Thermometry via light shifts in optical lattices: Supplemental material

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ANHARMONICITY FOR CARRIERS

To address the effects of anharmonicity, we consider the model potential

$$U(\mathbf{r}) \approx -U_0\, e^{-2\,(y^2+z^2)/w_0^2}\, \cos^2(2\pi x/\lambda) \tag{19}$$

for a 1D optical lattice, which is a good approximation near the trap center. This potential introduces three leading-order anharmonic corrections to (3), which are the quartic potentials

$$V_{xx}(\mathbf{r}) = -\left(M\omega_x^2\, x^2/2\right)^2/(3U_0) \tag{20}$$
$$V_{xr}(\mathbf{r}) = -\left(M\omega_x^2\, x^2/2\right)\left(M\omega_r^2\, r^2/2\right)/U_0 \tag{21}$$
$$V_{rr}(\mathbf{r}) = -\left(M\omega_r^2\, r^2/2\right)^2/(2U_0) \tag{22}$$

for the initial and likewise for the final lattice, where $r^2 \equiv y^2 + z^2$. Far from the axial trap center, a finite Rayleigh length introduces additional (e.g., cubic) leading-order corrections.

For a transition between a pair of known trap states in the initial and final lattices we may approximate the light shift of each $V_{ij}(\mathbf{r})$ by its first-order perturbation,

$$\delta E_{ij} \approx \langle n'_x n'_y n'_z|V'_{ij}|n'_x n'_y n'_z\rangle - \langle n_x n_y n_z|V_{ij}|n_x n_y n_z\rangle, \tag{23}$$

where primes denote final-lattice values. These shifts introduce the corrections

$$W_{ij} = \langle \delta E_{ij}\rangle \tag{24}$$

to the total light shift W of (7), where the brackets denote a thermal average over the allowed pairs of initial and final trap states. For axial sideband (SB) transitions, the effects of n_x-dependent excitation rates must be included in this average, as described in the next section. In the Lamb-Dicke (LD) and resolved-sideband regimes with suppressed transverse SB transitions, the trap state pairs satisfy

$$n'_x = n_x + D,\ n'_y = n_y,\ \text{and}\ n'_z = n_z, \tag{25}$$

where the integer D is introduced to distinguish between axial carrier ($D = 0$) and first-order axial SB transitions ($D = \pm 1$).

Surprisingly, carrier transitions are nearly unchanged by the leading-order corrections (20–22), because the first-order light shifts (23,24) are zero:

$$\delta E_{ij} = W_{ij} = 0 \quad \text{if} \quad D = 0. \tag{26}$$

Before evaluating these quantities explicitly in the next section, we can explain this general result as follows. First, note that any form for $U(\mathbf{r})$ must be proportional to the polarizability α. Thus, any anharmonic corrections to (3), such as (20–22), must also be proportional to α. Next, note that the expectations $\langle n_x|x^2|n_x\rangle \propto 1/\sqrt{\alpha}$ and $\langle n_x|x^4|n_x\rangle \propto 1/\alpha$ for harmonic oscillator states. The matrix elements in (23) for the V_{ij} of (20-22) are therefore independent of α' and α, respectively, and must be equal, thus producing no differential shift. This general insensitivity of the carrier light shift to quartic anharmonicities also applies to the model potentials $-U_0\, e^{-2\,(z/w_0)^2}\, \cos^2(2\pi x/\lambda)\cos^2(2\pi y/\lambda)$ and $-U_0 \cos^2(2\pi x/\lambda)\cos^2(2\pi y/\lambda)\cos^2(2\pi z/\lambda)$ for 2D and 3D optical lattices.

AXIAL SIDEBAND TRANSITIONS

For axial SB transitions with $D \neq 0$, the total light shift W of (7) due to the harmonic potential (3) must be modified as follows. First, there is an "axial-SB shift" from the final lattice,

$$W_s = \hbar\omega'_x\, D, \tag{27}$$

which must be added as a fourth part to W. Next, if $D < 0$, the populations of the initial lattice with $n_x < |D|$ will not participate in the transition, so the expectation $\langle n_x + 1/2\rangle$ must be computed accordingly. This asymmetry also leads to the relation (2) between temperature and the ratio of SB areas.

Additionally, for SB transitions the excitation rates depend on n_x. The expectation $\langle n_x + 1/2\rangle$ is no longer solely thermal, but must account for this inhomogeneous excitation by weighting each value of n_x with the square of its Rabi frequency for the transition,

$$\Omega(n_x, D)^2 \propto |\langle n'_x|e^{ikx}|n_x\rangle|^2 \approx \begin{cases} 1 & D = 0 \\ \eta^2\, n_x & D = -1 \\ \eta^2\,(n_x + 1) & D = +1, \end{cases} \tag{28}$$

where the LD parameter $\eta = k\sqrt{\hbar/(2M\omega_x)}$ and the axial wavenumber $k = 2\pi/\lambda$. As before, we assume the trap states are approximately orthonormal, $\langle n'_x|n_x\rangle \approx \delta_{n'_x,n_x}$, which may need to be modified if α'/α is far from unity. After normalizing the probabilities for each n_x, the weighted expectations are

$$\langle n_x + \frac{1}{2} \rangle = \begin{cases} \coth\left[\Delta_x/2\right]/2 & D = 0 \\ \coth\left[\Delta_x/2\right] + 1/2 & D = -1 \\ \coth\left[\Delta_x/2\right] - 1/2 & D = +1 \end{cases} \quad (29)$$

where as before $\Delta_x = \hbar\omega_x/(k_B T)$.

Hence, although the form of $W_x = \langle \delta E_x \rangle$ given by (10),

$$W_x = \left(\sqrt{\alpha'/\alpha} - 1\right) \hbar\omega_x \langle n_x + 1/2 \rangle, \quad (30)$$

will be unchanged for SBs, the value of W_x will depend on D following (29). Note that the form and value of $W_r = \langle \delta E_r \rangle$ given by (11),

$$W_r = \left(\sqrt{\alpha'/\alpha} - 1\right) \hbar\omega_r \langle n_r + 1 \rangle, \quad (31)$$

is the same for SBs as for carriers.

The anharmonic corrections (20–22) are important for SBs, unlike carriers, especially for state-insensitive 'magic' traps with $\alpha'/\alpha = 1$. The contributions (24) to the shift W from these corrections are

$$W_{xx} = -\frac{W_s}{4U_0}\left(\sqrt{\frac{\alpha}{\alpha'}}\,\hbar\omega_x \langle n_x + 1/2 \rangle + \frac{W_s\,\alpha}{2\,\alpha'}\right) \quad (32)$$

$$W_{xr} = -\frac{W_s}{4U_0}\sqrt{\frac{\alpha}{\alpha'}}\,\hbar\omega_r \langle n_r + 1 \rangle \quad (33)$$

$$W_{rr} = 0 \quad (34)$$

for both carrier and SB transitions, as derived below. Importantly, note that all these contributions are zero for carriers as argued above, since $W_s = 0$ if $D = 0$.

The expression (32) for W_{xx} follows from the expectation $\langle n_x | (M\omega_x^2 x^2/2)^2 | n_x \rangle = 3(\hbar\omega_x)^2(2n_x^2 + 2n_x + 1)/16$ [1], which gives the matrix elements

$$\langle n_x n_y n_z | V_{xx} | n_x n_y n_z \rangle = -\frac{(\hbar\omega_x)^2}{16U_0}(2n_x^2 + 2n_x + 1), \quad (35)$$

and from noting that $(\omega_x')^2/U_0' = \omega_x^2/U_0$ and $2(n_x')^2 + 2(n_x') + 1 = 2n_x^2 + 2n_x + 1 + 4D(n_x + 1/2) + 2D^2$. The expression for W_{xr} follows from expectations of the form $\langle n_x | (M\omega_x^2 x^2/2) | n_x \rangle = \hbar\omega_x(n_x + 1/2)/2$, which give the matrix elements

$$\langle n_x n_y n_z | V_{xr} | n_x n_y n_z \rangle = -\frac{\hbar\omega_x \hbar\omega_r}{4U_0}(n_x + 1/2)(n_r + 1), \quad (36)$$

and from noting that $\omega_x'\omega_r'/U_0' = \omega_x\omega_r/U_0$. The shift W_{rr} of (34) is then zero because the condition (25) includes only radial carrier transitions. That is, V_{rr} of (22) contributes no shift for the same reasons that $W_{xx} = W_{xr} = 0$ if $D = 0$.

To demonstrate the effects of anharmonicity on the lineshape of SB transitions, let us treat the case of a magic lattice with $\alpha'/\alpha = 1$ where there is no thermal broadening of the carrier. In this case, broadening comes only from the thermal distribution of the anharmonic shifts δE_{xx} and δE_{xr}. Using (36) with (23), we find

$$\delta E_{xr}(n_r) = -D(n_r + 1)\,\hbar\omega_r\,\hbar\omega_x/(4U_0). \quad (37)$$

Similarly, using (35) with (23) and (27),

$$\begin{aligned} \delta E_{xx}(n_x) &= -\left[2D(n_x + 1/2)(\hbar\omega_x)^2 + W_s^2\right]/(8U_0) \\ &\approx -D(n_x + 1/2)(\hbar\omega_x)^2/(4U_0), \end{aligned} \quad (38)$$

where the second line follows from neglecting a constant offset (half the lattice-photon recoil energy) that contributes no broadening. Note that (32,33) are related to (38,37) via (24) with $\alpha'/\alpha = 1$.

Together, the shifts (37,38) lead to similar lineshapes as derived for carrier transitions. As before, we introduce a function to replace Boltzmann exponents,

$$v(\delta E) = -\delta E/[k_B T\,\hbar\omega_x\,D/(4U_0)] \geq 0. \quad (39)$$

The discrete step size of $v(\delta E_{xx})$ is $\Delta_x = \hbar\omega_x/(k_B T)$ and of $v(\delta E_{xr})$ is $\Delta_r = \hbar\omega_r/(k_B T)$. Since the probability distribution for n_r is unchanged, the probability for the discrete variable δE_{xr} follows from the p_r of (14),

$$p_{xr}(\delta E_{xr}) = \frac{1}{Z_r^2 \Delta_r}\, v(\delta E_{xr})\, e^{-v(\delta E_{xr})}. \quad (40)$$

Likewise, for $D \geq 0$ the probability p_x of (12) for n_x is unchanged. However, we now need to account for inhomogeneous excitation, so the probability for the discrete variable δE_{xx} is

$$p_{xx}(n_x) \propto \Omega(n_x, D)^2\, p_x(n_x). \quad (41)$$

For $D = 1$, using (28) and normalizing, this evaluates to

$$p_{xx}(\delta E_{xx}) = \frac{v(\delta E_{xx}) + \Delta_x/2}{Z_x \Delta_x (1 + e^{-\Delta_x/2} Z_x)}\, e^{-v(\delta E_{xx})}. \quad (42)$$

Likewise, for $D = -1$ where only $n_x \geq 1$ participate,

$$p_{xx}(\delta E_{xx}) = \frac{v(\delta E_{xx}) - \Delta_x/2}{Z_x^2 \Delta_x}\, e^{-v(\delta E_{xx}) + \Delta_x/2}. \quad (43)$$

In the continuum limit, these probabilities simplify to

$$\overline{p}_{xi}[v(\delta E_{xi})] = \lim_{\Delta_i \to 0} \frac{p_{xi}(\delta E_{xi})}{\Delta_i} = v\, e^{-v} \quad (44)$$

for both $i = x, r$ and $D = \pm 1$.

Following (15), the distribution for the total shift $\delta E(n_x, n_r) = \delta E_{xx}(n_x) + \delta E_{xr}(n_r)$ is the convolution

$$p(\delta E) = \sum_{\{n_x, n_r\}_{\delta E}} p_{xx}(n_x) p_{xr}(n_r), \quad (45)$$

over the pairs of n_x and n_r satisfying $\delta E(n_x, n_r) = \delta E$. In the continuum limit this reduces to a Gamma distribution similar to (17),

$$\overline{p}[v(\delta E)] = \lim_{\Delta_x, \Delta_r \to 0} \frac{p(\delta E)}{\Delta_x \Delta_r} = \frac{1}{6} v^3 e^{-v}, \qquad (46)$$

for both $D = \pm 1$ SBs. As expected and demonstrated in Fig. 2(a), the sharp edge of this lineshape is furthest from the carrier. To extract axial trap frequencies ω_x from spectra like Fig. 2(a), we fit the natural logarithm of the data (to account for linear probe absorption) with the lineshape (46) to determine the spacing between the $v = 0$ points of the red and blue SBs.

The dimensionless FWHM of (46) is approximately 4.131. Using this with (39) gives the relation

$$\Gamma_{\mathrm{SB}} \approx 1.033 f_x |D| k_B T / U_0 \qquad (47)$$

between the FWHM Γ_{SB} (in temporal frequency units) of the lineshape (46) and the temperature T. Equation (18) then follows from this together with Eq. (4), $|D| = 1$, and rewriting $T = T_{\mathrm{SB}}$. Note that for non-magic lattices, the competition of harmonic and anharmonic shifts will lead to both broadening and narrowing effects for SB transitions.

[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-relativistic Theory), 3rd edition* (Butterworth-Heinemann, Oxford, 1976).