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A modified Rosen–Zener calculation of surface-ion neutralization

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Abstract. We suggest two modified versions of the Rosen–Zener theory of surface-ion neutralization, originally proposed by Amos and his colleagues. In the first, we retain the assumption of zero bandwidth, and use a more accurate form of the Rosen–Zener conjecture. In the second, we also allow the band to have some width.

The dynamics of surface-ion neutralization has been, and continues to be, a focus of considerable theoretical interest (Amos *et al* (1989a) and references therein). In the analysis of this problem, one assumes that a fast ion moving in the vicinity of a surface captures an electron from a band of the solid. The process can occur even if the bound atomic level occupied by the electron in the final state does not exactly coincide in energy with any electron in the initial state of the solid, since compensation for energy defects can be provided by the kinetic energy of the atomic mass centre. The usual approach, which shall be followed here, is semiclassical—the ion moves along a rectilinear path at constant speed and generates a time-dependent potential which interacts with the electrons. If the Fourier transform of this potential is appreciable at the energy difference between initial and final states, there will be a significant capture probability P_n. For slow ions, P_n will be negligible, unless the vacancy in the free atom coincides in energy with electrons in the band of the solid.

One can see this effect most simply in first-order perturbation theory. Let $U_{k0}(t)$ be the time-dependent matrix element coupling a particular electron in the band of interest to the vacant ionic state. (We can evidently also look upon the process as the transfer of a hole from the ion to the surface.) The amplitude for the process is, in atomic units (which we use here and throughout the paper),

$$a_k = -\mathrm{i}\int_{-\infty}^{\infty} U_{k0}\exp[-\mathrm{i}(\Omega_k - \Omega_0)t]\,\mathrm{d}t \tag{1}$$

where Ω_k, Ω_0, are the energies of the electron in the surface and atomic states, respectively. The integral on the right-hand side of equation (1) is the Fourier transform (FT) of the coupling potential. Only if the FT is appreciable at $(\Omega_k - \Omega_0) = \delta_k$ will there be a significant transition probability. Thus, as noted, neutralization will

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be negligible for slow ions unless the bound state lies *within* the band of surface states. We will discuss the slow-ion case elsewhere.

The identification of the first-order amplitude with the FT of the coupling pulse is quite general, i.e., is not dependent on the temporal form of U_{k0}. This is fortunate, since, in realistic problems, this function is not normally known very well. In effect, the FT becomes an unknown function to be inferred from experiment.

Amos and co-workers (Amos *et al* 1986, 1989a, b) have devised a very clever way, based on the Rosen–Zener conjecture for two-level systems (Rosen and Zener 1932, Robiscoe 1978), to extend the first-order theory, with its single unknown function, to strong coupling, for cases where the width of the initial band may be considered to be zero. The purpose of this note is to modify their approach.

First, we shall describe a way to further characterize the presumably unknown coupling function U_{k0} by a parameter. Then, as a separate exercise, we shall demonstrate how one may modify the original result to allow for a non-zero, but small, width for the initial band.

If the initial band is sufficiently narrow, one may proceed along the lines followed by Amos *et al* (1986)—treat the system as equivalent to one of two levels. We shall begin by reviewing the quantum mechanics of two-level problems.

Let a_1, a_2 be the probability amplitudes of states $|1\rangle$ and $|2\rangle$. Instead of equation (1), we must solve the fully-coupled time-dependent Schrödinger equation

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -\mathrm{i}\,U_{12}(t)\exp(\mathrm{i}\delta t)a_2 \tag{2a}$$

$$\frac{\mathrm{d}a_2}{\mathrm{d}t} = -\mathrm{i}\,U_{12}(t)\exp(-\mathrm{i}\delta t)a_1 \tag{2b}$$

where now $\delta = \Omega_1 - \Omega_2$ is the frequency separation of the two states. Equations (2) are to be integrated subject to the initial conditions $a_1 = 1$, $a_2 = 0$, as $t \longrightarrow -\infty$. The desired transition amplitude is $a_2(+\infty)$. For the special case where $U(t)$ is a hyperbolic secant (one of the few pulse shapes where exact solutions to the two-level problem are known), the form of the solution is extremely simple, namely

$$a_2(+\infty) = -\mathrm{i}\,F(\delta)\sin A \tag{3}$$

where A is the so-called 'pulse area', i.e., the integral of U_{12} between $t = \pm\infty$, and F is the FT of U_{12} divided by A. Since AF is the approximation to a_2 given by first-order perturbation theory, the probability amplitude is the product of two factors—its first-order approximant and $(\sin A)/A$. In their original paper, Rosen and Zener (1932) surmised that the same form might hold for all smooth pulses, with the proviso that one replace F for the hyperbolic secant by the FT of the actual pulse. If this conjecture were true, solving a given problem with two levels in perturbation theory would also generate the exact solution. Amos and co-workers (1986, 1989a, b) postulate the correctness of the assumption, and apply it to the ion neutralization problem. We shall develop their ideas further.

Now the Rosen–Zener conjecture (RZC) is valid for arbitrary pulse shapes if $\delta = 0$. However, it is manifestly false for non-resonant coupling pulses that are asymmetric functions of the time. Bambini and Berman (1981) demonstrated this by constructing explicit solutions to a particular class of asymmetric-coupling problems, and Robinson (1981) generalized their conclusion to arbitrary asymmetric shapes. In addition, the RZC is false even for a symmetric pulse whose Fourier transform has a discontinuous derivative at $\delta = 0$ (Robinson 1984). On the other hand, the conjecture *is* approximately correct for symmetric coupling pulses whose Fourier transforms possess a derivative at $\delta = 0$ (Robinson 1984), provided that δ is 'small'. That is, it was shown for the symmetric pulses with differentiable FT that

$$a(+\infty) = -\mathrm{i}\, F(\delta) \sin A + \mathrm{O}(\delta^2) \tag{4}$$

where F is the FT of the actual pulse, not necessarily a hyperbolic secant (Robinson 1984). The work of Amos and colleagues seems eminently sensible in the light of equation (4). In fact, the agreement they obtained (Amos *et al* 1989b) between an exact calculation which modelled both pulse shape and state distribution within the valence band of the solid seems so good that an improved formulation might not be needed. We proceed in order to allow for the possibility that the quality of the agreement might be worse in other cases.

In the following, we assume that the indicated conditions (symmetric pulses with differentiable FT) for approximate validity of the RZ conjecture apply.

One may obtain equation (4) from the infinite-product representation of the probability amplitude (Robinson 1985a, b). We summarize this formulation. An exact expression of $a_2(+\infty)$ is given by

$$a_2(+\infty) = -\mathrm{i}\, A F(\delta) \prod_N (1 - A^2/A_N^2) \tag{5}$$

where A_N^2 is a 'restoring eigenvalue' of the square of the pulse area (Robinson 1981, 1984), i.e., the squares of those pulse areas for which the system is restored to its initially prepared state. The eigenvalues in a particular problem depend on the pulse shape and δ. In some sense, equation (4), which we emphasize is not an approximation is a generalization to arbitrary pulse shapes of the Rosen–Zener solution for the hyperbolic secant.

It can happen that there are pulse shape-detuning combinations for which none of the eigenvalues is real (for example, asymmetric pulses with δ different from zero). This means that there are no physical pulses of the particular shape and δ that can restore the system to its initially prepared condition. In such cases, not only is the RZC not valid, but the chief qualitative property of the transition probability given by equation (3), that it oscillates with A and passes through zero an infinite number of times, is absent. For the hyperbolic secant, $A_N^2 = (N\pi)^2$, independent of δ, while for other symmetric pulses with differentiable transforms,

$$A_N^2 = (N\pi)^2 - \mathrm{O}(\delta^2). \tag{6}$$

Equation (6) does *not* apply for large detunings, although there are scaling laws that are valid in that asymptotic regime (Robinson and Berman 1983) in some cases.

We are now prepared to offer our first modification to the formulation of Amos *et al.* We shall use a result that is implied in previous work (Robinson 1984, 1985a), but which has not been made explicit.

It has been shown, via a variational calculation, that the quadratic correction term in equation (6) is approximately independent of the index N (Robinson 1984). Let us designate this correction by $(a\delta)^2$, so that equation (6) becomes

$$A_N^2 \approx (N\pi)^2 - (a\delta)^2. \tag{6a}$$

If the shape of the pulse is unknown, a is a free parameter of the theory. Substituting the eigenvalues of equation (6) into equation (5), the infinite product is identified as

$$a_2(+\infty) \approx \frac{-\mathrm{i}\,F(\delta)\sin[\sqrt{A^2+(a\delta)^2}]a\delta}{\sqrt{A^2+(a\delta)^2}\sin[a\delta]}. \tag{7}$$

This is an improved form of equation (4). Amos *et al* also obtained an oscillatory result, but with the maxima occurring at the Rosen–Zener $A = N\pi$. Here, in equation (7), the argument of the sinusoidal functions resembles that of a square pulse. In fact, equation (7) is *exact* for a square pulse, with $a = T/2$, where T is the duration of the interaction. Thus, contrary to the surmise of Rosen and Zener, the transition amplitude for a square pulse is given by an expression related to the RZ form! One does not require a smoothly varying pulse for the (approximate) validity of the modified form of the conjecture—rather the pulse must be symmetric in time, and be characterized by a differentiable FT, i.e., the smoothness requirement refers to the frequency domain, not the time domain. In effect, the transition amplitude for such a pulse will combine square-pulse and hyperbolic-secant characteristics.

Now, in the present problem, neither the coupling strength nor the shape function is subject to the control of the experimenter. Since both F and a depend on U, one may hope to infer the shape U empirically, by exploring the dependence of P_n on the normal component of ion velocity. For example, one might guess a form for U and a value for A based on calculations performed in the Hartree–Fock approximation. With the assumed form, the parameter a and the FT F are determined. If the experimental transition probability is not a good fit to equation (7) with a particular F and a, adjust the shape of the potential U, and continue until a good fit is obtained.

Both the oscillatory result in equation (7) and the original form of Amos *et al* are consequences of the assumption that the valence band may be treated as a single level. In the opposite extreme, where the band is broad, the oscillations will be greatly reduced or absent.

It is also of interest to infer the form of the capture probability between the two extremes of infinite continuum and zero-width band. To model the broadening of $|2\rangle$, we consider a two-level system in which the excited state decays exponentially to an unrelated continuum, not driven by the pulse. In this model, the only parameter is the decay width Γ. The exponential time dependence implies that the shape function of the 'band' will be a Lorentzian. This is, of course, usually unphysical, but since we mainly desire to see the effect of non-zero width, this detail should not be too important.

Since, in our picture of the problem, $|a_2\rangle$ decays away, the probability of neutralization is given by

$$P = 1 - |a_2(\infty)|^2 \tag{8}$$

and our task is to calculate $a_1(\infty)$. We shall proceed by writing a suitable expression for a_1 that is valid for zero width, and analytically continue it to the case where state $|2\rangle$ decays. From equation (7), in the non-decaying limit, the modulus for finding the system in its initially prepared state is

$$|a_1(+\infty)| = \left[\!\!\left[1 - \frac{A^2F^2(\delta)\sin^2[A^2+(a\delta)^2]a^2\delta^2}{[A^2+(a\delta^2)]\sin^2(a\delta)}\right]\!\!\right]^{1/2}$$
$$= \left\{\cos^2\sqrt{A^2+(a\delta)^2} + \sin^2\left[\sqrt{A^2+(a\delta)^2}\right]\right.$$
$$\left.\times\left[1-\left(AF(\delta)a\delta/\sqrt{A^2+(a\delta)^2}\sin(a\delta)\right)^2\right]\right\}^{1/2}. \qquad (9)$$

Thus, without loss of generality, we may write the infinite-time initial state probability as

$$a_1(\infty) = \exp(\mathrm{i}\phi)\left\{\cos\sqrt{A^2+(\delta a)^2} \pm \mathrm{i}[1-A^2F^2(a\delta/\sin a\delta)^2]/[A^2+(\delta a)^2)]^{1/2}\right.$$
$$\left.\times\sin\sqrt{A^2+(\delta a)^2}\right\} \qquad (10)$$

where ϕ is a phase factor that varies with the pulse shape, detuning and area. That the sine and cosine factors in this equation are in phase quadrature guarantees that it satisfies equation (9) and unitarity. However, unitarity alone does not fix the relative sign of the sine and cosine terms. We shall show how to remove the ambiguity in sign that is present in equation (10) later. At this point, we merely state the result

$$a_1(\infty) = \exp[\mathrm{i}\phi]\left\{\cos\sqrt{A^2+(\delta a)^2} - \mathrm{i}\sqrt{[1-A^2F^2(a\delta/\sin a\delta)^2]/[A^2+(\delta a)^2)]}\right.$$
$$\left.\times\sin\sqrt{A^2+(\delta a)^2}\right\}. \qquad (11)$$

The exponential prefactor acquires a decaying part in the actual problem of interest, but we shall not have to determine it explicitly.

The equations of motion for a two-level system with a decaying excited state may be written

$$\frac{\mathrm{d}a_1}{\mathrm{d}t} = -\mathrm{i}\,U_{12}(t)\exp(\mathrm{i}\delta t)a_2 \qquad (12a)$$

$$\frac{\mathrm{d}a_2}{\mathrm{d}t} = -\mathrm{i}\,U_{12}(t)\exp(-\mathrm{i}\delta t)a_1 - \Gamma a_2/2. \qquad (12b)$$

Following Robiscoe (1978), we define $a_2 = b_2 \exp[-\Gamma t/2]$. $a_1 = b_1$, so that equations (12) become

$$\frac{\mathrm{d}b_1}{\mathrm{d}t} = -\mathrm{i}\, U_{12}(t) \exp[\mathrm{i}(\delta + \mathrm{i}\Gamma/2)t] b_2 \tag{13a}$$

$$\frac{\mathrm{d}b_2}{\mathrm{d}t} = -\mathrm{i}\, U_{12}(t) \exp[-\mathrm{i}(\delta + \mathrm{i}\Gamma/2)t] b_1 . \tag{13b}$$

Thus, insofar as the ground state amplitude is concerned, the width of the excited state merely imparts an imaginary part to the detuning, and equation (11), with δ complex, applies to this case.

However, the presence of the factor $\exp(\mathrm{i}\phi)$, with ϕ unknown, makes it impossible to directly apply equation (11). Instead, we shall use that equation to write an expression for b_1 in terms of a certain set of eigenvalues, which are the squares of the roots of equation (11). The eigenvalue formulation will also enable us to deduce the relative signs of the sine and cosine terms in equation (10).

It has previously been shown that this infinite product representation for b_1, analogous to equation (5), exists (Robinson 1985b). In this case, we have

$$b_1 = \prod_Q (1 - A^2/A_Q^2) . \tag{14}$$

The A_Q^2 are the squares of those pulse areas that depopulate the initially prepared state. They depend on pulse shape and detuning, and, like their restoring counterparts, need not be real.

It is convenient to recall the origin of equation (14), which is exact. One may rewrite equations (13) as uncoupled second-order differential equations, namely

$$\frac{\mathrm{d}^2 b_1}{\mathrm{d}z^2} - \mathrm{i}\frac{\delta}{f}\frac{\mathrm{d}b_1}{\mathrm{d}z} + A^2 b_1 = 0 \tag{15a}$$

$$\frac{\mathrm{d}^2 b_2}{\mathrm{d}z^2} + \mathrm{i}\frac{\delta}{f}\frac{\mathrm{d}b_2}{\mathrm{d}z} + A^2 b_2 = 0 \tag{15b}$$

where

$$A = \int_{-\infty}^{\infty} U_{12}(t)\, \mathrm{d}t \qquad f = U_{12}(t)/A$$

and the 'compressed time' is

$$z = \int_{-\infty}^{t} f(t')\, \mathrm{d}t' - \tfrac{1}{2} .$$

The eigenvalues A_Q^2 are those squares of the pulse area for which $b_1 = 1$ at $z = -\frac{1}{2}$ and vanishes at $z = +\frac{1}{2}$. The A_Q^2 are also given in terms of the eigenfunctions b_N

by

$$A_Q^2 = -\int_{-1/2}^{1/2} (b_N b_N'' - \mathrm{i}(\delta/f) b_N' b_N) \exp(-\mathrm{i}\delta t)\, \mathrm{d}z \tag{16}$$

where $'$ denotes differentiation with respect to z, and where the eigenfunctions are normalized according to

$$\int_{-1/2}^{1/2} b_N^2 \, \mathrm{d}z = 1. \tag{17}$$

The eigenvalues are, as noted, in general complex, whether or not δ is real. When $\delta = 0$, the eigenvalues are given by $[(N + \frac{1}{2})\pi]^2$, $N = 0, 1, 2, \ldots$, and the eigenfunctions by $b_n = \sqrt{2}\cos[(N + \frac{1}{2})\pi(z + \frac{1}{2})]$.

At this point, the sign ambiguity in equation (10) will be resolved. We recall that Rosen–Zener is a valid approximation for pulse shapes that are symmetric in the real and compressed times, t and z, provided f has a Fourier transform that is differentiable at $\delta = 0$, with small detuning (Robinson 1984). Then, $A_Q^2 = [(N + \frac{1}{2})\pi]^2 + g(\delta)$, where g is small. We shall expand the correction term g as a power series in δ, and retain the leading non-vanishing term. Its sign will determine that of the sine and cosine terms in equation (10).

We proceed by treating the term proportional to δ in equation (16) as a perturbation. Then, A_{Q1}^2, the first-order correction to the zero-detuning eigenvalue, is given by

$$\begin{aligned} A_{Q1}^2 = \int_{-1/2}^{1/2} \mathrm{d}z\, b_N b_N' (\mathrm{i}\delta/f) &= -2\mathrm{i}(N + \tfrac{1}{2})\pi \int_{-1/2}^{1/2} \mathrm{d}z\, \sin(N + \tfrac{1}{2})\pi(z + \tfrac{1}{2}) \\ &\quad \times \cos(N + \tfrac{1}{2})\pi(z + \tfrac{1}{2})/f \\ &= -\mathrm{i}(N + \tfrac{1}{2})\pi \int_{-1/2}^{1/2} \mathrm{d}z\, \sin(2N + 1)\pi(z + \tfrac{1}{2})/f \\ &= (-1)^{N+1}\mathrm{i}(N + \tfrac{1}{2}) \int_{-1/2}^{1/2} \mathrm{d}z\, \cos(2N + 1)\pi(z)/f. \end{aligned} \tag{18}$$

The cosine function in the final integrand of equation (18) undergoes $(N + \frac{1}{2})$ cycles between $z = -\frac{1}{2}$ and $z = +\frac{1}{2}$, and, since f increases monotonically between $z = -\frac{1}{2}$ and $z = 0$ for reasonable pulse shapes, the sign of the integral will be the same as that possessed by the integrand near its end points. That is, the first-order correction to the eigenvalue is proportional to $-\mathrm{i}$. In the particular case of the hyperbolic secant pulse, $f = (\operatorname{sech} \pi t/T)/T$, the eigenvalues are given by

$$A_Q^2 = [(N + \tfrac{1}{2})\pi - \mathrm{i}\delta T/2]^2. \tag{19}$$

The hyperbolic secant result is exceptional in that it is not restricted to the small detuning regime.

For small detunings,

$$F = 1 - b^2\delta^2$$
$$(a\delta/\sin a\delta)^2 = 1 + (a\delta)^2/3$$
$$A^2/[A^2 + (a\delta)^2] = 1 - (a\delta/A)^2$$

so that equation (9) becomes

$$|a_1(\infty)|^2 = \cos^2(A + (a\delta)^2/2A) + (\delta q)^2 \sin^2(A + (a\delta)/2A) \tag{20}$$

where

$$q^2 = (b^2 - a^2/3 + a^2/A^2).$$

We note that q^2 must be real and non-negative in order that $|a_1|^2$ have the significance of a probability for arbitrary pulse areas. This can be achieved only if $a^2 \leqslant 3b^2$. Clearly, a^2 cannot be negative, so that $0 \leqslant a^2 \leqslant 3b^2$. Since $a^2 = 0$ for the hyperbolic secant pulse, while $a^2 = 3b^2$ for the square pulse, we note that these two exactly solvable problems represent opposite limiting cases, and the ratio $(a/b)^2$ measures how closely a given pulse shape will approximate one of the extremes.

Using the approximate form of equation (20), equation (10) becomes

$$a_1(\infty) = \exp(\mathrm{i}\phi)[\cos(A + (a\delta)^2/2A) \pm \mathrm{i}\delta q \sin(A + (a\delta)^2/2A)]. \tag{21}$$

We must choose the sign in equation (20) so that its roots yield a sign that agrees with that of the small detuning eigenvalue determined previously. The probability amplitude given by equation (21) vanishes for pulse areas that are given by

$$-\cot(A + (a\delta)^2/2A) = \mathrm{i}\delta q \tag{22}$$

or

$$-\tan[(2N+1)\pi/2 - A - (a\delta)^2/2A] = \mathrm{i}\delta q = (2N+1)\pi/2 - A - (a\delta)^2/2A \tag{23}$$

since the deviation from the zero-detuning-restoring eigenvalues is presumed to be small. In order that the eigenvalue shift be negative imaginary for real positive detuning, it is necessary that we choose the negative sign in equation (20). To find the eigenvalues in cases where $|2\rangle$ decays, we must simply replace δ by $(\delta + \mathrm{i}\Gamma/2)$ in the formula (23).

Thus, the neutralization probability is given by

$$P_n = \prod_Q (1 - A^2/A_Q^2) \tag{24}$$

where the eigenvalues are computed for the complex detuning $\delta + i\Gamma/2$.

To see how the width modifies the character of the transition probability, we examine the case of the hyperbolic secant, $f = \mathrm{sech}(\pi t/T)$. The eigenvalues are given by

$$A_Q^2 = [\pi(N + \tfrac{1}{2}) + \Gamma T/4 - i\delta T/2]^2. \tag{25}$$

The transition probability is, retaining only corrections linear in δ,

$$P_n = \sin^2 A\,\mathrm{sech}^2\,\delta T/2 + [\sin^2(A)\,\mathrm{sech}^2(\delta T/2 - 1)][\mathrm{Re}\,\Gamma T/2\pi(2\psi(\tfrac{1}{2} - i\delta T/2\pi) \\ - \psi(\tfrac{1}{2} - i\delta T/2\pi - A/\pi) - \psi(\tfrac{1}{2} - i\delta T/2 + A/\pi))] \tag{26}$$

where ψ designates the digamma function. As compared to the case of zero bandwidth, equation (26) suggests an overall increase in the neutralization probability, on average, and an introduction of contributions that do not oscillate with pulse area.

Qualitatively similar behaviour is manifest for a rectangular pulse of duration T. Again retaining only terms linear in the width, we obtain, using the exact solution for the square pulse, the expression

$$P_n = 1 - \exp(-\Gamma T/2)\Big\{1 - [1 + (\delta T/2)^2]/[A^2 + (\delta T/2)^2]\sin^2\sqrt{A + (\delta T/2)} \\ + \Gamma T^3\delta^2/8[A^2 + (\delta T)^2] + (\Gamma T(1 - (\delta T)^2)/2(A^2 + (\delta T)^2)) \\ \times \sin^2\sqrt{A^2 + (\delta T/2)^2}/4\sqrt{A^2 + (\delta T/2)^2}\Big\}. \tag{27}$$

To summarize, we have proposed modified versions of the Rosen–Zener type result for fast ion neutralization, which had been originally proposed by Amos and his colleagues. In the first form, we retain their assumption of a zero-width band, and make use of a more general form of the RZ conjecture, which should yield higher accuracy. In this formula, the zeroes of the neutralization probability occur at $(N\pi)^2 - (a\delta)^2$, instead of the $(N\pi)^2$ which characterize the hyperbolic secant. The parameter a is determined by the coupling pulse, so that no information beyond that required by Amos and colleagues is needed here. The oscillations predicted by Amos and co-workers appear in this calculation, but shifted.

In addition to improving the accuracy of the method, we have also observed that our approach facilitates the parametrization of the driving pulse, and sets limits on the variation of the results. In addition to the constant a, there is a term containing a characteristic coefficient b, defined as $(b\delta)^2 = 1 - F^2$. In the small detuning limit, where the Rosen–Zener approximation is valid, the square pulse and hyperbolic secant represent opposite limits for the ratio $(a/b)^2$. Thus, one expects the behaviour of an arbitrary pulse to fall somewhere between the two.

In our second modification, we allow the band from which the electron is extracted to have a non-zero width. This width becomes an additional parameter of the theory. Results are expressed in terms of an infinite product, whose roots are obtained by solving an equation that is trancendental in the Fourier transform of the driving pulse, the parameter a, the detuning and the width. For the small detuning limit, this equation reduces to a simple algebraic form, which may be solved explicitly.

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