_{n_1+k,n_1+k'}=\sum_{l=1}^{n}Y_{lk}^{*}S_{bb}^{(l)}Y_{lk'}+\sum_{l=n+1}^{n_2}Y_{lk}^{*}Y_{lk'}$$
$$\times\exp(-iV_{ll}^{(b)}(t'+t'')-i\beta(t''^2-t'^2)/2), \tag{20b}$$

$$S_{j,n_1+k'}=\sum_{l=1}^{n}X_{lj}^{*}S_{ab}^{(l)}Y_{lk'}, \tag{20c}$$

$$S_{n_1+k,j'}=\sum_{l=1}^{n}Y_{lk}^{*}S_{ba}^{(l)}X_{lj'}, \tag{20d}$$

where $1\leqslant j\leqslant n_1$, $1\leqslant j'\leqslant n_1$, $1\leqslant k\leqslant n_2$, and $1\leqslant k'\leqslant n_2$. This solution constitutes the quasidegeneracy approximation.

Whenever $S_{aa}^{(l)}$ or $S_{bb}^{(l)}$ are l independent, and $n=n_1$ (or $n=n_2$), transitions between states within the corresponding set of n_1 (or n_2) parallel potentials become forbidden due to the unitarity of matrices X_{lj} and Y_{jk}. Such an effect may take place if the couplings g_l are close in magnitude or very small. If $n<n_1$ (or $n<n_2$) such transitions vanish only at low couplings, in which case $|S_{aa}^{(l)}|$ (or $|S_{bb}^{(l)}|$) are close to unity. When one of the sets contains only one potential ($n_1=1$ or $n_2=1$), Eqs. (20) are reduced to the transition amplitudes obtained in Ref. [19].

IV. APPLICABILITY CRITERIA

The quasidegeneracy approximation described in Sec. II 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

$$\Delta S_{ll'}^{(a)}=\int_{-t'}^{t''}a_l^{(0)*}(t)V_{ll'}^{(a)}a_{l'}^{(0)}(t)dt, \tag{21}$$

and analogous expressions for $\Delta S_{ll'}^{(b)}$, obtained by replacing a with b everywhere in Eq. (21).

An overestimate for these amplitudes can be obtained by substituting $a_l^{(0)}(t)=b_l^{(0)}(t)=1$, resulting in the criteria

$$(t'+t'')\Delta V_{1,2}\ll 1, \tag{22}$$

where the bandwidths of the potential sets ΔV_1 and ΔV_2 are defined by Eq. (7). However, in certain situations less stringent criteria may exist, as can be shown by the use of approximate expressions for the unperturbed wave functions [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/β, i.e.,

$$t'+t_l\gg g_l/\beta,\quad t''-t_l\gg g_l/\beta\quad(\text{for all } l). \tag{23}$$

In this case, an asymptotic expansion of the confluent hypergeometric function (see [30]) on the the left-hand asymptote $t'+t_l>-t+t_l\gg g_l/\beta$ yields

$$a_l^{(0)}(t)\approx a_l^{(0)}(-t')(|t|/t')^{i\lambda_l}\exp[-iV_{ll}^{(a)}(t'+t)],$$
$$b_l^{(0)}(t)\approx b_l^{(0)}(-t')(|t|/t')^{-i\lambda_l}$$
$$\times\exp(-iV_{ll}^{(b)}(t'+t)-i\beta(t^2-t'^2)/2), \tag{24}$$

and on the right-hand asymptote $g_l/\beta\ll t-t_l<t''-t_l$ it yields

$$a_l^{(0)}(t)\approx a_l^{(0)}(t'')(t/t'')^{i\lambda_l}\exp(-iV_{ll}^{(a)}(t-t'')),$$
$$b_l^{(0)}(t)\approx b_l^{(0)}(t'')(t/t'')^{-i\lambda_l}$$
$$\times\exp(-iV_{ll}^{(b)}(t-t'')-i\beta(t^2-t''^2)/2). \tag{25}$$

Whenever $l>n$, Eqs. (24) and (25) become exact [see Eqs. (11)]. Hereafter one should set $\lambda_l=0$ if $l>n$.

The first-order corrections to the amplitudes Eq. (21) can therefore be estimated as

$$\Delta S_{ll'}^{(a)} \approx \frac{V_{ll'}^{(a)}}{1+i\lambda_{l'}-i\lambda_l}[t' a_l^{(0)*}(-t')a_{l'}^{(0)}(-t') + t'' a_l^{(0)*}(t'')a_{l'}^{(0)}(t'')], \quad (26)$$

for the horizontal set, and a similar expression, with *b* replacing *a*, for the slanted set.

Finally, using Eq. (6) one can write the applicability criteria in the form

$$(t'+t'')\Delta V_{1,2} \ll |1+i\lambda_{l'}-i\lambda_l|. \quad (27)$$

Let us consider now the second limiting case, in which both boundaries $-t'$ and t'' lie way inside the two-state transition ranges g_l/β, i.e.,

$$t'+t_l \ll g_l/\beta, \quad t''-t_l \ll g_l/\beta \quad (\text{for all } l). \quad (28)$$

In addition, let $\lambda_l \gg 1$, in order to obtain an adiabatic evolution. Within the range defined by Eq. (28), the adiabatic energies are approximately $V_{ll}^{(a)} \pm g_l$, and

$$\begin{pmatrix} a_l^{(0)}(t) \\ b_l^{(0)}(t) \end{pmatrix} \approx \frac{a_l^{(0)}(-t')+b_l^{(0)}(-t')}{2} \times \exp(-i(V_{ll}^{(a)}+g_l)(t'+t)) \pm \frac{a_l^{(0)}(-t')-b_l^{(0)}(-t')}{2} \times \exp(-i(V_{ll}^{(a)}-g_l)(t'+t)). \quad (29)$$

Substitution of Eqs. (29) in Eq. (21), taking into account Eq. (6), gives the applicability criteria

$$(t'+t'')\Delta V_{1,2} \ll 1+|g_l-g_{l'}|(t'+t''). \quad (30)$$

Criteria combining the cases Eqs. (22), (27), and (30) can be written with the help of Eq. (13) as the single expression

$$(t'+t'')\Delta V_{1,2} \ll 1+|g_l-g_{l'}|\min(t'+t'',(g_l+g_{l'})/\beta). \quad (31)$$

These criteria allow for an interpretation that stems from the viewpoint of the uncertainty principle. Equation (31) means that the potentials become indistinguishable within a limited time interval. The second term on the right-hand side of Eq. (31) 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 [25]). 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 $2\to 1$, $3\to 4$, $3\to 5$, and $4\to 5$, 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.

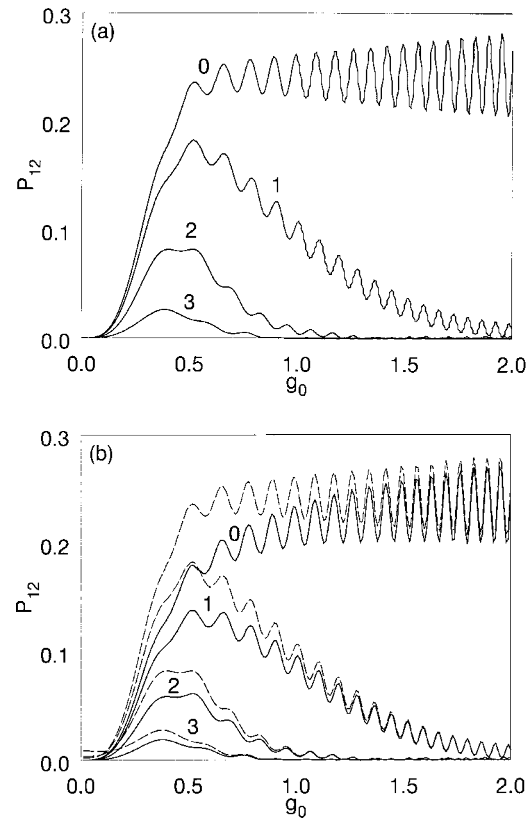

FIG. 2. Counterintuitive transition probabilities vs the coupling strength g_0 [see Eq. (32)] for a truncated linear grid with the bounds $t'=t''=100$ (on a scale in which the potential slopes $\beta=1$) and the potential gaps: (a) $\Delta V=0$, and (b) $\Delta V=2.5\times 10^{-3}$. The numbers denote the values of the phase parameter *m* in Eq. (32). The results of numerical integration of the coupled equations (1) are presented by solid lines. The dashed-line plots in (b) are calculated with the quasidegeneracy approximation using Eqs. (20).

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 [19]. Such transitions are present in truncated linear grids as well, since the transformations Eq. (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

$$g_{jk}=g_0\begin{pmatrix} 1/1.2 & 1 \\ 1 & 1.2\exp(im\pi/4) \end{pmatrix}, \quad (32)$$

with integer values of *m*, or the equal-coupling form, with

$$g_{11}=g_{12}=g_{21}=g_{22}=g_0. \quad (33)$$

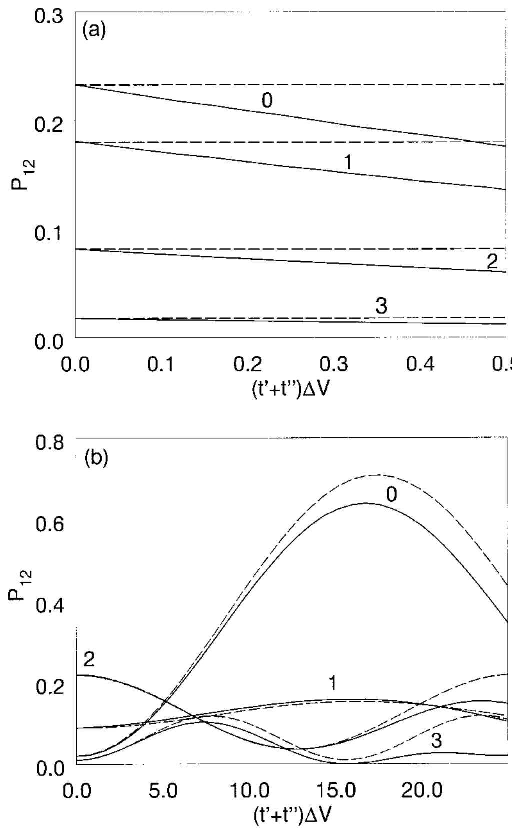

FIG. 3. Counterintuitive transition probabilities vs the potential gap ΔV, calculated for (a) $t'=t''=100$, $g_0=0.5$, or (b) $t'=t''=20$, $g_0=5$. Other notations as in Fig. 2.

All the following calculations are performed for the slope $\beta=1$. The results can be readily expanded to other β 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 Eq. (31). At low values of g_0 the amplitudes $S_{aa}^{(l)}$ and $S_{bb}^{(l)}$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. (20)]. In cases in which the singular values are quite similar, the probabilities of such transitions become small at high coupling strengths, since $S_{aa}^{(l)}$ and $S_{bb}^{(l)}$are small for all l (see, for example, the plots for $m=3$ in Fig. 2, 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 $S_{aa}^{(l)}$ (or $S_{bb}^{(l)}$) 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 nonseparable one, and therefore changes the behavior of the transition probability at high values of the coupling strengths.

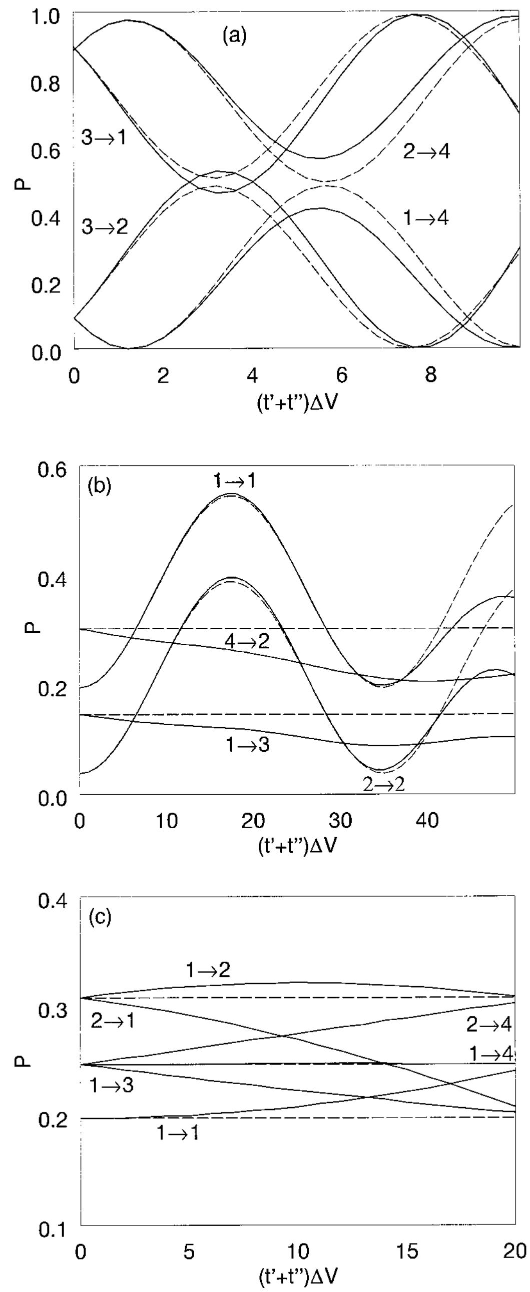

FIG. 4. Probabilities of specified state-to-state transitions vs the potential gap ΔV for a truncated linear grid with $t'=t''=50$ and $g_0=5$. Parts (a) and (b) correspond to the coupling matrix Eq. (32) with $m=4$ and $m=0$, respectively, while part (c) corresponds to the case of equal couplings [see Eq. (33)]. Other notations as in Fig. 2.

Counterintuitive transitions persist at finite values of the potential gap ΔV as well [see Figs. 2(b) and 3]. As one can see, the higher is the coupling strength, the better the results of the quasidegeneracy approximation [in agreement with the criteria Eq. (31)]. At low coupling strengths the predictions of the quasidegeneracy approximation are correct as long as

$(t'+t'')\Delta V \leqslant 0.2$ [see Fig. 3(a)], while at high coupling strengths they are correct as long as $(t'+t'')\Delta V \leqslant 0.2\lambda$ [see Fig. 3(b)].

Probabilities of counterintuitive transitions [see Fig. 3(b)] 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 Stückelberg 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. 3 and 4.) The period of the Stückelberg oscillations is $\Delta V/\beta$; i.e., it is dependent on the potential gap ΔV but independent of the time interval $t'+t''$. These properties, as well as the magnitude of the Stückelberg oscillation period, are not in agreement with the behavior of the oscillations presented in Figs. 3(b) and 4.

The quasidegeneracy approximation relates the oscillations reported here to the interference of the terms in Eqs. (20), corresponding to different decoupled channels. The dependence on ΔV is due to exponents in Eqs. (12) and in the second sum of each of the two equations (20a) and (20b). The oscillation period in ΔV is $2\pi\rho/(t'+t'')$, where $\rho=\Delta V/(V_{22}^{(a)}-V_{11}^{(a)})=\Delta V/(V_{22}^{(b)}-V_{11}^{(b)})$ is the ratio of the potential gaps in the original and decoupled representations. For the coupling matrix Eq. (32) 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(b) these oscillations are absent just for the transitions for which one would expect Stückelberg oscillations ($4\rightarrow2$ and $1\rightarrow3$). The reason for not seeing Stückelberg oscillations in our figures is simple. The scale of the plot is too small to show even a single Stückelberg period. In the case of equal coupling [see Eq. (33)] $V_{ll}^{(a)}=V_{ll}^{(b)}=0$ for all l. This property results in the absence of oscillations in Fig. 4(c).

There is still another kind of oscillation possible. It has been demonstrated in the case of a truncated two-state linear curve crossing, in which oscillations may show up as a function of each of the two truncation times (see [23]). In principle, such oscillations should also appear in our model in the ΔV dependence, since the crossing points move as the potential gap is varied. However, the period of these oscillations, too, is too large to show up in Figs. 3 and 4.

In the limit of high coupling strengths or slow potential variation ($\lambda\gg1$) the semiclassical approach of independent crossings predicts nonvanishing transitions only for one final state per a given initial state. If $n_1=n_2$ all the nonvanishing transitions lead from one set of the parallel potentials to another set, leading to a complete population transfer between the sets. This property was used in a recent proposal of single-electronics devices, based on transitions between quantum dots (Refs. [14,15]). In contrast, the quasidegeneracy approximation predicts more nonvanishing transitions (see Figs. 3 and 4). In the case of $n<n_1=n_2$, a finite probability may remain for transitions within the same set of parallel potentials [see Figs. 3, 4(b), and 4(c)], 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 of incomplete population transfer may interfere with the operation of the single-electronics devices mentioned above.

VI. CONCLUSIONS

Equations (20) represent the transition amplitudes in a truncated linear potential grid as a coherent sum of amplitudes for parallel two-state crossings. These amplitudes become exact in the case of strict degeneracy, and are approximately applicable to nondegenerate systems whenever the criteria Eq. (31) are observed. The results also can be applied 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. (20) for the quasidegenerate groups. Thus the approximation can be used in a wide variety of physical problems in which multistate curve crossing occurs.

Although the derived analytical expressions are not simple looking, they allow us to predict certain features of multistate curve crossing, such as properties of counterintuitive transitions, the existence of a new kind of quantum oscillations, and conditions for incomplete population transfer at high coupling strengths. For a qualitative analysis one can use the simplified form based on Landau-Zener amplitudes [see Eqs. (17)]. The more accurate amplitudes [see Eqs. (15) and (12)] are expressed in terms of confluent hypergeometric functions and require numerical evaluation. However, the required computer resources are proportional to the number of channels N, whereas close-coupling calculations require a memory proportional to N^2 and a computation time proportional to N^3.

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