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Resonances crossing and electric field quantum sensors*

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Abstract

We propose a theoretical model for a quantum sensor that can determine in a very simple way whether the intensity of an electric field has an assigned value or not. It is based on the fact that when an exact crossing of the imaginary parts of the resonances occurs in a double-well quantum system subject to an external DC electric field, a damped beating phenomenon occurs, which is absent if there is no such a crossing. This result is then tested numerically on an explicit one-dimensional model.

Introduction

Quantum sensors are devices that measure physical quantities, such as electric or magnetic fields, using the laws of Quantum Mechanics. The first devices with these characteristics include the Ramsey interferometer [1], based on a two-level system. Currently, many other quantum sensors have been developed, from those based on silicon carbide to those based on nitrogen-vacancy (NV) centers in nanodiamonds, with numerous applications, from rechargeable batteries to biomedical devices (see [2–5] and references therein).

The typical model of a quantum sensor consists of an Hamiltonian $H = H_i + V_e$, where H_i is the internal (or unperturbed) Hamiltonian, and V_e is an external potential to be measured or that represents an element of control used to set the quantum sensor appropriately [6]. For example, in some quantum sensors the external field is a DC electric field, and $V_e(x)$ represents a linear Stark potential.

Assume that H_i is a two-level system with energy levels $E_1 \leq E_2$, and that $\omega = E_2 - E_1$ is the transition frequency between the two states; therefore, in the case where $\omega \neq 0$, an interference effect generates a periodic beating motion with period $T = 2\pi/\omega$. The basic idea is that the effect of the perturbation dues to V_e is to produce a shift in energy levels, and a change in the transition frequency ω ; therefore, a periodic beating motion of the quantum system described by H is still observed, but with a modified period. A relationship is then established between the period of the beating motion and the external field that can be used to obtain an estimate of the intensity of the perturbation V_e . The protocol of such a quantum sensor is essentially based on two steps: in the first step, it is necessary to measure the period of the beating motion with sufficient precision and then, in the second step, to calculate the electric field strength as a function of the measured period.

In this paper we propose a theoretical model for a quantum sensor with an asymmetrical double-well internal Hamiltonian H_i . In this case it is well known [7] that two energy levels of the fundamental states E_1 and E_2 become quantum resonances and have a crossing/avoided crossing behaviour when the the strength of the external electric field varies. The novelty of our analysis consists in applying a criterion to establish the kind of crossing and, furthermore, in showing that some quantum observables, e.g. the survival amplitude, exhibits a beating motion only when the imaginary part of the two quantum resonances cross each other. This fact makes it easier to check whether or not the strength of an external DC electric field is close to a predefined value simply by observing the presence or absence of a beating motion, without the need to measure its period and without performing any calculations. The advantage of such a device is its simplicity and speed of response; on the other hand, with this method, it is not possible to determine exactly the value of the electric field strength, but only to verify whether it is within a given range.

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In this way, it is possible to check very quickly and easily whether, for example, the charge value of a nanobattery [8] becomes lower (or higher, during battery charging) than a predetermined threshold. Also in medical diagnostics, this device could have applications in ultra-dense Electric Field Encephalography [9] in order to monitor the presence/absence of electrical activity in a certain area of the scalp surface.

Such a device can be made with double-well nano-heterostructures presenting essentially one-dimensional features. For example, the analytical study of the behaviour of bound states (when a confining external potential is present) as the electric field strength varies was analysed for a 200 Å Ga_sAl_{1-s}As/60 Å GaAs/ 60 Å Ga_sAl_{1-s}As/50 Å GaAs/200 Å Ga_sAl_{1-s}As heterostructure with s = 0.8 (see section 3.13 [7]); [10] also performed a similar analysis in the case of double-well heterostructures with s = 0.3. We also mention the paper [11] where a detailed analysis of the resonance states was carried out in the case of double-well heterostructures with s = 0.33. Finally, we would like to point out that experimental investigations on electron transport in asymmetrical double-barrier heterostructures have recently been carried out, see [12] and references therein; the techniques are therefore ready to realise a similar device in which there is a double-well instead of a double-barrier.

An essentially one-dimensional double-well potential can also be obtained in Bose–Einstein condensates by superimposing a three-dimensional harmonic trapping potential on a one-dimensional optical lattice, strongly confining along the direction perpendicular to the optical lattice [13]; if the boson scattering length is rather small and if the optical lattice is directed along the vertical axis, the same theoretical model is obtained in which, in this case, the linear potential is due to gravity.

Finally, we emphasise that the above-mentioned devices have essentially one-dimensional characteristics. This fact is very important because in this case the analytical calculation can be carried out with relative ease. The case where the dimension is greater than one can nevertheless, at least in principle, be dealt with even though, as explained in the conclusions, several technical problems arise.

Interference effect at the resonances crossing point. Let the internal one-dimensional Hamiltonian $H_i = -\frac{d^2}{dx^2} + V_i$ be associated with an asymmetrical double-well potential V_i , and let the external potential be a linear Stark potential $V_e(x) = -Fx$, where *F* is the DC electric field strength. If we consider the ground state of a single well, e.g. the left-hand-side (l.h.s.) one, the effect of the second well is to slightly perturb it, and we denote by E_1 the corresponding energy; similarly, let us denote by E_2 the energy of the ground state of the right-hand-side (r.h.s.) well treating the l.h.s. well as a perturbation. The two-level system consists by restricting H_i to these two states, and the effect of the linear Stark potential V_e is, in the first instance, to change the splitting ω as described above.

We can observe, however, that a second effect, associated with the crossing of energy levels, is generated for an appropriate choice of parameters. In fact, if the l.h.s. well of V_i is deeper than the r.h.s. well, then, for F = 0, the energy level E_1 is less than the energy level E_2 . As F increases, these two levels will come closer until they almost cross each other for a critical value of F, and we denote by E their (almost) common value. Since in dimension one the energy levels are always non-degenerate, exact crossing is not possible, and so we have an avoided-crossing picture.

At this (almost) common *E* value of the two levels at the avoided crossing point, the two wells are separated by an inner barrier, where 'classical motion' is forbidden since the potential $V(x) = V_i(x) + V_e(x)$ exceeds the energy level *E*; furthermore, there is an outer barrier (see figure 1). We can measure the length of these barriers by means of Agmon's metric, which in dimension one is simply $\rho_i = \int_{X_2}^{X_3} \sqrt{V(x) - E} \, dx$, for the inner barrier,

and $\rho_e = \int_{X_*}^{X_5} \sqrt{V(x) - E} \, dx$ that of the outer barrier.

In fact, for any F > 0 the stationary states become metastable states associated to quantum resonances $E_1(F)$ and $E_2(F)$ depending on F and with negative imaginary part, and in the complex plane the crossing phenomenon between these two levels may be of:

- type I crossing when there is an exact crossing of their imaginary parts $\Im E_1(F)$ and $\Im E_2(F)$, and an avoidedcrossing of their real parts $\Re E_1(F)$ and $\Re E_2(F)$ (see, e.g. figure 2), which occurs when $\rho_i < 2\rho_e$;
- type II crossing when there is an exact crossing of their real parts, and an avoided-crossing of their imaginary parts (see, e.g. figure 3), which occurs when $\rho_i > 2\rho_e$.

Crossing phenomenon of resonances was analyzed as early as Avron's work in 1982 [14], and was later taken up by [15–17] providing the above criterion for determining the type of crossing. This theoretical result is valid in the semiclassical limit, which in the present context means that the parameter *F* and the depth of the two wells (i.e. α_1 and α_2 in the toy model (1)) are very large in absolute value so that the two resonances are very narrow, that is their imaginary parts are very small in absolute value. However, from a practical point of view, we will see in a numerical experiment that this criterion is already useful even if these parameters are not excessively large.

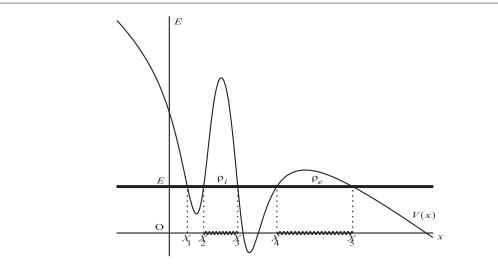
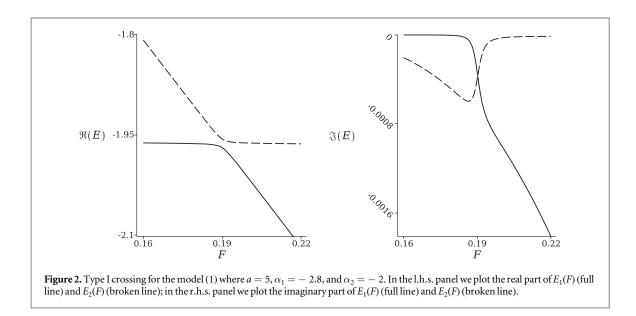


Figure 1. Asymmetrical double-well model with potential $V = V_i + V_e$. The abscissa axis represents the spatial variable *x*, while the ordinate axis represents the energy *E*. For a given value of *E* we may have, as in the figure, two wells, one between X_1 and X_2 and the other one between X_3 and X_4 , and two barriers, the inner barrier with Agmon length ρ_i is between X_2 and X_3 , and the outer barrier with Agmon length ρ_e is between X_4 and X_5 . There are no stable states for *H*, but metastable ones.

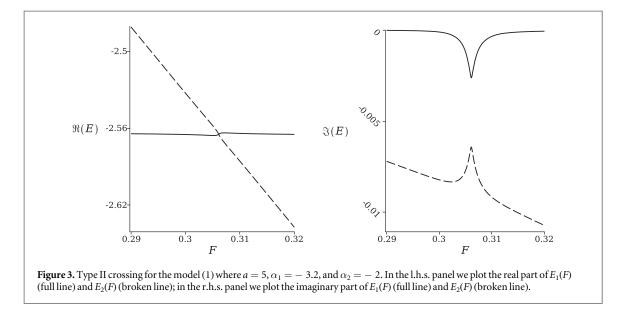


We should mention that the question of resonances crossing is of great interest both in a general context [18, 19], and even in experimental applications [20, 21]; furthermore, it has also been analyzed in the case of symmetric double-well potential [22]. Here we extend these studies by considering the criterion based on the Agmon distances ρ_i and ρ_e to determine whether the resonance crossing is of type I or II. This improvement allows us to tune the parameters of the double-well model to design a quantum sensor for DC electric fields.

Indeed, when the imaginary parts of the two resonances $E_1(F)$ and $E_2(F)$ are sufficiently different from each other then the lifetimes of the two metastable states are quite different, and the phenomenon of interference will not be triggered because one of the two metastable states decays much faster than the other one. In fact, a very slight beating effect can be observed for small times, as pointed out by [23], but it quickly disappears and only the exponential decay associated with the narrowest resonance remains as the dominant term.

On the other side, this picture changes markedly at values of model parameters for which the imaginary parts of the two resonances coincide $\Im E_1(F) = \Im E_2(F)$; in this case, which can occur only in the case of type I crossing, the interference effect is triggered, and thus we observe a damped beating effect with (pseudo-)period $T = 2\pi/(\Re(E_2) - \Re(E_1))$ for large time intervals.

In this way, we have a theoretical model for a quantum sensor that makes it possible to verify whether the intensity F of the external field assumes the specific value for which type I crossing and beating effect occur; we observe that this specific value can be appropriately selected by adjusting the value of the parameters of the internal double-well potential V_i .



Quantitative analysis. To verify this idea on an explicit one-dimensional toy model, we consider the doublewell potential with two attractive singular interactions due to two Dirac's δ ,

$$V_i(x) = \alpha_1 \delta_{x_1} + \alpha_2 \delta_{x_2}, \, x_1 < x_2, \, \alpha_1 < \alpha_2 < 0, \tag{1}$$

where δ_y is such that $\int_{\mathbb{R}} \delta_y f(x) dx = f(y)$. The idea of using Dirac's δ to model wells or barriers goes back to Enrico Fermi [24], and in this context it has been extensively used for the study of the Stark effect on both a single well [25–30], and on double-well [22, 23, 31, 32] cases.

The spectrum of *H* is purely continuous and it coincides with the entire real axis. Therefore, no stable states are possible. It is possible, however, to have resonances *E* associated with metastable states ψ such that $H\psi = E\psi$ where ψ satisfies the outgoing conditions [22] $\psi(x) = C_i^+(x)$ for x > a, where $C_i^\pm(x) = B_i(x) \pm iA_i(x)$, A_i and B_i being the two Airy functions. Resonances of *H* can be equivalently defined as the complex poles of the analytic continuation of the kernel of the resolvent operator $[H - z]^{-1}$ from the upper half-plane $\Im z > 0$ to the lower half-plane $\Im z < 0$ (see [32] and references therein). If we denote by $K_0 = K_0^{\pm}$, if $\pm \Im z > 0$, the kernel of the resolvent operator $[H_0 - z]^{-1}$, where $H_0 = -\frac{d^2}{dx^2} - Fx$, then it is known that

$$K_{0}^{\pm}(x, y; z) = \frac{\pi}{F^{1/3}} \begin{cases} Ci^{\pm} \left(-\frac{Fy+z}{F^{2/3}} \right) Ai \left(-\frac{Fx+z}{F^{2/3}} \right), x \leq y \\ Ci^{\pm} \left(-\frac{Fx+z}{F^{2/3}} \right) A_i \left(-\frac{Fy+z}{F^{2/3}} \right), y < x \end{cases}$$
(2)

The kernel $K = K^{\pm}$, if $\pm \Im z > 0$, of the resolvent operator $[H - z]^{-1}$ can be obtained by K_0^{\pm} as follows [33]:

$$K^{\pm}(x, y; z) = K_0^{\pm}(x, y; z) + \frac{R^{\pm}(x, y; z)}{D^{\pm}(z)},$$
(3)

where

$$R^{\pm}(x, y; z) = \sum_{n,m=1}^{2} K_{0}^{\pm}(x, x_{n}; z) M_{n,m}^{\pm}(z) K_{0}^{\pm}(x_{m}, y; z),$$
(4)

and where, adopting the shortcut notation $k_{j,\ell}^{\pm}(z) = K_0^{\pm}(x_j, x_{\ell}; z)$,

1

$$D^{\pm}(z) = \frac{[1 + \alpha_1 k_{1,1}^{\pm}(z)][1 + \alpha_2 k_{2,2}^{\pm}(z)]}{\alpha_1 \alpha_2} - k_{1,2}^{\pm}(z) k_{2,1}^{\pm}(z),$$
(5)

and

$$M^{\pm}(z) := \begin{pmatrix} \frac{1}{\alpha_2} + k_{2,2}^{\pm}(z) & -k_{1,2}^{\pm}(z) \\ -k_{2,1}^{\pm}(z) & \frac{1}{\alpha_1} + k_{1,1}^{\pm}(z) \end{pmatrix}.$$
 (6)

Then resonances *z* for *H* are the zeros such that $\Im z < 0$ of the analytic continuation of the function $D^+(z)$ from the upper half-plane $\Im z > 0$ to the lower half-plane $\Im z < 0$, and it is possible to compute them numerically once parameter values *F*, α_1 , α_2 , x_1 and x_2 are assigned.

The two resonances have respectively real parts close to the values of the two single-well ground states: $\Re E_1 \sim -\alpha_1^2/4$ and $\Re E_2 \sim -\alpha_2^2/4 - Fa$, where ~means the asymptotic value for large $|\alpha_{1,2}|$, and where we set, to fix the ideas and without losing in generality, $x_1 = 0$ and $x_2 = a > 0$. Thus, crossing phenomenon occurs when *F* is close to the critical value

$$F_C \sim \frac{\alpha_1^2 - \alpha_2^2}{4a},\tag{7}$$

and for these values we have that the Agmon lengths of the inner and outer barriers are given by $\rho_i \sim (\alpha_1^3 - \alpha_2^2)/12F_C$ and $\rho_e \sim \alpha_2^3/12F_C$. Thus a type I crossing occurs when $\sqrt[3]{3} \gtrsim \alpha_1/\alpha_2$, and type II when $\alpha_1/\alpha_2 \gtrsim \sqrt[3]{3}$. Actually, this theoretical result, which holds true exactly only in the semiclassical limit in which $|\alpha_{1,2}|$ and |F| go to infinity, retains good validity even when the parameters are finite. For example, for a = 5, $\alpha_1 = -2.8$, and $\alpha_2 = -2$, a type I crossing is observed in figure 2; from the semiclassical result (7), it turns out that the theoretical value of F_C is 0.192, and this result is in good agreement with the numerical experiment in which F_C takes the value of 0.190(2). For a = 5, $\alpha_1 = -3.2$, and $\alpha_2 = -2$ a type I cross is observed in figure 3, and again there is good agreement between (7) and the result of the numerical experiment.

An important remark concerns the fact that from the type of crossing will follow a different behaviour of observables. Let us consider, for example, the survival amplitude $A(t) = \langle \psi_0 | \psi_t \rangle$ where ψ_0 is the wave function of the initial state, and where $\psi_t = e^{-iHt}\psi_0$ is the wave function of the state at instant *t*. In absence of stable states the survival amplitude decreases in time [32]. This decay is, for a generic Hamiltonian without stable states, the contribution of two terms: one of exponential type that is dominant for intermediate time intervals, and one of power type that instead becomes dominant for longer times; see [34] where it was numerically conjectured that a transition effect between the two different types of decay starts around a certain instant *t*, see also [35–42] for rigorous results, and [43] for the experimental evidence of the deviation from exponential decay. However, in our model the power law decay does not play any role because the spectrum of *H* is not bounded from below [44], and thus we expect to observe only the exponential decay. In particular, since there are only two narrow resonances $E_1(F)$ and $E_2(F)$ having small imaginary part then from the residue theorem it follows that the dominant term of the survival amplitude is given by [27]

$$\langle \psi_0 | e^{-itH_0} \psi_0 \rangle + \sum_{j=1}^2 c_j e^{-itE_j(F)},\tag{8}$$

where

$$c_j = R_j \sum_{n,m=1}^{2} M_{n,m}^+(E_j(F)) q_{n,j} p_{m,j},$$
(9)

and

$$q_{n,j} = \int_{\mathbb{R}} K_0^+(x, x_n; E_j(F)) \, \bar{\psi}_0(x) \, dx \tag{10}$$

$$p_{m,j} = \int_{\mathbb{R}} K_0^+(x_m, y; E_j(F)) \,\psi_0(y) \,dy \tag{11}$$

and where R_j is the value of the residue of the function $1/D^+(z)$ at $z = E_j(F)$. The evolution operator e^{-itH_0} is an integral operator with kernel [45]

$$U_0(x, y; t) = \frac{\exp\left\{\frac{i}{2}\left[\frac{(x-y)^2}{2t} - \frac{1}{6}F^2t^3 + tF(x+y)\right]\right\}}{\sqrt{4\pi i t}},$$
(12)

and the term $\langle \psi_0 | e^{-itH_0} \psi_0 \rangle$ decays more rapidly than the exponential $e^{-t|\Im E_j(F)|}$ in the case of narrow resonances. Then, the asymptotic behaviour of A(t) is governed only by the contributions given by the two resonances. If we are in the type II crossing case, where e.g., $|\Im E_1(F)| < |\Im E_2(F)|$ for each value of F as in figure 3, then the dominant contribution to the exponentially decreasing behaviour of |A(t)| is given by $|c_i|e^{-t|\Im E_1(F)|}$. If, on the other hand, we are in the case of type I crossing, and if we call F_C the value of F at which $\Im E_1(F) = \Im E_2(F)$, then we still observe an exponentially decreasing behaviour given by $|c_j|e^{-t|\Im E_j(F)|}$, where j = 1 if $F < F_C$, and j = 2 if $F > F_C$ as in figure 2; eventually, only for F close to F_C there is a damped oscillating behaviour due to the interference between the two resonances, and in this case the dominant behaviour of |A(t)| is given by:

$$e^{-t|\Im E_1(F_C)|}|c_1 + c_2 e^{-i\omega t}], \tag{13}$$

with pseudo-period $T = 2\pi/\omega$ where $\omega = \Re E_2(F_C) - \Re E_1(F_C)$.

We consider a numerical experiment where ψ_0 is a normalized wavefunction localized on the l.h.s. well corresponding to x = 0; for argument's sake let us assume that ψ_0 is the Gaussian function

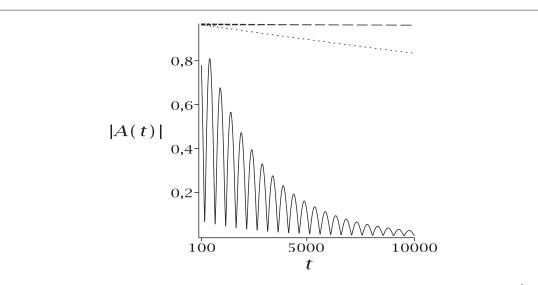


Figure 4. In the case of type I crossing corresponding to a = 5, $\alpha_1 = -2.8$, and $\alpha_2 = -2$, we can observe in the interval $t \in [10^2, 10^5]$, a damped beating behaviour (full line) of |A(t)| when *F* is close to the critical value $F_C = 0.190(2)$ for which we have exact crossing of the imaginary parts of the two resonances; if $F = 0.17 < F_C$ (broken line) or $F = 0.21 > F_C$ (dot line) no significant oscillation is observed.

Table 1. Table of values of the resonances E_j and of the coefficients c_j , j = 1, 2, for different values of F_j where a = 5, $\alpha_1 = -2.8$, and $\alpha_2 = -2$ correspond to a type I crossing.

	$F = 0.17 < F_C$	$F = F_C = 0.190(2)$	$F=0.21>F_C$
$\Re E_1$	-1.96(3)	-1.97(0)	-2.06(6)
$\Im E_1$	$-0.35(1) \cdot 10^{-8}$	$-0.36(8) \cdot 10^{-3}$	$-0.13(7) \cdot 10^{-2}$
$\Re E_2$	-1.86(0)	-1.95(7)	-1.96(3)
$\Im E_2$	$-0.32(9) \cdot 10^{-3}$	$-0.36(8) \cdot 10^{-3}$	$-0.14(6) \cdot 10^{-4}$
$\Re c_1$	$0.41(0) \cdot 10^{-2}$	0.44(8)	0.96(5)
$\Im c_1$	$0.85(1) \cdot 10^{-7}$	-0.027(6)	$0.13(0) \cdot 10^{-3}$
$\Re c_2$	0.96(6)	0.52(1)	$0.34(9) \cdot 10^{-2}$
$\Im c_2$	$-0.11(2) \cdot 10^{-4}$	0.027(5)	$-0.14(4) \cdot 10^{-3}$

$$\psi_0(x) = (2\pi\sigma^2)^{-1/4} e^{-x^2/4\sigma^2}$$
, where $\sigma = 1/2$, (14)

and we go on to study the behaviour of A(t) for $t \in [10^2, 10^5]$ and for some $F < F_C$, $F > F_C$, and for $F = F_C$. For a = 5, $\alpha_1 = -2.8$, and $\alpha_2 = -2$, we have a type I crossing when F takes the value $F_C = 0.190(2)$; for the values of the resonances E_j , and of the coefficients c_j , j = 1,2, see table 1. As expected, in figure 4 (full line) a damped oscillating behaviour is observed for |A(t)| when the intensity F of the external field is close to F_C . On the other hand, when F is different from this value a damping without significant oscillations is observed (see figure 4 - broken lines) because one of the two metastable states decays much faster than the other one, and therefore it is not possible to have a long times interference phenomenon. In this case the damping effect is slower than in the first case, because one of the two resonances is much narrower than those obtained when $F = F_C$.

We remark that the critical value F_C does not depend on the initial state; instead, as the parameters α_1 , α_2 and a vary, one can tune the critical value F_C as desired.

As a consequence of this numerical experiment, it can be stated that for this choice of parameters significant oscillations of the survival probability are observed when *F* is close to the predetermined value F_C , while for *F* outside the range $[F_C - \delta_F, F_C + \delta_F]$, where the measurement tolerance δ_F is less that the 10% of F_C , the imaginary parts of the two resonances are substantially different and therefore no significant oscillations occur.

Conclusions. In conclusion, this paper analyses in detail the time evolution of the survival amplitude for a Schrödinger operator with an asymmetrical double-well potential under the effect of a Stark perturbation. It is verified in a numerical experiment that this is a useful theoretical model for designing a quantum sensor for which the response to an external DC electric field has two distinctly different behaviours depending on whether the field strength is close to or different from a predetermined value F_C of the external field strength, with a precision on the order of 10% of the value F_C . By means of (7) the value F_C can be chosen by tuning the internal potential parameters.

The novelty is that it is possible to verify a specific value of the DC electric field simply by observing whether or not significant oscillations of the survival probability are present, regardless of their period. In some ways we have a phenomenological analogy with RLC electrical circuits that resonate at a specific external frequency; in our model, similarly, only at a specific value of the DC electric field strength does a long-term interference between two metastable states occur, producing a periodic beating effect.

Future research may be directed towards addressing the following problems:

- Experimental validation of the theoretical model can be considered in the case where the double-well potential is realised by means of heterostructures instead of two Dirac δ . In fact, although in this case the formulas (8)–(11) cannot simply be applied since the kernel of the resolvent operator is not easy to deal with, the resonances can be calculated by applying the outgoing boundary conditions and the numerical calculation of the survival amplitude can be performed, for example, by the spectral splitting method.
- Extension of the model to 2D or 3D devices. We must emphasise that in this case a rather serious technical problem arises, since in dimension greater than one the calculation of Agmon distances ρ_i and ρ_e becomes difficult, and the evaluation of the ratio ρ_i/ρ_e is essential to decide whether the resonance crossing is of type I or II.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflict of interest statement

The author has no competing interests to declare that are relevant to the content of this article.

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