Lattice-depth measurement using continuous grating atom diffraction

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We propose a new approach to characterizing the depths of optical lattices, in which an atomic gas is given a finite initial momentum, which leads to high amplitude oscillations in the zeroth diffraction order which are robust to finite-temperature effects. We present a simplified model yielding an analytic formula describing such oscillations for a gas assumed to be at zero temperature. This model is extended to include atoms with initial momenta detuned from our chosen initial value, before analyzing the full finite-temperature response of the system. Finally we present a steady-state solution to the finite-temperature system, which in principle makes possible the measurement of both the lattice depth, and initial temperature of the atomic gas simultaneously.

I. INTRODUCTION

There is much interest in the precise measurement of optical lattice [1] depths in the field of atomic physics, particularly for accurate determination of transition matrix elements [2–6], better knowledge of these matrix elements can be used to improve the black body radiation correction for ultraprecise atomic clocks [7, 8], and allows quantitative modeling of atom-light interaction [9]. Other areas of interest include atom interferometry [10, 11] and many body quantum physics [12, 13], where knowledge of the lattice depth is essential for interpreting experimental results.

Commonly used lattice depth measurement schemes include Kapitza–Dirac scattering [13–17], parametric heating [18], Rabi oscillations [19], and, more recently, the sudden phase shift method [20]. For the case of a weak lattice (V≤0.01ER for any atom, where V is the lattice depth and ER is the atomic recoil energy), methods based on multipulse atom diffraction have been explored [21, 22], with a view to reducing signal-to-noise considerations in the measurement of the resultant diffraction patterns. In previous work we have presented improved models for the expected multipulse diffraction patterns for a given lattice depth. We have also noted that when considering a gas with initial momentum hK/2, the functional form of these models is markedly simpler and therefore easier to fit to data to make an accurate measurement of the lattice depth [23].

In this paper we explore such a measurement scheme for a lattice which is not pulsed but instead continuously present throughout the experimental sequence, which we show to be more robust to finite-temperature effects than a multipulse approach. In Sec. II, we describe our model system and experimental considerations. In Sec. III, we introduce a simplified analytic approach for determining the time evolution of the atomic population in the zeroth diffraction order, and make a comparison to exact numerical calculations. Finally, in Sec. IV, we present an approximate analytic model for the finite-temperature response of the system, and discuss how these may be used to determine both the lattice depth and initial temperature of the atomic gas.

II. MODEL SYSTEM: ATOMIC GAS IN AN OPTICAL GRATING

A. Experimental setup and Hamiltonian

We consider a two-level atom in an assumed noninteracting Bose-Einstein condensate exposed to a far off resonance optical grating, the Hamiltonian of which is given by Eq. (1):

\[ H_{\text{Latt}} = \frac{\tilde{p}^2}{2M} - V \cos \left( K \left( \hat{x} + \nu_G t \right) \right), \]  

where \( \tilde{p} \) is the momentum operator along the lattice axis, \( V \) is the lattice depth, \( K \) is twice the laser wavenumber \( k_L \), \( M \) is the atomic mass and \( \nu_G \) is the phase velocity of the grating in the x direction (\( \nu_G = 0 \) for a static grating). For the simpler case of a static grating, we consider a BEC initially prepared in a momentum state with \( p = hK/2 \). As shown in Fig. 1(a), the BEC is diffracted by the static optical grating for a time \( t \), before a time of flight measurement interrogates the population of the gas in each of the allowed momentum states. In principle there is an infinite ladder of such states, each separated by integer multiples of \( hK \), though here we show only the zeroth and first diffraction orders. We note that an initial state \( p = hK/2 \) can be achieved for instance by Bragg diffraction, or equivalently we may prepare the BEC in a state with \( p = 0 \) and impart an appropriately tuned time-dependent phase \( \nu_G t \) to the standing wave as in Fig. 1(b). We show this equivalency in Sec. II B below.

B. Gauge transformations and momentum kicks

The Hamiltonian of Eq. (1) can be transformed to a frame comoving with the walking grating by use of the unitary trans-
The spatial periodicity of Eq. (3) allows us to invoke Bloch theory [26], by rewriting the momentum operator in the following basis:
\[
\hat{\beta}(\hbar K)^{-1} p = k + \beta, \quad (4a)
\]
\[
\hat{k}(\hbar K)^{-1} p = k + \beta = k(\hbar K)^{-1} p = k + \beta, \quad (4b)
\]
\[
\hat{\beta}(\hbar K)^{-1} p = k + \beta = \beta(\hbar K)^{-1} p = k + \beta. \quad (4c)
\]
We may speak of \( k \in \mathbb{Z} \) as the discrete part of the momentum, and \( \beta \in [-1/2, 1/2) \) as the continuous part or quasimomentum [27]. Here \( \beta \) is a conserved quantity, as such, only momentum states separated by integer multiples of \( \hbar K \) are coupled [24, 25]. This simplification allows us to construct the time evolution operator for a lattice pulse of duration \( t \) from the lattice Hamiltonian (3) as follows:
\[
\hat{U}(\beta, \tau)_{\text{Latt}} = \exp \left( -i \left[ \frac{\hbar^2 k^2}{2} - \frac{2\hbar \beta \cos(\hat{\theta})}{2} - V_{\text{eff}} \cos(\hat{\theta}) \right] \tau \right), \quad (5)
\]
in which \( \beta \) is simply a scalar value such that overall phases which depend solely on \( \beta \) can be neglected. Here \( V_{\text{eff}} = VM/\hbar^2 k^2 \) is the dimensionless lattice depth, \( \hat{\theta} = K\hat{x} \) and \( \tau = t\hbar K^2/M \) is the rescaled time.

By using Eq. (5) to calculate \( |\psi(\tau)\rangle = \sum_j c_j(\tau) |j\rangle \), the population in each discrete momentum state \( |k\rangle \) following an evolution for a rescaled time of \( \tau \) is given by the absolute square of the coefficients \( P_j(\tau) = |c_j(\tau)|^2 \). In this paper we employ the well-known split-step Fourier approach [25, 28] to determine \( |\psi(\tau)\rangle \), as well as an analytic approach based on a simpler two-state model.

The dynamics of a single atom in the BEC standing-wave system can be understood in terms of the scattering process given by the semiclassical energy diagram of Fig. 1(c) (see also [29–33]). A two-level atom begins in a state with momentum \( p = hK/2 \), before absorbing a photon with momentum \( p = -hK/2 \), and subsequently emits a second photon with the momentum \( p = hK/2 \). This is the only scattering process which classically conserves energy, whilst also conserving the quasimomentum. We therefore expect that scattering into states with momentum \( p > |hK/2| \) ought to be strongly suppressed even under the fully quantum time evolution. We explore this simplified picture in Sec. III.

### III. REDUCTION TO AN EFFECTIVE 2-STATE SYSTEM

#### A. Simplification

We may test the conjecture that population transfer into states with \( k < -1 \) or \( k > 0 \) is strongly suppressed by computing the full time evolution of the system numerically, the results of such calculations on an exhaustive basis of momentum states are displayed in Fig. 2. Over the 13 basis states displayed, we can clearly see that, though population transfer into higher order modes does occur, the oscillation of population between the \( k = -1 \) and \( k = 0 \) states is the dominant
process in the system. We therefore expect that a representa-
tion of the system in a truncated momentum basis composed
of only these two states ought to capture the essential dynam-
ics, and explore this simplified two-state model below.

B. Two-state model analytics

We may represent the Hamiltonian (3) in the \( \beta = 1/2 \) sub-
space using the following two-state momentum basis:

\[
|k = 0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (6a)
\]

\[
|k = -1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (6b)
\]

yielding:

\[
H_{\text{Latt}}^{2 \times 2} = \begin{pmatrix} 1/4 & -V_{\text{eff}}/2 \\ -V_{\text{eff}}/2 & 1/4 \end{pmatrix}, \quad (7)
\]

We recognize Eq. (7) as a Rabi matrix with zero detuning, the
eigenvectors and eigenvalues of which are well known [34],
and can be used to straightforwardly determine the time evolu-
tion of the population in the \( |k = 0\rangle \) and \( |k = -1\rangle \) states, respectively:

\[
P_0 = \cos^2(V_{\text{eff}} \tau/2), \quad (8a)
\]

\[
P_{-1} = \sin^2(V_{\text{eff}} \tau/2), \quad (8b)
\]

as outlined in Appendix A. This analytic result is compared to
our exact numerics in Figs. 2 and 3, both of which show excel-
 lent agreement for a wide range of experimentally relevant
values of the effective lattice depth \( V_{\text{eff}} \). We note in particular
that the form of Eqs. (8a) and (8b) is such that there is an ex-
ant universality between \( \tau \) and \( V_{\text{eff}} \), which is elucidated in Fig.
3(b), where all population curves fall on top of each other.

IV. FINITE-TEMPERATURE RESPONSE

A. Other values of \( \beta \)

In the following section we consider the effect of evolving
initial states with quasimomentum different to \( \beta = 1/2 \) in or-
der to gain insight into the dynamics of a finite-temperature
gas. Numerically, this is achieved by computing the evolution
of an initial state \( |k + \beta\rangle \) under the time evolution operator (5).
We make the assumption from the outset that the initial mo-
mentum distribution of the gas (centred at \( \beta = 1/2 \)) spans less
than half of each of the \( k = 0 \) and \( k = -1 \) Brillouin zones for
a static grating (or falls within the \( k = 0 \) Brillouin zone with a
momentum distribution centered on \( \beta = 0 \) for a walking grating).
Our results in this low temperature regime are displayed in
Fig. 4, which indicates a \( k = 0 \) Brillouin zone with high
amplitude but low-frequency oscillations in the population of
the zeroth diffraction order centered around \( |\beta| = 1/2, \) and
low amplitude but rapidly oscillating solutions as \( \beta \) is detuned
from this value. We may also use our simplified semiclassical
model of Sec. III to derive an approximate analytic result for
the same calculation, in which the quasimomentum \( \beta \) is en-
coded as a detuning to be included in our initial Rabi model
of Eq. (7). These additions yield the following \( 2 \times 2 \) Hamiltoni-
nian matrix:

\[
H_{\text{Latt}}^{2 \times 2}(\beta) = \begin{pmatrix} \beta^2/2 & -V_{\text{eff}}/2 \\ -V_{\text{eff}}/2 & (1 - 2\beta + \beta^2)/2 \end{pmatrix}, \quad (9)
\]

in which \( \beta \) is now a free parameter. The time evolution of
the zeroth diffraction order population governed by this matrix
can be found using the approach given in Appendix B, thus:

\[
P_0(\beta) = 1 - \frac{V_{\text{eff}}^2}{(\beta - 1/2)^2 + V_{\text{eff}}^2} \sin^2\left(\sqrt{(\beta - 1/2)^2 + V_{\text{eff}}^2} \tau\right), \quad (10)
\]

which is similar to the result reported in [15] for a zero tem-
perature gas, and agrees excellently with the exact numerics
for physically relevant parameters as shown in Fig. 4. We
therefore expect that thermal averaging of this result should
produce an accurate description of the full finite-temperature
response.

B. Finite temperature analysis

To find the finite temperature response of the system we
weight the contribution of Eq. (10) for each individual quasi-
momentum subspace according to the Maxwell-Boltzmann
distribution:

\[
D_{k=0}(\beta, w) = \frac{1}{w \sqrt{2\pi}} \exp\left(-\frac{(\beta - 1/2)^2}{2w^2}\right), \quad (11)
\]

where the dimensionful temperature is given by \( T_w = h^2 K^2 w^2/Mk_B \) [35]. Mathematically this corresponds to the integ-
ral:

\[
P_0(w) = \int_0^\infty D_{k=0}(\beta, w) P_0(\beta) \, d\beta. \quad (12)
\]

Inserting Eqs. (11) and (10), we have:

\[
P_0(\rho) = \frac{1}{\sqrt{2\pi} \rho} \int_{-1}^1 \exp\left(-\gamma^2\right) \left[ 1 - \frac{1}{\gamma^2 + 1} \sin^2\left(\frac{\sqrt{\gamma^2 + 1}}{2} \phi\right) \right] \, d\gamma, \quad (13)
\]

where we have introduced \( \gamma = (\beta - 1/2)/V_{\text{eff}} \), \( \phi = V_{\text{eff}} \tau \) and
\( \rho = w/V_{\text{eff}} \) for simplicity. The exponential and trigonometric
terms can be power expanded, and the integral (13) solved
term by term, giving:

\[
P_0(\rho) = 1 - \sum_{s=0}^{\infty} \sum_{q=0}^{s} u_s(\phi) M_{s,q} v_q(\rho), \quad (14)
\]

where \( u_s(\phi) = (-\phi^2)^s s!(2s + 1)! \), \( M_{s,q} = -(2q)!/[2(q!)^2](s-q)! \) and \( v_q(\rho) = (\rho^2/2)^q \) (see Appendix
Though the full sum over $q$ diverge, meaning that a preferred truncation of the sum is not obvious.

However, given the well-behaved nature of the integrand, Eq. (13) can be straightforwardly integrated numerically, for instance using the trapezium rule. We compare this numerical integration to our full finite-temperature numerics in Fig. 5, which shows excellent agreement across a large range of initial momentum widths in the weak lattice regime [Figs. 5 (a), (b)], and for $V_{\text{eff}} = 0.1$ in the strong lattice regime [Fig. 5 (d)]. However, for $V_{\text{eff}} = 0.5$ [Fig. 5 (c)] the agreement is relatively poor, as in this regime the semiclassically motivated two-state model is no longer valid. We therefore expect that numerically fitting Eq. (13) to experimental data, with $\phi = V_{\text{eff}} \tau$ and $\rho = w/V_{\text{eff}}$ as free parameters, would give an accurate value of the effective lattice depth, if the time $\tau$ is known to high precision and the lattice depth is sufficiently small.

Further, we note that using standard integral results, we may also extract the steady state solution to Eq. (13) as $\phi \to \infty$:

$$P_{0,\phi \to \infty}(\rho) = \frac{1}{2\rho} \sqrt{\frac{\pi}{2}} \exp\left(\frac{1}{2\rho^2}\right) \text{Erfc}\left(\frac{1}{\sqrt{2\rho}}\right),$$

Where $q = 0$, Eq. (15) reduces to the zero temperature result of Eq. (8a), as such we should expect the finite temperature behavior of the system to be captured in terms with $q > 0$. Though the full sum over $q$ is always convergent, the presence of the $(\phi/2)^{2(q+1)}$ term guarantees that all individual terms with $q \geq 1$ diverge, meaning that a preferred truncation of the sum is not obvious.

With $q = 0$, Eq. (14) can in principle be solved numerically by recursively populating the elements of a sufficiently large pair of $u(\phi), v(\rho)$ vectors and M matrix, though the elements of the vectors will grow with $s$ and $q$ respectively unless $\phi$ and $\rho$ are sufficiently small, and this condition is only satisfied for certain experimentally relevant regimes. Nonetheless, Eq. (14) yields some insight when expressed as a sum over derivatives of sinc functions (see Appendix D):

$$P_0(\rho) = 1 - \sum_{q=0}^{\infty} \left(\frac{\rho}{2}\right)^{2q} \frac{2q!}{q!^2} \left(\frac{\phi}{2}\right)^{2(q+1)} \left(\frac{2}{\phi} \frac{d}{d(\phi/2)} \left[\frac{\sin^2(\phi/2)}{(\phi/2)^2}\right]\right).$$

(15)

FIG. 2. (Color online) Time evolved momentum distributions for an atomic gas initially prepared in the $|k = 0, \beta = 1/2\rangle$ momentum state (corresponding to the $|k = 0, \beta = 0\rangle$ state in the lab frame for a walking grating), as calculated numerically on a basis of 2048 momentum states. The top row of false color plots [(a), (c), (e)] shows the population in the first 13 momentum states, to be read on the logarithmic colorbar to the right, a cutoff population of $P_{\text{cutoff}} = 10^{-11}$ has been applied to accommodate the log scale. The labels $P_{\text{static}}$ and $P_{\text{walking}}$ denote the momentum as measured in the lab frame for the case of a static and a walking grating respectively. The bottom row of plots [(b), (d), (f)] shows the time evolution of the population in the $|k = 0\rangle$ (red circles) and $|k = -1\rangle$ (blue squares) states, where the solid line through each curve is given by the analytic solution of Eqs. (8a) and (8b). Also shown is the population in the $|k = 1\rangle$ state (green points). Each column of plots corresponds to a simulation for a fixed value of the effective lattice depth $V_{\text{eff}}$, here, from left to right $V_{\text{eff}} = 0.07, 0.10, 0.13$ respectively.
which depends only on $\rho = w/V_{\text{eff}}$. Here, ‘Eríć’ is the complementary error function \[36\].\footnote{When evaluating Eq. (16) for physically relevant values of $\rho = w/V_{\text{eff}}$, the exponential term becomes large as the error function takes a correspondingly such that $p_{0\beta\rightarrow0}(\rho)$ remains bounded between 0 and 1. This complication can present a problem for numerical evaluation using standard numerical routines. In practice, we numerically implement Eq. (16) exclusively in terms of rational numbers in Mathematica, before requesting a numerical evaluation to a specified precision.} In essence, by measuring the steady state population experimentally, and numerically fitting Eq. (16), $\rho = w/V_{\text{eff}}$ can be straightforwardly determined and substituted into Eq. (13), leaving a fit in only one parameter $\phi = V_{\text{eff}}\tau$. The steady state population can be found either by allowing the atomic gas to evolve in the lattice for a sufficient time, or taking the average value of $p_0$ in time for an appropriate number of oscillations. In fact, this improved fitting approach not only allows $\phi = V_{\text{eff}}\tau$, and therefore the effective lattice depth $V_{\text{eff}}$ to be determined more accurately, but also allows the initial effective temperature to be determined from $w = \rho V_{\text{eff}}$.

V. CONCLUSIONS

We have presented a simplified model system yielding an analytic zero-temperature formula for the evolution of the zeroth diffraction order population, and demonstrated the validity of this approach across a wide range of lattice depths. We have extended this model to incorporate finite-temperature effects and discussed from where they arrive mathematically. We have shown that there is excellent agreement between this analytic model and exact numerical calculations if the lattice depth is sufficiently small, and shown that a steady state so-
The same level of precision, however, there is no need for any stationary BEC; it is unlikely that this can be achieved with simulation measurements. With regard to potential experimental implementations, we note that the phase velocity of a walking optical lattice can be calibrated extremely precisely, however, does require optical elements to be in place which will reduce the intensity of the laser beam and therefore the lattice. The alternative is to impart a specified momentum to an initially stationary BEC; it is unlikely that this can be achieved with the same level of precision, however there is no need for any additional optical elements affecting the lattice depth.

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**Appendix A: Derivation of the two-state model**

To calculate the time-evolution of the population in the zeroth diffraction order, we construct the time evolution operator in the momentum basis from the Hamiltonian of Eq. (7), reproduced here for convenience:

$$H_{\text{att}}^{2\times2} = \begin{pmatrix} 1/4 & -V_{\text{eff}}/2 \\ -V_{\text{eff}}/2 & 1/4 \end{pmatrix}. \tag{A1}$$

The diagonal terms simply represent an energy shift that can be transformed away, thus the eigenvalues of Eq. (7) can simply be read from the off-diagonal: $$E_{\pm} = \pm V_{\text{eff}}/2$$. We may now solve the eigenvalue equation:

$$\begin{pmatrix} 0 & -V_{\text{eff}}/2 \\ -V_{\text{eff}}/2 & 0 \end{pmatrix} \begin{pmatrix} v^+ \v_0^- \\ v_0^+ \end{pmatrix} = \pm V_{\text{eff}}/2 \begin{pmatrix} v_0^+ \\ v^+ \end{pmatrix}. \tag{A2}$$

Equation (A2) leads directly to $$v_0^+ = \pm v^+$$, yielding eigenvectors:

$$|E_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |E_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{A3}$$
We may now construct our initial condition in the energy basis, in which the matrix representation of the time evolution operator
\[ \hat{U}(\tau) = \exp(-i\hat{H}_{\text{Latt}}\tau) \]
is diagonal:
\[ |\psi(\tau = 0)\rangle = |k = 0\rangle = \frac{1}{\sqrt{2}} (|E_+\rangle + |E_-\rangle). \]  
(A5)

The time evolution of the population in the zeroth diffraction order is given by:

\[ P_0 = \left| \langle E_+ | + \langle E_- | \hat{U}(\tau) (|E_+\rangle + |E_-\rangle) \right|^2, \]
\[ = \frac{1}{4} \left| e^{-iE_+ \tau} + e^{-iE_- \tau} \right|^2, \]
\[ = \frac{1}{2} \cosh^2(V_{\text{eff}} \tau / 2), \]  
(A6)

which corresponds to Eq. (8a).

**Appendix B: Derivation of \( \beta \) dependent two-state model**

To calculate the time-evolved population for a given quasi-momentum subspace, we follow the same procedure as in Appendix A. Equation (9), reproduced here for convenience
\[ H_{\text{Latt}}^{2\times2}(\beta) = \begin{pmatrix} 0 & V_{\text{eff}}/2 \\ -V_{\text{eff}}/2 & -2\beta + \beta^2/2 \end{pmatrix}, \]
is nothing other than a Rabi matrix, the eigenvalues of which are
\[ E_\pm = \left(1/2 - \beta + \beta^2\right) \pm \sqrt{\beta - 1/2)^2 + V_{\text{eff}}^2/2}, \]
and the corresponding eigenvectors:
\[ |E_+\rangle = \begin{pmatrix} \cos(\alpha/2) \\ \sin(\alpha/2) \end{pmatrix} \]
\[ = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \cos(\alpha)} & 0 \\ 1 - \sqrt{1 + \cos(\alpha)} & 0 \end{pmatrix} |k = 0\rangle, \]
\[ |E_-\rangle = \begin{pmatrix} -\sin(\alpha/2) \\ \cos(\alpha/2) \end{pmatrix} \]
\[ = -\frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 - \cos(\alpha)} & 0 \\ 1 + \sqrt{1 - \cos(\alpha)} & 0 \end{pmatrix} |k = 0\rangle, \]  
(B1)

where \( \cos(\alpha) = (\beta - 1/2) / \sqrt{(\beta - 1/2)^2 + V_{\text{eff}}^2} \). This leads directly to:
\[ |\psi(\tau = 0)\rangle = |k = 0\rangle = \cos(\alpha/2)|E_+\rangle - \sin(\alpha/2)|E_-\rangle \]
\[ = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \cos(\alpha)} & \sqrt{1 - \cos(\alpha)} \end{pmatrix} |E_+\rangle - \sqrt{1 - \cos(\alpha)}|E_-\rangle. \]

We may now simply calculate the time-evolved state from the action of the time evolution operator
\[ \hat{U}(\tau, \beta) = \exp(-i\hat{H}(\beta)_{\text{Latt}}\tau), \]
on this initial state thus:
\[ |\psi(\tau, \beta)\rangle = \exp(-i\hat{H}(\beta)_{\text{Latt}}\tau)|k = 0\rangle \]
\[ = \frac{1}{\sqrt{2}} \left( \sqrt{1 + c \cos(\alpha/2)}|E_+\rangle + \sqrt{1 - c \cos(\alpha/2)}|E_-\rangle \right). \]

Here we have introduced \( c \equiv \cos(\alpha) \). The time-evolved population in the zeroth diffraction order for a given \( \beta \) subspace is then given by:
\[ P_0(\tau, \beta) = \langle k = 0 | \psi(\tau, \beta) \rangle^2 \]
\[ = \frac{1}{4} \left( 1 + c \right) \cos^2(\alpha/2) + \frac{1}{4} \left( 1 - c \right) \sin^2(\alpha/2) \]
\[ = 1 - \frac{V_{\text{eff}}^2}{(\beta - 1)^2} + \frac{V_{\text{eff}}^2}{2} \sin^2 \left( \sqrt{(\beta - 1)^2 + V_{\text{eff}}^2} \right), \]
(C2)

which corresponds to Eq. (10).

**Appendix C: Derivation of finite-temperature matrix equation**

To derive the matrix equation for the finite-temperature response of the zeroth diffraction order population, we begin from Eq. (12), into which we insert Eqs. (11) and (10), yielding:
\[ P_0(w) = 1 - \frac{1}{\sqrt{2\pi w}} \int_{-\infty}^{\infty} \frac{V_{\text{eff}}}{\alpha^2 + V_{\text{eff}}^2} \exp \left( -\alpha^2 \right) \sin^2 \left( \sqrt{\alpha^2 + V_{\text{eff}}^2} \right), \]
\[ = 1 - P_{-1}(w) \]
(C1)

where we have introduced \( \alpha = (\beta - 1) / 2 \). For simplicity, we now refer to \( P_{-1}(w) \), the population in the \( |k = -1\rangle \) state. The sinusoidal term can be rewritten using \( \sin^2(\theta) = [1 - \cos(2\theta)]/2 \), thus:
\[ P_{-1}(w) = \frac{V_{\text{eff}}}{\sqrt{2\pi w}} \int_0^{\infty} \frac{1}{\alpha^2 + V_{\text{eff}}^2} \exp \left( -\alpha^2 \right) \sin^2 \left( \sqrt{\alpha^2 + V_{\text{eff}}^2} \right) \]
\[ = \frac{V_{\text{eff}}}{\sqrt{2\pi w}} \sum_{s=0}^{\infty} (-1)^s \frac{2s+1}{(2s+1)!} \int_0^{\infty} \frac{1}{2} \exp \left( -\alpha^2 \right) \left( \alpha^2 + V_{\text{eff}}^2 \right)^s, \]
(C3)
such that the square root in the argument no longer appears, and the \((\alpha^2 + V^2_{\text{eff}})^{s}\) term can be binomially expanded thus:

\[ P_{-1}(w) = \frac{V^2_{\text{eff}}}{\sqrt{2\pi}w} \sum_{s=0}^{\infty} \left( -1 \right)^s \frac{r^{2(s+1)}s!}{(2s + 1)!} \sum_{q=0}^{s} \frac{V^{2(s-q)}}{q!(s-q)!} \int_0^{\infty} \alpha^2q \exp \left( -\frac{\alpha^2q}{2w^2} \right) \, dq. \]

(C4)

Further, introducing \( \xi \equiv \alpha^2/(2w^2) \), the remaining integral can be rewritten as:

\[ \int_0^{\infty} \alpha^2q \exp \left( -\frac{\alpha^2q}{2w^2} \right) = w^{2q+1}e^{-\xi/2} \int_0^{\infty} d\xi \exp(-\xi)\xi^{q-1/2}, \]

\[ = w^{2q+1}e^{-\xi/2}\Gamma(q + 1/2), \]

which, when substituted into Eq. (C4) leads to:

\[ P_{-1}(w) = \frac{1}{2 \sqrt{\pi}} \sum_{s=0}^{\infty} \left( -1 \right)^s \frac{(V_{\text{eff}}r)^{2(s+1)}s!}{(2s + 1)!} \sum_{q=0}^{s} \frac{1}{q!(s-q)!} \left( \frac{2w^2}{V^2_{\text{eff}}} \right)^q \Gamma(q + 1/2). \]

(C5)

Finally, noting that \( \Gamma(s + 1/2) = (2s)! \sqrt{\pi}/(2^s s!) \), Eq. (C5) can be rewritten, thus:

\[ P_{-1}(w) = \sum_{q=0}^{\infty} \sum_{s=q}^{\infty} \left( -V^2_{\text{eff}}r^2 \right)^{s+1} s! \left( -\frac{1}{2} \right) (2q)! \frac{1}{(2s+1)!}(q!)^q \left( \frac{2w^2}{V^2_{\text{eff}}} \right)^q \Gamma(q + 1/2), \]

\[ = u_{s}(V_{\text{eff}}r)M_{s,q}v_q(w/V_{\text{eff}}), \]

(C6)

or, equivalently, with \( \phi = V_{\text{eff}}r \) and \( \rho = w/V_{\text{eff}} \):

\[ P_0(\rho) = 1 - P_{-1}(\rho) = 1 - \sum_{q=0}^{s} \sum_{s=q}^{\infty} u_{s}(\phi)M_{s,q}v_q(\rho), \]

which corresponds to Eq. (14).

**Appendix D: Expression of Eq. (14) in terms of Sinc functions**

Equation (C6) can be rewritten as:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \sum_{s=q}^{\infty} \frac{s!}{(2s+1)!}(s-q)!(-\phi^2)^{s+1} \]

where we have used \( \phi = V_{\text{eff}}r \) and \( \rho = w/V_{\text{eff}} \). We now introduce \( \tau = \phi^2 \) and re-index the sum in \( s \), yielding:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \sum_{s=q+1}^{\infty} \frac{(s-1)!}{(2s)!}(s-1-q)!(-1)^s \tau \]

which corresponds to Eq. (15).

Expanding the factorial terms in \( s \) and rearranging in \( \tau \) in the following way:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \sum_{s=1}^{\infty} \frac{(s-1)(s-2)...(s-q)}{(2s)!}(-1)^s \tau^{-q-1} \]

which we recognize can be expressed as a derivative in \( q \), thus:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \frac{d^q}{d\tau^q} \sum_{s=1}^{\infty} \frac{(-1)^s \tau^{-s-1}}{(2s)!} \]

(D1)

Equation (D1) can be rewritten:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \left[ \frac{d^q}{d\tau^q} \left( \frac{1}{\tau} \left[ \frac{\sin^2(\sqrt{\tau}/2)}{\tau} \right] \right) \right] \]

such that the sum in \( s \) can now be recognized as a sinusoidal term, yielding:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \left[ \frac{d^q}{d\tau^q} \left( \frac{1}{\tau} \left[ \frac{\sin^2(\sqrt{\tau}/2)}{\tau} \right] \right) \right] \]

Reintroducing \( \phi \) leads to:

\[ P_{-1}(\rho) = \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{-1}{2} \right) \left[ \frac{d^q}{d\phi^q} \left( \frac{\sin^2(\phi/2)}{\phi^2} \right) \right] \]

\[ = \frac{1}{2} \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{\phi^2}{2} \right)^{q+1} \left[ \frac{1}{\phi} \frac{d}{d\phi} \left( \frac{\sin^2(\phi/2)}{\phi^2} \right) \right], \]

\[ = \frac{1}{2} \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{\phi^2}{2} \right)^{q+1} \left[ \frac{1}{\phi} \frac{d}{d\phi} \left( \frac{\sin^2(\phi/2)}{\phi^2} \right) \right] \]

\[ \times \left( \frac{\phi^2}{2} \right)^{q+1} \left[ \frac{1}{\phi} \frac{d}{d\phi} \left( \frac{\sin^2(\phi/2)}{\phi^2} \right) \right] \]

Equivalently,

\[ P_0(\rho) = 1 - P_1(\rho) \]

\[ = 1 - \sum_{q=0}^{\infty} \left( \frac{\rho^2}{2} \right)^q \frac{(2q)!}{q!^2} \left( \frac{\phi^2}{2} \right)^{q+1} \left[ \frac{1}{\phi} \frac{d}{d\phi} \left( \frac{\sin^2(\phi/2)}{(\phi/2)^2} \right) \right], \]

which corresponds to Eq. (15).
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