Vibronic “Rabi resonances” in harmonic and hard-wall ion-traps for arbitrary laser intensity and detuning

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We investigate laser-driven vibronic transitions of a single two-level atomic ion in harmonic and hard wall traps. In the Lamb-Dicke regime, for tuned or detuned lasers with respect to the internal frequency of the ion, and weak or strong laser intensities, the vibronic transitions occur at well isolated “Rabi Resonances”, where the detuning-adapted Rabi frequency coincides with the transition frequency between vibrational modes. These vibronic resonances are characterized as avoided crossings of the dressed levels (eigenvalues of the full Hamiltonian). Their peculiarities due to symmetry constraints and trapping potential are also examined.

PACS numbers: 03.75.Be, 32.80.Lg, 32.80.Qk, 42.50.Vk

I. INTRODUCTION

Laser cooled trapped ions have been much studied, both theoretically and experimentally, because of metrological applications as frequency standards, high precision spectroscopy, or the prospects of realizing quantum information processing [1]. The coupling between internal and vibrational degrees of freedom of the ion in harmonic traps due to laser light has in particular been examined as a way to implement the Jaynes-Cummings model or other simple model Hamiltonians for quantum gate design, motional cooling or state preparation [2, 3, 4]. This coupling has been predominantly considered for weak fields, $\Omega_R << \omega_T$, where $\omega_T$ is the trap’s lowest (angular) frequency (for direction $x$, we assume that the two other frequencies in $y$ and $z$ directions are so large that the ion motion is effectively one dimensional), and $\Omega_R$ is the optically “on-resonance” Rabi frequency, i.e., for the zero-detuning case in which the laser frequency $\omega_L$ and the ion transition frequency $\omega_0$ between two internal levels coincide, $\Delta := \omega_L - \omega_0 = 0$ [20]. In the laser adapted interaction picture, after applying the usual (optical) rotating wave approximation and dropping the constant term of the zero point energy, the Hamiltonian reads for a classical laser field,

$$ H = H_{\text{trap}} + H_A + V(\Omega_R), $$

where

$$ H_{\text{trap}} = \hbar \omega_T a^\dagger a, $$

$$ H_A = -\frac{\hbar \Delta}{2} \sigma_z, $$

$$ V = \frac{\hbar \Omega_R}{2} \left[ e^{i\eta(a+a^\dagger)} |e\rangle \langle g| + h.c \right], $$

$\eta := k_L x_0$ is the Lamb-Dicke (LD) parameter, with $x_0$ being the characteristic length of the oscillator $x_0 = \sqrt{\frac{\hbar}{2 \omega_T k_L}}$, and $k_L$ the laser wavenumber; also $\sigma_z = |e\rangle \langle e| - |g\rangle \langle g|$, and $a$ and $a^\dagger$ are the annihilation and creation operators for the vibrational states $\{|n\rangle\}, n = 0, 1, 2, \ldots$. We are assuming that the internal states $\{|g\rangle, |e\rangle\}$ of the ion have an infinite lifetime, thus neglecting spontaneous emission.

At this point it is customary to separate the Hamiltonian as

$$ H = H_B + V(\Omega_R), $$

$$ H_B = H_{\text{trap}} + H_A, $$

to carry out a second interaction picture with respect to $H_B = H(\Omega_R = 0)$, i.e., the free motion of the electronic and vibrational degrees of freedom of the ion or “bare part”. If the rapidly oscillating terms are neglected in a “second” or vibrational rotating wave approximation and, in addition, the Lamb-Dicke regime is assumed, $\eta << 1$, three possible resonance conditions arise between the detuning and the vibrational frequency. They define motional sidebands and state subspaces with simplified, effective Hamiltonians:

- $\Delta = 0$: “carrier” sideband, a purely internal resonance between bare states $|g, n\rangle$ and $|e, n\rangle$, without vibrational excitation.
- $\Delta = -\omega_T$: first red sideband for vibronic transitions between $|g, n+1\rangle$ and $|e, n\rangle$ represented by a Jaynes-Cummings model Hamiltonian.
- $\Delta = \omega_T$: first blue sideband for vibronic transitions between $|g, n\rangle$ and $|e, n+1\rangle$ (anti-Jaynes-Cummings model).

These transitions are the basis of the Cirac-Zoller and related controlled-NOT quantum gates [2, 3, 5]. By choosing larger detunings, one can obtain in principle further vibronic resonances (motional sidebands) with non-linear couplings depending on higher orders of the Lamb-Dicke parameter, but they are not easy to realize in the laboratory since efficient motional cooling is usually performed in the Lamb-Dicke regime [4].

The vibrational rotating wave approximation breaks down for larger $\Omega_R$. This is but a particular example of the failure of the “secular approximations” for a strong perturbation [5]. There are however good reasons for exploring also stronger fields since one of the consequences
of weak fields is that the vibronic transitions involving
one vibrational quantum occur slowly: the effective Rabi frequencies for them scale with \( \eta \Omega_R \). Looking for faster quantum gates, Jonathan, Plenio and Knight\[6\] considered the possibility of using instead stronger fields for the optically resonant case, \( \Delta = 0 \), finding a different vibronic resonance condition, \( \Omega_R = \omega_T \), for transitions involving one motional quantum and laser adapted internal states \( | \pm \rangle = (1/\sqrt{2})(|g \rangle \pm |e \rangle) \). These transitions had been already noticed by Moya-Cessa et al.\[10\] in a study of super-revivals, by means of a unitary transformation leading to the transformed Hamiltonian

\[
H_{MC} = H_{\text{trap}} + \frac{\hbar \Omega_R}{2} \sigma_z + \frac{\hbar}{2} (\sigma_- + \sigma_+) + \frac{i \hbar \eta \omega_T}{2} (a - a^\dagger) (\sigma_- + \sigma_+),
\]

where \( \sigma_- = |g \rangle \langle e | \) and \( \sigma_+ = |e \rangle \langle g | \). Going to an interaction picture with respect to \( H_{\text{trap}} + \frac{\hbar \eta \omega_T}{2} \sigma_z \), and applying again a rotating wave approximation to get rid of rapidly oscillating terms gives the vibronic resonance condition \( | \Omega_R | = \omega_T \) and suppresses any dependence on the detuning, but, mirroring the previously commented failure of the RWA for “large” \( \Omega_R \), this scheme is clearly not valid for sufficiently large detuning \( \Delta \), and requires \( \Delta << \omega_T \). As pointed out in \[11\], in the weak field limit the last term (“spin flip term”) in Eq. (6) does not go to zero so it does not provide a good perturbative scheme. Note also that higher, nonlinear resonances, of the type \( \Omega_R = k \omega_T \), \( k = \pm 2, \pm 3, \ldots \), are not immediately obvious using a second rotating wave approximation although, in principle, could be identified with a more sophisticated treatment\[12\].

Aniello, Porzio, and Solimeno\[11\] could go beyond these two partial approaches, valid for weak fields or weak detunings, and set a more general resonance condition for the principal vibronic resonance, namely for \( \Omega = \omega_T \), where

\[
\Omega = (\Omega_R^2 + \Delta^2)^{1/2} \geq 0
\]

is the detuning-adapted Rabi frequency\[21\]. Their treatment, however, required a somewhat complicated series of transformations and relied on finding a zeroth order Hamiltonian diagonal in the bare basis of the bare Hamiltonian \( H_B = H(\Omega_R = 0) \). We shall present here a simpler treatment in which the initial Hamiltonian\[11\] is separated into the following zeroth order and perturbation terms

\[
H = H_{SD} + W(\eta),
\]

where the “semidressed” Hamiltonian is given by \( H(\eta = 0) \),

\[
H_{SD} = \hbar \omega_T a^\dagger a + \frac{\hbar \Delta}{2} \sigma_z + \frac{\hbar \Omega_R}{2} (|e \rangle \langle g | + |g \rangle \langle e |),
\]

and represents the ion in the trap with a laser field which does not induce any motional coupling, whereas

\[
W(\eta) = \frac{\hbar \Omega_R}{2} \left[ (e^{i\eta (a + a^\dagger)} - 1) |e \rangle \langle g | + h.c. \right]
\]

represents the coupling term. The explicit dependence in the argument of \( W(\eta) \) emphasizes that \( H = H_{SD} \) when \( \eta = 0 \). Notice that the leading term in Eq. (11) depends \( \eta \Omega_R \), whereas \( H_{SD} \) depends parametrically on \( \omega_T, \Delta \) and \( \Omega_R \). This will determine the parameter domains appropriate for a perturbative scheme based on Eq. (3).

All vibronic resonances discussed so far for weak field, or weak detuning will be identified directly from the degeneracies of the “semidressed” eigenenergies of \( H_{SD} \). With the coupling term \( W(\eta) \), they become avoided crossings and their width and energy splitting are well characterized by perturbation theory. In this way, the vibronic resonance condition of Aniello et al. may be obtained and generalized from the crossings of the energy levels of a zeroth order Hamiltonian in the whole range of \( \Omega_R \) and \( \Delta \) values. Since the vibronic resonances correspond to Rabi frequencies equal to the vibrational transition frequencies, the term “Rabi resonance”, which we proposed previously for a related waveguide confinement\[13\], seems appropriate for the general case.

For small Lamb-Dicke parameters (the smallness criterion depends on the particular resonance as we shall see), the resonances are well isolated, which facilitates state manipulation and control. Other factors affecting any possible use of the resonances for information processing or state preparation are the speed of the transition, determined by the effective Rabi frequency at the vibronic resonance, and its width, which will tell us the minimum stability required in the laser detuning and/or intensity. We shall see that both factors as well as the isolation of the resonances can be deduced from the energy splitting, for which we shall provide explicit and resonance-dependent expressions.

The formalism is also easy to apply for a hard-wall trap, and comparisons are made with the harmonic one. The hard-wall trap has been experimentally realized optically\[14\] or in a microelectronic chip version\[15\], and has generated recently much theoretical work in the field of ultracold atoms in low dimensions\[16\].

In the next section we shall first rephrase the weak field case in a time independent framework following\[3\]. This will be a useful reference since the more general case of arbitrary laser intensity in Sec. III can be treated very similarly. In Section IV we compare the results for harmonic and square traps and the paper ends with a discussion and technical appendices.

II. LOW INTENSITY FIELDS; TIME INDEPENDENT APPROACH

In this section we present a time independent approach\[3\] which is essentially equivalent to the usual time-dependent treatment based on a second application of the RWA\[1, 3\]. For \( \Omega_R \ll \omega_T \)[21], it is natural to regard the coupling between the laser and the ion as a small perturbation of the bare system consisting on the trapped ion, and decompose the Hamiltonian\[11\] as in Eq. (4),
The matrix elements of the coupling potential do not cross as the strength of the perturbation.

Note that the degeneracies are removed and the crossings become avoided crossings when the states are dressed ($k^{th}$ motional sidebands).

$$H = H_B + V(\Omega_R)$$

The bare part, $H_B = H(\Omega_R = 0)$, is diagonal in the bare basis \{|g, n\}, \{|e, n\}\} with eigenvalues

$$\epsilon_{g, n} = E_n + \frac{\hbar \Delta}{2}, \quad \epsilon_{e, n} = E_n - \frac{\hbar \Delta}{2},$$

where $E_n = n\hbar \omega_T$ are the energy levels of the oscillator. These bare energy levels cross each other whenever the detuning is on-resonance with the vibrational-level spacing, see Fig. 1 (dashed line),

$$\Delta = k\omega_T,$$

with $k = 0, \pm 1, \pm 2, \ldots$. When the laser is applied, these degeneracies are removed and the crossings become avoided crossings, see Fig. 1 (solid line). This is just a particular case of the “no level crossing theorem”, which states that a pair of energy levels connected by a perturbation do not cross as the strength of the perturbation is varied. The matrix elements of the coupling potential are

$$\langle g, n | V(\Omega_R) | e, n' \rangle = \frac{1}{2} \hbar \Omega_{nn'}^e,$$

$$\langle e, n | V(\Omega_R) | g, n' \rangle = \frac{1}{2} \hbar \Omega_{nn'}^g,$$

(the rest of terms are zero), where the effective Rabi frequency $\Omega_{nn'}$, defined by

$$\Omega_{nn'} := \Omega_R \langle n | e^{i\eta(n-n')} | n' \rangle = \Omega_{nn'},$$

is the coupling strength between the motional levels $n$ and $n'$, calculated in Appendix A. These matrix elements are in general different from zero, so that all the ground and excited levels are connected by the perturbation and therefore do not cross. Moreover, these avoided crossings will be well-localized and isolated, because of the assumption of a low intensity laser. Good approximations to the dressed states at avoided crossings will be obtained by diagonalizing the $2 \times 2$ reduced matrix in the degenerate subspace. If we consider the crossing of the $|g, n\rangle$ and $|e, n'\rangle$ levels at the $\Delta = \pm \omega_T = k\omega_T$ ($k = n' - n$) resonance, the matrix in the degenerate subspace spanned by $|g, n\rangle$ and $|e, n'\rangle$ reads

$$\hat{V}_{\Delta}(|g, n\rangle, |e, n'\rangle) = \hbar \left( \begin{array}{cc} 0 & \Omega_{n'n}^* \tilde{\Omega} \\ \Omega_{nn'}^* \tilde{\Omega} & 0 \end{array} \right).$$

This operator governs the dynamics of the system at the resonance, leading to Rabi Oscillations with a frequency $\Omega_{n'n}$ between bare states $|g, n\rangle \leftrightarrow |e, n'\rangle$. These resonances are nothing but the $k^{th}$ motional sidebands mentioned before.

The eigenvalues of the matrix \(\Omega\) provide the energy splitting in the avoided crossing,

$$\Delta \epsilon_{nn'} = \hbar |\Omega_{nn'}|.$$  

In leading order (see Appendix A), $\Delta \epsilon_{nn'} \propto \Omega_R |n-n'|$. A criterion for resonance isolation is $\Delta \epsilon_{nn'} \ll \hbar \omega_T$, since $\hbar \omega_T$ is the energy difference between consecutive resonances. This leads to the condition $\Omega_R \ll \omega_T$ for the carrier, and $\eta\Omega_R \ll \omega_T$ for the first sidebands, which leaves some room for a relatively high $\eta$ beyond the LD regime.

### III. ARBITRARY INTENSITY FIELDS

If more intense lasers are to be used, e.g. for $\Omega_R \gtrsim \omega_T$, the resonances described before are not isolated and new transitions with different sidebands occur. It is possible however, to find well isolated avoided crossings for higher intensity lasers if we work in the Lamb-Dicke regime where it is more natural to regard the LD parameter $\eta$ as the perturbative parameter, as in Eq. 8, $H = H_{SD} + W(\eta)$, instead of the on-resonance Rabi frequency used in the decomposition 4.

The semi dressed Hamiltonian $H_{SD}$ is easily diagonalized, with eigenvalues and corresponding energy eigenstates

$$\epsilon_{n, \pm} = E_n \pm \frac{\hbar \Omega}{2},$$

$$|\epsilon_{n, \pm}\rangle = \frac{1}{\sqrt{N_{\pm}}} \left( \frac{\Delta \pm \Omega}{\Omega R} |g, n\rangle + |e, n\rangle \right),$$

where the $N_{\pm}$ are dimensionless normalization factors,

$$N_{\pm} = \frac{(\Delta \pm \Omega)^2}{\Omega_R^2} + 1 = \frac{2\Omega}{\Omega_R} (\Omega \pm \Delta).$$
These semidressed energy levels are degenerate at “Rabi Resonances”, where the detuning-adapted Rabi frequency is resonant with some vibrational transition,

$$\Omega = \frac{|E_{n'} - E_n|}{\hbar} = |n' - n|\omega_T, \quad (22)$$

or $$\Omega^2_R + \Delta^2 = (n' - n)^2\omega_T^2$$. This also provides the motional sideband resonances in the low intensity limit ($\Omega_R \ll \omega_T, \Delta$): the semidressed states in Eq. (20) reduce to the bare states and are resonant at $\Delta = (n' - n)|\omega_T$. A peculiarity of the present approach compared to the one in Sec. II is that, since $\Omega$ is defined as a positive number, red and blue sidebands are formally treated in the same manner, see also [11] [28].

At Rabi Resonances, the semidressed states involved in the crossing are coupled. The strength of this coupling is given by

$$\langle \epsilon_{n,s}|W(\eta)|\epsilon_{n',s'} \rangle = \frac{\hbar}{2\sqrt{N_sN_{s'}}} \left[ (\Delta + s'\Omega)\langle n|e^{i\eta(a + a^\dagger)} - 1|n' \rangle + (\Delta + s\Omega)\langle n|e^{-i\eta(a + a^\dagger)} - 1|n' \rangle \right]$$

$$= \frac{\hbar\Delta}{\sqrt{N_sN_{s'}}} [C_{nn'} - \delta_{nn'}] + \frac{s'\hbar\Omega}{\sqrt{N_sN_{s'}}} \left( C_{nn'} - \delta_{nn'} \right) \text{ if } s = s'$$

$$+ \frac{s\hbar\Omega}{\sqrt{N_sN_{s'}}} \left( iS_{nn'} \right) \text{ if } s \neq s'$$

(23)

where $s = \pm 1$ is a shorthand notation to represent the “sign” of each state and

$$C_{nn'} = \langle n| \cos \eta(a + a^\dagger)|n' \rangle, \quad (24)$$

$$S_{nn'} = \langle n| \sin \eta(a + a^\dagger)|n' \rangle. \quad (25)$$

From parity arguments it is clear that, generically, all these coupling elements may be different from zero, connecting all the semidressed states among them. For the $\Delta = 0$ case, however, only states with different vibrational parity will be connected, see Fig. 2, where only alternate crossings are avoided.

The eigenvalues of the $2 \times 2$ reduced matrix in the degenerate subspace,

$$\hat{W}_{n,n'} = \begin{pmatrix} \langle \epsilon_{n,+}|W|\epsilon_{n,+} \rangle & \langle \epsilon_{n,+}|W|\epsilon_{n',-} \rangle \\ \langle \epsilon_{n,-}|W|\epsilon_{n,+} \rangle & \langle \epsilon_{n,-}|W|\epsilon_{n',-} \rangle \end{pmatrix},$$

provide the energy splitting in the avoided crossing,

$$\Delta\epsilon_{nn'} = \frac{\hbar\Omega_R}{\Omega} \leq \frac{\hbar\Omega_R}{\Omega} \times \sqrt{\Omega^2_R (C_{nn'} - C_{nn})^2 + 4(\Delta^2C^2_{nn'} + \Omega^2S^2_{nn'})},$$

(26)

with leading order in $\eta$ (see Appendix A)

$$\Delta\epsilon_{n,n+1} = \frac{\hbar\Omega_R\eta}{\Omega} \left\{ \begin{array}{ll} \frac{1}{\sqrt{2}} & \text{if } l \text{ even} \\ 1 & \text{if } l \text{ odd} \end{array} \right\}. \quad (28)$$

In particular, $\Delta\epsilon_{n,n+1} = \hbar\eta\Omega_R \sqrt{n+1}$. Keep in mind that $\Omega_R$ in these expressions has to satisfy the resonance condition $\Omega_R \ll \omega_T$.

The criterion for isolated resonances is $\Delta\epsilon_{n,n+1} \ll \hbar\omega_T$ whereas the resonance width with respect to $\Omega$ can be estimated from the slopes in Eq. (19) to be given also by the energy splitting.

All vibronic transitions in Sec. II can be described in this manner, in particular we recover the splitting of Eq. (10) for $\Delta >> \Omega_R$ in leading order. At the sideband-motion resonances for $k = \pm 1, \pm 2, \ldots$, $\Delta$ is a multiple of $\omega_T$ so this condition is well satisfied. The energy splitting of the carrier sideband, a purely internal transition, is also recovered in that limit, but it is clear that this resonance does not require $\Delta >> \Omega_R$. In fact in Section II, the expression for the carrier splitting is obtained for $\Delta = 0$ and a small, finite $\Omega_R << \omega_T$. Notice that in this regime $H(\eta = 0)$ already provides the carrier transition splitting, so this regime lies outside the range of our perturbative scheme based on $W(\eta)$ breaking the degeneracy.

For the first vibronic resonance $n = 0, n' = 1$ at $\Delta = 0$ the resonance condition is $|\Omega_R| = \omega_T$ which implies a splitting $\hbar\eta\omega_T$ and an isolation condition $\eta << 1$ equivalent to the LD condition. The isolation condition is therefore more stringent on $\eta$ for these resonances than for the motional weak-field sidebands described in Sec. II.

Another difference is the dependence of the effective Rabi frequency and the isolation condition on $\omega_T$. Let’s recall that, for a given laser wavenumber, $\eta \propto \omega^{-1/2}_T$. Thus $\Omega_R \eta << \omega_T$ is satisfied better and better for in-
increasing $\omega_T$, i.e., for tighter confinement irrespective of the type of resonance: for small $\Omega_R$ as in Sec. II, or for small $\Delta$. However, the splitting, and thus the speed of the transition, decreases with increasing $\omega_T$ in the first case, whereas it increases in the second, because $\Omega_R \approx \omega_T$.

IV. HARD-WALL TRAP

We now consider the confinement of the ion in a hard-wall trap

$$V(x) = \begin{cases} 0 & \text{if } |x| < \frac{a}{2} \\ \infty & \text{if } |x| > \frac{a}{2} \end{cases}. $$

The treatment is essentially the same as for the harmonic trap, replacing $\exp[i\eta(a+a^*)]$ by $\exp(ikLx)$, and the energies and eigenstates of the harmonic oscillator by those of the square potential. Now the motional energies

$$E_n = \frac{\hbar^2}{2m} \left( \frac{n\pi}{a} \right)^2, \quad (29)$$

with $n = 1, 2, \ldots$ are no longer equally spaced. Note that the ground state in this trap is labelled with $n = 1$ in contrast to the ground $n = 0$ state of the harmonic potential. The hard-wall coupling strengths between the different motional levels (playing the role of $\Omega_{nn'}$ in the harmonic wall) are

$$\chi_{nn'} = \Omega_R \langle \phi_n | e^{ikLx} | \phi_{n'} \rangle = \Omega_R \int \frac{\hbar}{2} dx \phi_n(x) \phi_{n'}(x) e^{ikLx},$$

which are explicitly calculated in Appendix [14]

The crossing of the semidressed energy levels define the resonances as in the harmonically trapped ion. In the case of a hard-wall trap, the Rabi Resonance condition is given by [13]

$$\Omega = \frac{|E_n - E_{n'}|}{\hbar} = \frac{\hbar \pi^2}{2ma^2} |n^2 - n'^2|. \quad (31)$$

The energy splitting in a given Rabi Resonance will be given by the same formal expressions as for the harmonic case, replacing $\Omega_{nn'}$ by $\chi_{nn'}$. In leading order in $\eta$, defined now as $k_L a / \pi$,

$$\Delta \epsilon_{n,n+l} = \hbar 4 \Omega_R n(n+l) \left\{ \begin{array}{ll} \eta^2 \xi \frac{\Delta}{\pi} & \text{if } l \text{ even} \\ \frac{2\eta}{\pi} & \text{if } l \text{ odd} \end{array} \right. , \quad (32)$$

which should be compared with Eq. [26]. Different dependencies on the LD parameter $\eta$ are observed. Note that for zeroth, first and second sidebands ($l = 0, 1, 2$), both splittings are of the same order, while for higher order multi-phonon transitions ($l > 2$), transitions in the rigid wall potential become faster if a strong confinement is assumed (LD regime), see Fig. [3]. In fact numerical comparison shows that the carrier transition is also stronger in a hard wall for typical values of the LD parameter, see Fig. [4].

V. DISCUSSION

The perturbative schemes based on different decompositions of the Hamiltonian $H$ in Eq. [1], to treat the effects of a laser on an ion in a harmonic trap, lead naturally to the identification of different families of vibronic resonances, i.e., transitions localized in a relatively small range of some varying parameter (such as the detuning, the laser intensity, a combination of both, or even the Lamb-Dicke parameter [25]) in which the populations of both vibrational and internal levels oscillate. A well known family corresponds to the “motional sidebands” which appear as avoided crossings in the dressed level structure with respect to laser-ion detuning for weakfields. Less studied are the vibronic resonances for zero detuning and varying laser intensity [4, 10, 11]. They may also be identified as avoided crossings with respect to the optically on-resonance Rabi frequency [12].

It is in fact possible to identify and characterize all the above resonances with the same perturbative scheme [11], including moreover generalized resonances with respect to the detuning-adapted Rabi frequency. Our first contribution in this paper has been to simplify the treatment originally proposed by Anniello et al. [11]. Our approach is based on a straightforward decomposition of the Hamiltonian [11] into a zeroth order, “semidressed” term corresponding to $H$ with zero Lamb-Dicke parameter, and a coupling term responsible for vibrational coupling. The resonances are at the degeneracies of a semidressed Hamiltonian (in the $\{\Delta, \Omega_R\}$-plane on concentric circles.
The formalism is very easy to adapt to hard-wall traps so that the results for harmonic and square traps can be compared. This comparison is our second main contribution. The main result is that, to leading order in \( \eta \), the carrier transition, and vibronic resonances implying the interchange of three or more vibrational quanta are more effective (i.e., faster, more strongly coupled) for the hard wall trap. Explicit expressions have been provided and possible applications of this intriguing behaviour are left for future research.

Acknowledgments

We thank J. I. Cirac and M. B. Plenio for useful comments on a preliminary version of this work presented in the XI edition of the workshop “Time in Quantum Mechanics” in La Laguna. This work has been supported by Ministerio de Educación y Ciencia (BFM2003-01003), and UPV-EHU (00039.310-15968/2004).

APPENDIX A: COUPLING STRENGTHS IN THE HARMONIC POTENTIAL

The coupling strength, or effective Rabi frequency, is given by

\[
\Omega_{nn'} = \Omega_{n'n} = \Omega_R \langle n' | e^{i\eta(a + a')} | n \rangle
= \Omega_R \int_{-\infty}^{\infty} dx \varphi_n(x) \varphi_{n'}(x) e^{ikLx},
\]

(A1)

where the \( \varphi_n(x) \) are the normalized eigenfunctions of the harmonic potential. This integral gives

\[
\Omega_{nn'} = \Omega_R \langle n' | e^{-\eta^2/2} (i\eta)^{|n-n'|} \sqrt{n_{<}!} L_n^{n_{<}} | n \rangle^2 (\eta^2).
\]

(A2)

The leading term is given by

\[
\Omega_{nn'} = \Omega_R (i\eta)^{|n-n'|} \sqrt{n_{<}!} n_{<}! |n-n'|!.
\]

(A4)

APPENDIX B: COUPLING STRENGTHS IN THE SQUARE POTENTIAL

For a hard wall trap of width \( a \),

\[
V(x) = \begin{cases} 
0 & \text{if } |x| < \frac{a}{2} \\
\infty & \text{if } |x| > \frac{a}{2}
\end{cases},
\]

the coupling strengths are given by the integral

\[
\chi_{nn'} = \Omega_R \langle \phi_n | e^{ikLx} | \phi_{n'} \rangle = \Omega_R \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \phi_n(x) \phi_{n'}(x) e^{ikLx},
\]

(B1)

where \( \phi_n(x) \) are the normalized eigenfunctions of the infinite well potential,

\[
\phi_n(x) = \langle x | \phi_n \rangle = \begin{cases} 
\sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & \text{if } n \text{ odd} \\
\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & \text{if } n \text{ even}
\end{cases},
\]

satisfying the boundary conditions \( \phi_n(-\frac{a}{2}) = \phi_n(\frac{a}{2}) = 0 \). This integral gives

\[
\chi_{nn'} = -(kLa)\Omega_R i^{n_n-n_{n'}} \frac{sn_{n'}\pi^2}{D} \begin{cases} 
sin \frac{kla}{2} & \text{if } n-n' \text{ even} \\
cos \frac{kla}{2} & \text{if } n-n' \text{ odd}
\end{cases},
\]

where \( D \) is a common denominator given by

\[
D = [(kLa)^2 - (n'-n)^2 \pi^2] [(kLa)^2 - (n'+n)^2 \pi^2]
\]
Note that, as in the harmonic case, these coupling strengths are real when connecting motional levels of the same parity, and purely imaginary otherwise.

We define the LD parameter for this type of potential in analogy with the harmonic case, in which the LD parameter could be written as \( \eta = \frac{\hbar k}{p_h} \) with \( p_h \) being the quasimomentum in \( \hbar \omega_T = \frac{p_h^2}{2m} \). For a hard-wall potential \( \eta \) can be written as \( \eta = \frac{\hbar k}{p_{hw}} \) with \( p_{hw} = \hbar \pi/a \), so that the LD parameter is defined as \( \eta := \frac{k}{L} \alpha/a \). In terms of this LD parameter the coupling strength reads

\[
\chi_{nn'} = -\eta \Omega R^\dagger|n-n'| \left\{ \begin{array}{ll}
\sin \frac{\pi n}{2} & \text{if } n - n' \text{ even} \\
\cos \frac{\pi n}{2} & \text{if } n - n' \text{ odd}
\end{array} \right.
\]

with

\[
\hat{D} = \left[ \eta^2 - (n' - n)^2 \right] \left[ \eta^2 - (n' + n)^2 \right].
\]

In the LD regime, the coupling strength to leading order in \( \eta \) is given by

\[
\chi_{nn'} \approx -\Omega R \frac{4|n| |n'| |n-n'|}{(n-n')^2(n+n')^2} \left\{ \begin{array}{ll}
\eta^2 & \text{if } n - n' \text{ even} \\
2\eta/\pi & \text{if } n - n' \text{ odd}
\end{array} \right.
\]

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[15] The laser frequency, and laser wavenumber are effective ones if a two photon Raman transition is used. \( \Omega_R \) is assumed to be real.
[16] Note that our notation convention and terminology may differ from the quoted papers. For example, our \( \Omega_R \) is twice the corresponding quantity in \([4, 10, 11]\), the detuning is defined quite often with opposite sign, or our Rabi frequency \( \Omega \) is called “corrected detuning” in \([11]\).
[17] The distinction occurs because the states \(|e, n, \pm\rangle \) in Eq. 24 tend to \(|g, n) \) or \(|e, n \rangle \) depending on the sign of \( \Delta \).