Vibrational Bloch-Siegert effect in trapped ions

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When trapped atoms are illuminated by weak lasers, off-resonant transitions cause shifts in the frequencies of the vibrational-sideband resonances. These frequency shifts may be understood in terms of Stark-shifts of the individual levels or, as proposed here, as a vibrational Bloch-Siegert shift, an effect closely related to the usual (radio-frequency or optical) Bloch-Siegert shift and associated with rapidly oscillating terms when the Rotating Wave Approximation is not made. Explicit analytic expressions are derived and compared to numerical results, and the similarities and differences between the usual and the vibrational Bloch-Siegert shifts are also spelled out.

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I. INTRODUCTION

A. Bloch-Siegert shift

The Rotating Wave Approximation (RWA) is applied to describe atoms interacting with near-resonant fields. It consists on neglecting the rapidly oscillating counter-rotating terms in a Hamiltonian. In 1940 Bloch and Siegert, studying magnetic resonances, showed that if the RWA is not applied, the counter rotating, fast oscillating terms give rise to a shift in the resonance frequency of the magnetic dipoles, i.e., the Bloch-Siegert shift [1, 2, 3].

Similar shifts exist in principle in the optical domain, although much smaller and difficult to detect.

In the treatment of laser driven trapped ions, apart from an optical RWA for the driven optical transition, a second or “vibrational RWA” is usually applied [4]. Within this approximation, the absorption spectrum of a harmonically trapped (two-level) ion consists of a carrier band centered at the transition frequency \( \omega_0 \) and sidebands separated from the carrier by multiples of the trap frequency \( \omega_T \). If this second RWA is not applied and vibrational counter-rotating terms are taken into account, the energy levels are distorted and thus the position of the sideband resonances are shifted, an effect that we shall call a “vibrational Bloch-Siegert shift”. Its analysis is the objective of the present paper in which we shall provide explicit expressions within a perturbative approach based on the resolvent method. The peculiarities of the Hamiltonian for the trapped ion lead to differences between the ordinary (in magnetic or optical resonances) and vibrational BS effects that we shall also discuss.

These sideband frequency shifts are important for optimizing the operation of quantum gates based on laser-driven trapped ions and can be observed and compensated experimentally [5, 6]. In this context they have been understood as the result of Stark-shifts of the individual levels due to off-resonant transitions. The connection between our compact treatment of the frequency shift (as a vibrational Bloch-Siegert effect) and the Stark-shifts will also be spelled out. Thanks to the systematic treatment with the resolvent method we find general expressions for the frequency shifts of arbitrary sidebands and correction terms that had been previously overlooked.

B. Vibrational Rotating Wave Approximation

We consider a two-level ion with (internal) ground and excited states \(|g\rangle\) and \(|e\rangle\), and transition frequency \( \omega_0 \) among them, moving in an effective one-dimensional harmonic potential of frequency \( \omega_T \) in \( x \)-direction (motion in \( y \) and \( z \) directions is unexcited and ignored throughout); this ion is illuminated by a (classical) laser beam with traveling wave of wavevector in \( x \)-direction and wavenumber \( k_L \). The system is described in the dipole approximation by

\[
H(t) = H_T + H_A + \hbar \Omega_R (\sigma_+ + \sigma_-) \cos(\omega_L t - k_L x),
\]

with

\[
H_T = \hbar \omega_T a^\dagger a,
\]

\[
H_A = \frac{\hbar \omega_0}{2} \sigma_z.
\]

where \( \sigma_z = |e\rangle\langle e| - |g\rangle\langle g|, \sigma_+ = |e\rangle\langle g|, \) and \( \sigma_- = |g\rangle\langle e|; \) \( \Omega_R \) is the on-resonance Rabi frequency, which plays the role of an atom-field coupling constant, and \( a^\dagger \) (\( a \)) are the creation (annihilation) operators of the harmonic potential.

In an interaction picture defined by \( H_T + H_A \) and neglecting the fast oscillating terms within the usual (opti-
cal) RWA, the Hamiltonian becomes

$$H_{TA}(t) = \frac{\hbar \Omega R}{2} \left( e^{i \eta [a(t) + a^\dagger(t)]} e^{-i \Delta t} \sigma_+ + H.c. \right),$$

(4)

where $H.c.$ means “Hermitian conjugate”, $a(t) = a e^{-i \omega_L t}$, $a^\dagger(t) = a^\dagger e^{i \omega_L t}$, and $\Delta = \omega_L - \omega_0$ is the detuning between the laser frequency and the internal atomic transition frequency. The parameter $\eta = k_L x_0$ is known as the Lamb-Dicke (LD) parameter, where $x_0 = \sqrt{\hbar/2m \omega T}$ is the extension (square root of the variance) of the ion’s ground state, i.e., $x_0 = x_0(a + a^\dagger)$. The LD parameter is a measure of the trap width on the scale of the laser wavelength. Let us denote by $|g, n \rangle$ (i.e., $|e, n \rangle$) the state of the ion in the ground (excited) internal state and in the $n$-th motional level of the harmonic oscillator. Using the so-called BCH identity $[8]$, 

$$e^{i \eta [a(t) + a^\dagger(t)]} \equiv e^{- \frac{\eta^2}{2}} e^{i \eta a^\dagger(t)} e^{i \eta a(t)},$$

(5)

and expanding the exponentials in power series of $\eta$, we end up with a Hamiltonian with terms containing a combination of $\sigma_\pm$, with $n$ $a^\dagger$-operators and $n'$ $a$-operators rotating with a frequency $(n - n') \omega_T$ $[4]$, 

$$H_{TA}(t) = \frac{\hbar \Omega R}{2} \left[ e^{- \frac{\eta^2}{2}} \sum_{n,n'} (i \eta)^{n+n'} a^\dagger a e^{i (n-n') \omega_T} e^{-i \Delta t} \sigma_+ \right] + H.c.$$

(6)

which in principle couples all the different vibrational levels via $a^\dagger$ and $a$ operators. The combinations satisfying the $\Delta \approx k \omega_T$ ($k = n - n'$) condition will be resonant, coupling the states $|g, n \rangle \leftrightarrow |e, n+k \rangle$, while the rest of rapidly oscillating terms are usually neglected in a second approximation of the RWA, a vibrational RWA (VRWA) $[4]$. Within this approximation, only co-rotating states $|g, n \rangle \leftrightarrow |e, n+k \rangle$ are coupled and the system becomes two-dimensional at each of these resonances. They are classified as: (i) $\Delta \sim 0$: Carrier resonance. The system is described by a Hamiltonian which is equivalent to a two level atom in a resonant field, coupling the states $|g, n \rangle \leftrightarrow |e, n \rangle$; (ii) $\Delta \sim -k \omega_T$: $k \hbar$ red sideband. The system is described by a $k$-photon Jaynes-Cummings type Hamiltonian, which couples $|g, n \rangle \leftrightarrow |e, n-k \rangle$; (iii) $\Delta \sim k \omega_T$: $k \hbar$ blue sideband. The system is described by a $k$-photon anti-Jaynes-Cummings type Hamiltonian, coupling the states $|g, n \rangle \leftrightarrow |e, n+k \rangle$.

The differences and similarities of both approximations (RWA and VRWA) are discussed in detail in Section III.B.

II. VIBRATIONAL BLOCH-SIEGERT SHIFT

If the VRWA is not applied and vibrational counter-rotating terms in the Hamiltonian $[3]$ are taken into account, a shift in the apparent position of each sideband resonance is observed, an effect that may be compared to the standard Bloch-Siegert shift in magnetic or optical resonances. This shift is more easily visualized and calculated if one writes the original Hamiltonian $[3]$ in a frame rotating with the field frequency, i.e., in a field-adapted interaction picture defined by the zeroth order Hamiltonian $\frac{\hbar}{2} \omega_L \sigma_z$. In this frame, and after applying the usual (optical) RWA, the Hamiltonian becomes time-independent,

$$H_{LA} = \hbar \omega_T a^\dagger a + \frac{\hbar \Delta}{2} \sigma_z + \frac{\hbar \Omega R}{2} \left[ e^{i \eta (a + a^\dagger)} \sigma_+ + H.c. \right].$$

(7)

The energy levels of this Hamiltonian are plotted in Fig. 1 as a function of the detuning. The bare ($\Omega_R = 0$) levels are given by straight lines

$$E^{(B)}_{g,n} = n \hbar \omega_T + \frac{\hbar \Delta}{2},$$

(8)

$$E^{(B)}_{e,n} = n \hbar \omega_T - \frac{\hbar \Delta}{2},$$

(9)

which are degenerate at each of the resonances mentioned before (dashed lines in Fig. 1), but the degeneracies are removed and become avoided crossings when the laser is turned on (solid lines in Fig. 1). These anti-crossings are nothing but the different sidebands mentioned in the previous section and lead to transitions between the different bare states. In this time independent approach, the VRWA corresponds to restricting the theory to a subspace spanned only by the two states involved in a given anti-crossing neglecting the rest of states, provided that the energy splitting of the avoided-crossing is well isolated $[8]$.
The bare states (eigenstates of $H_B$) of the system satisfy

$$H_B |\alpha, n\rangle = E^{(B)}_{\alpha,n}|\alpha, n\rangle,$$

where the index $\alpha = g, e$ accounts for the internal atomic state and the bare energy levels $E^{(B)}_{\alpha,n}$ are given in Eq. 8.

Let us now consider the $|g, n_g\rangle \leftrightarrow |e, n_e\rangle$ sideband transition, which corresponds to the crossing between the bare levels $E^{(B)}_{g,n_g}$ and $E^{(B)}_{e,n_e}$ at the point

$$E_0 = \frac{\hbar \omega_T}{2} (n_g + n_e),$$

$$\Delta_0 = (n_e - n_g) \omega_T$$

of the $(E, \Delta)$ plane, see Fig. 1. If these levels are close to each other but far from other levels, the time evolution of the system in the subspace spanned by the states $|g, n_g\rangle$ and $|e, n_e\rangle$ may be approximately described by an approximate Hamiltonian $\hat{H}$

$$\hat{H} = \begin{pmatrix}
E^{(B)}_{g,n_g} + R_{gg}(E_0) & R_{ge}(E_0) \\
R_{eg}(E_0) & E^{(B)}_{e,n_e} + R_{ee}(E_0)
\end{pmatrix},$$

where $R_{\alpha\beta}(E_0) = \langle \alpha, n_\alpha | R(E_0) | \beta, n_\beta \rangle$ are the matrix elements of the level shift operator defined by

$$R(E_0) = P V P + \sum_{n=1}^\infty PV \left( \frac{Q}{E_0 - H_B} V \right)^n P,$$

with $P = |g, n_g\rangle \langle g, n_g| + |e, n_e\rangle \langle e, n_e|$ and $Q = 1 - P$. Even though it is 2-dimensional, the approximate Hamiltonian $\hat{H}$ contains information about all the non-resonant states via the operator $Q$, the projector onto the counter-rotating subspace. The eigenvalues of $\hat{H}$ will then give, for weak fields, the correct energy levels, including non-resonant effects. It can be easily shown that the maximum (or minimum) of these perturbed energy levels are shifted from their non-perturbed position $\Delta_0$ by

$$\delta \omega = \left[ R_{ee}(E_0) - R_{gg}(E_0) \right]/\hbar,$$

which is the vibrational Bloch-Siegert shift of the position of the resonances due to the effect of counter-rotating (vibrational) terms, see Fig. 2.

Moreover, if the states are coupled by $R_{ge}$, their corresponding levels form an avoided crossing with an energy splitting given by

$$\delta \epsilon = |R_{ge}(E_0)| = \frac{\hbar |\Omega_{n_e,n_g}|}{2},$$

1 The resonant method is capable of providing the exact levels substituting $E_0$ by the unknown eigenvalue $E$ in the approximate Hamiltonian. Finding $E$ requires iterative procedures, see e.g. 10. The simplest, explicit, rather than implicit, approximate treatment followed here provides the correction to the energy in leading order in the perturbation.

2 Solve $dE_{\alpha,n_\alpha}/d\Delta = 0$, where $E_{\alpha,n_\alpha}$ are the eigenvalues of $\hat{H}$.
where \( \Omega_{n,n'} = \Omega_R(n|e^{i\eta(a + a^\dagger)}|n'|) \) are the coupling strengths between the different vibrational levels of the trap [11 12], see the explicit expressions in Appendix A. As we have already pointed out, the approximate Hamiltonian [13] will only be valid if the anti-crossing is well isolated. A criterion for resonance isolation is \( \delta \epsilon \ll \omega_T \), since \( \omega_T \) is the energy difference between consecutive resonances. As low intensity lasers (\( \Omega_R \ll \omega_T \)) are being assumed, this criterion will be readily fulfilled and all the crossings will be well isolated.

In order to give an explicit expression of \( \delta \omega \) we need the matrix elements \( R_{gg} \) and \( R_{ee} \) of the level shift operator. To lowest order in the perturbation, they are given by (see Appendix A for the explicit calculation)

\[
R_{gg}(E_0) = \langle g, n_g | R | g, n_g \rangle = \sum_{k=0}^{\infty} \frac{|\Omega_{n_e,k}|^2}{E_0 - E_{g,k}^B},
\]

\[
R_{ee}(E_0) = \langle e, n_e | R | e, n_e \rangle = \sum_{k=0}^{\infty} \frac{|\Omega_{n_e,k}|^2}{E_0 - E_{e,k}^B}, \tag{19}
\]

Then, using the expressions of the bare energies (8) and the crossing point of these bare levels (13) one has from (17) that the position of the \( |g, n_g \rangle \leftrightarrow |e, n_e \rangle \) resonance is given by \( \Delta = \Delta_0 + \delta \omega \), where

\[
\delta \omega = \frac{1}{4\omega_T} \left( \sum_{k=0}^{\infty} \frac{|\Omega_{n_e,k}|^2}{n_g - k} - \sum_{k=0}^{\infty} \frac{|\Omega_{n_e,k}|^2}{n_e - k} \right), \tag{20}
\]

which is in principle valid for all values of \( \eta \) provided low intensity fields are assumed. We have verified the validity of this expression by comparing with the frequency shifts that result from diagonalizing the time independent Hamiltonian [7] with a large basis of bare states (\( n \gg 1 \)) and numerically finding the maximum or minimum of a given energy level, see Fig. 3 (solid lines).

Note that Eq. (20) can also be understood as the sum of the Stark shifts for the excited state minus the Stark shifts for the ground state due to all non-resonant transitions, which provides a connection with previous treatments [3 11].

### B. LD regime: \( \eta \ll 1 \)

A particularly interesting and common regime is the so-called LD regime, in which the recoil frequency of the ion is much smaller than the trapping frequency, i.e., \( \eta \ll 1 \). Up to quadratic terms in \( \eta \), only the same or consecutive vibrational levels are coupled, reducing the infinite sum in (20) to one where only “off-resonant carrier terms” \( k = n_e \) in \( R_{ee} \) and \( k = n_g \) in \( R_{gg} \) or coupling between adjacent vibrational levels is considered. Thus, we find that, see Fig. 3 (dashed lines)

\[
\delta \omega = \frac{\Omega_R^2}{2(n_g - n_e)\omega_T} \left[ 1 - \eta^2(n_g + n_e + 1) \right] + \frac{\eta^2\Omega_R^2}{4\omega_T} \sum_{k=\pm 1}^{n_g + n_e + 1} \frac{n_g + n_e + 1}{n_g - n_e + k} + O(\eta^4), \tag{21}
\]

which is valid for \( n_g \neq n_e \), since it follows directly from (20) that the position of the central (carrier, \( n_g = n_e \)) resonances are not shifted to any order in \( \eta \): the shifts from both sides (positive and negative) detunings are compensated and canceled. (Contrast this with [13], where a different type of shift of the carrier was studied, defined by the excitation peak position rather than by the level structure).

The first line in Eq. (21) is nothing but the (off-resonant) carrier contribution to the vibrational Bloch-Siegert shift, while the second line is the contribution of the adjacent sideband transitions. It is remarkable that in the LD-regime the main contribution to any sideband frequency shift is always given by the coupling to off-resonant carrier transitions, no matter how far the sideband is from the carrier.

Note that in the strict LD (\( \eta = 0 \)) limit, the states \( |g, n_g \rangle \) and \( |e, n_e \rangle \) are not connected by the perturbation \( V \), and \( R_{ge} \) will be zero to all orders. The energy lev-
The vibrational Bloch-Siegert shift. Compared to previous results in [3, 13], our formulation is more general and applies to arbitrary sidebands. In [3], Steane et al. describe the shift on the first red sideband as the result of the light shifts of the levels because of off-resonant transitions. Aniello et al. [13], after a series of unitary transformations of the Hamiltonian end up with a resonance condition which gives a shift also for the first red sideband. In both cases the calculated shift is given by

$$\delta \omega = \frac{\Omega_R^2}{2 \omega_T} + \frac{\eta^2 \Omega_R^2}{4 \omega_T}.$$  

(22)

\((n_g = 1, n_e = 0),\) which differs from our result in (21) by the \(\eta^2\) correction from off-resonant carrier transitions. This correction is indeed easy to miss (in particular, it is overlooked if \(\langle n | e^{i \eta (a + a^\dagger)} | n \rangle\) is approximated by keeping only terms up to linear order in \(\eta\)), but it becomes quite significant at moderate values of \(\eta\), as shown by the numerical comparison of the exact result (from diagonalization of the Hamiltonian with a large basis), and the shifts given by Eqs. (21) and (22) in Fig. 3(b).

B. RWA vs. vibrational RWA

In order to highlight the differences between the usual RWA and the VRWA (and thus the differences between the usual Bloch-Siegert shift and its vibrational version), we shall now compare our trapped ion system with the interaction of a two-level atom and a quantized field mode of frequency \(\omega\). These two systems are in many ways similar if the ion is assumed to be trapped within the LD regime [20, 21]. Since the RWA has to do with co-rotating and counter-rotating terms in a time dependent Hamiltonian, the different nature of both RWA’s is more clearly understood if the Hamiltonians describing both systems are written in an interaction picture where the free evolution of the amplitudes is removed, i.e.,

$$H_F(t) = \frac{\hbar \Omega_R}{2} \left[ \left( a e^{-i \omega_T t} + a^\dagger e^{i \omega_T t} \right) e^{i \omega_T t} \sigma_+ + H.c. \right],$$

$$H_{T.A.LD}(t) = \frac{\hbar \Omega_R}{2} \left[ \left( 1 + i \eta q e^{-i \omega_T t} + i \eta a e^{i \omega_T t} \right) e^{-i \Delta t} \sigma_+ + H.c. \right],$$  

(23)

where the subscript \(F\) refers to the atom-quantized field case, and \(T,A,LD\) to the trapping case, see Eq. (6), in the Lamb-Dicke regime. The creation and annihilation operators have different meaning depending on the system: they increase or decrease the number of photons of a given Fock state in the first case or they add or remove

III. DISCUSSION

A. Comparison with previous works

We have shown that the effect of the vibrational counter-rotating terms is to shift the position of the sidebands, an effect that may be related to the ordinary Bloch-Siegert shift. Compared to previous results in [3, 13], our formulation is more general and applies to arbitrary sidebands. In [3], Steane et al. describe the shift on the first red sideband as the result of the light shifts of the levels because of off-resonant transitions. Aniello et al. [13], after a series of unitary transformations of the Hamiltonian end up with a resonance condition which gives a shift also for the first red sideband. In both cases the calculated shift is given by

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$$H_{T.A.LD}(t) = \frac{\hbar \Omega_R}{2} \left[ \left( 1 + i \eta q e^{-i \omega_T t} + i \eta a e^{i \omega_T t} \right) e^{-i \Delta t} \sigma_+ + H.c. \right],$$  

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where the subscript \(F\) refers to the atom-quantized field case, and \(T.A,LD\) to the trapping case, see Eq. (6), in the Lamb-Dicke regime. The creation and annihilation operators have different meaning depending on the system: they increase or decrease the number of photons of a given Fock state in the first case or they add or remove
a vibrational quantum in the trapped ion case. Despite these conceptual differences, both systems look formally very similar.

If near resonant processes are considered ($\omega \sim \omega_0$) in $H_P$, counter-rotating terms like $\sigma_+ a$ and $\sigma_- a^\dagger$ can be neglected since they oscillate with a frequency $\sim \omega$, much faster than the co-rotating terms, whose frequency of oscillation is $\delta = \omega - \omega_0$. Counter-rotating terms can never be resonant since both the mode frequency $\omega$ and the transition frequency $\omega_0$ are positive quantities. The main effect of keeping these counter-rotating terms is a shift on the apparent resonant frequency of the atom $\omega_0$, i.e., the ordinary Bloch-Siegert shift [10].

In the trapped ion case, the role of $\omega_0$ is played by the frequency difference or detuning $\Delta = \omega_L - \omega_0$, which may happen to be positive (blued detuned) or negative (red detuned). Terms like $\sigma_+ a$ will be resonant if the laser is tuned to the first red sideband. This is similar to the atom-field coupling case, since after all the interaction is described by a Jaynes-Cummings type Hamiltonian. However terms like $\sigma_- a^\dagger$, which would be counter rotating in the atom-field coupling case, are resonant in the trapped ion system when the laser is tuned to the first blue sideband and the system is approximately described by an anti Jaynes-Cummings Hamiltonian.

Another important difference between these systems is that for the atom in the quantized-field, transitions where only the internal state of the atom changes (with no photon absorption or emission) do not happen, while in the trapped ion case these carrier-type transitions give no photon absorption or emission (do not happen), while the apparent resonant frequency of the atom $\omega_0$, i.e., the ordinary Bloch-Siegert shift.

APPENDIX A: CALCULATION OF MATRIX ELEMENTS OF THE LEVEL SHIFT OPERATOR

In this Appendix the matrix elements of the levels shift operator are explicitly calculated to leading order in the perturbation $V$, see Eq. (11). We will consider the crossing between the $|g, n_g\rangle$ and $|e, n_e\rangle$ bare states, with $P = |g, n_g\rangle\langle g, n_g| + |e, n_e\rangle\langle e, n_e|$ and $Q = 1 - P$. The first order term $\langle g, n_g|V|g, n_g\rangle$ vanishes, since the perturbation does not connect states with the same internal atomic state. The next order will be given by

$$
R_{gg}(E_0) = \langle g, n_g|V|E_0 - H_B\rangle\langle g, n_g|
$$

where

$$
\chi_{nn'} = \langle n|e^{i\eta(\sigma_+ a + a^\dagger)}|n'\rangle = e^{-\eta^2/2} \sqrt{n_n! n_{n'}!} L_n^{n'}(\eta^2),
$$

$L_n^{n'}$ the generalized Laguerre functions,

$$
L_n(X) = \sum_{k=0}^{n} (-1)^k \frac{(n + a)!}{(n - k)!} X^k.
$$

In an analogous way, $R_{ee}$ is obtained:

$$
R_{ee}(E_0) = \sum_{k \neq n_e} \frac{|\Omega_{n_e,k}|^2}{E_0 - E_{g,k}^{(B)}}.
$$

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where

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R_{gg}(E_0) = \langle g, n_g|V|E_0 - H_B\rangle\langle g, n_g|
$$

where

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\chi_{nn'} = \langle n|e^{i\eta(\sigma_+ a + a^\dagger)}|n'\rangle = e^{-\eta^2/2} \sqrt{n_n! n_{n'}!} L_n^{n'}(\eta^2),
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R_{ee}(E_0) = \sum_{k \neq n_e} \frac{|\Omega_{n_e,k}|^2}{E_0 - E_{g,k}^{(B)}}.
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