Non-Adiabatic Contributions to Bragg Regime Dynamics in the Atomic Kapitza-Dirac Effect

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The primary mechanism of the atomic Kapitza-Dirac effect is a multi-photon process in which the electronic state is virtually excited while the direct product state is altered as the velocity of the atom undergoes spatial quantization. The Bragg resonance is a virtual multi-photon stimulated Raman scattering in which counterpropagating photons act as pump and probe imparting transverse velocity to the atom through recoil while the energy in the field is lowered such that the energy of the system is conserved. The bulk of the literature for the past three decades has presumed that the energy-nonconserving intermediate states which are described by non-adiabatic contributions could be neglected once the perturbative effects of next-order off-resonant states were included. This paper demonstrates the necessity of including higher-order non-adiabatic contributions of energy-nonconserving momentum states in calculating the final populations of Bragg resonances as a function of field strength. As the field strength is increased, the Pendellö sung frequency varies while generally decreasing dramatically, requiring a greater number of intermediate states to calculate. This paper demonstrates that \( n \propto \sqrt{\beta/\delta} \) states must be included to precisely calculate the populations of diffracted atoms as a function of field strength in better agreement with experiment.

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I. INTRODUCTION

The Kapitza-Dirac effect (KDE), first suggested by P.L. Kapitza and P.A.M. Dirac in 1933 at a meeting of the Cambridge Physical Society [1], demonstrates the analog between matter and light in the form of matter-wave diffraction through a light crystal. The reciprocity of electrons and photons in quantum electrodynamics suggests that one could observe Bragg diffraction of matter from a periodic light source analogous to X-ray diffraction from crystalline solids in the regular Laue geometry. Kapitza and Dirac imagined an electron beam diffracting from a strong, periodic light source which would mimic a system of X-rays and a crystalline solid. In the energy conserving or Bragg regime, the outcome of this effect is the spatially quantized diffraction of the electron beam into undeflected and deflected trajectories whose momenta and kinetic energies are conserved when considered in conjunction with the photons exchanged in the process.

The first proposal for observing the Kapitza-Dirac effect using lasers was by J.H. Eberly in 1965 when he calculated the Compton scattering for the electron in a KDE type experiment [2]. The small coupling of light with electrons requires the use of pulsed lasers with intensities of 0.3 GW cm\(^{-2}\). Such an experiment was performed in 2002 by H. Batelaan et. al. [3], however, the vast majority of subsequent KDE type experiments involve a definition of the Kapitza-Dirac effect which has been expanded to include atoms diffracting from periodic light crystals created by counter-propagating lasers [4]. Rather than the simpler photon-electron interaction, the system analyzed in this paper is complicated by the internal structure of the atom. Figure 1 depicts the energy level scheme presumed in the subsequent calculations.

For experimental ease, we utilize a Doppler-shifted Laue geometry wherein the atom beam is cooled transverse to its classical trajectory such that the angle of incidence is perpendicular to the light grating. In the standard Laue geometry, the atom enters the light grating at the Bragg angle and exits undeflected or at the mirror Bragg angle whereas in the Doppler-shifted geometry, the incoming atomic beam is normal to the laser axis. To achieve this, the laser in one direction is tuned to a higher frequency, which is analogous to finding Bragg resonances in X-ray diffraction by selectively imparting velocity to the material sample. The relative ease of detuning allows the experimentalist to set the incoming beam position normal to the laser direction while adjusting only the detector’s angle and the relative laser frequencies. Here, a real exchange of the higher frequency photon for a lower
frequency photon in the antiparallel direction is accomplished by scattering from a far off-resonant electronic state of the atom while imparting a transverse momentum to the scattering atom. Thus the momentum is conserved as the counter-propagating fields have each lost or gained a photon respectively, and the atom now has gained a transverse momentum equal to the change of the photon momentum sum. As field strength is varied, Pendellösung in the populations of the outgoing beams is observed analogous to Bragg scattering of X-rays in crystals in a Laue geometry where the thickness of the sample is varied. In the atomic frame, the interaction is that of an atom experiencing two counter-propagating pulses with an envelope defined by the laser profile after which the atom is left as it started or has gained transverse velocity from the multi-photon recoil.

Atomic Kapitza-Dirac Bragg scattering is a resonant two-photon process in which there is stimulated scattering from an off-resonant internal atomic state which takes one photon from one field and returns it to the antiparallel field. The particle is left with a momentum shift of \(2\hbar k\) and its initial internal ground state energy. The Bragg conditions require that the characteristic time, given by \(\frac{\text{beam width}}{\text{particle speed}}\), must be large compared to the line width. If this condition is not met, momentum, as always, is conserved creating spatially quantized deflections of outgoing atoms such that the number of photons reflected from the atom is matched by a change of velocity as the mass is fixed. The change in field energy is not necessarily equal to the change in mechanical energy of the atom. This short time interaction which allows exchange through a velocity perpendicular to the atomic beam \([6]\). In this manner, one creates a travelling standing wave analogous to moving the crystalline sample in X-ray diffraction, to excellent approximation, wherein the group velocity is used to match the Bragg conditions much the way moving the sample does in X-ray diffraction. The incident atomic beam can then be perpendicular to the light crystal and any Bragg condition can be met by an appropriate detuning of the lasers. These geometries are compared in Fig. 3.

In the Doppler-shifted Laue geometry, one sets the initial transverse speed to 0 and the field frequencies the atom sees are \(\Omega + \delta\) and \(\Omega\) respectively. Momentum conservation requires the change in the field momentum to equal the transverse momentum \(\hbar \Omega/c + \hbar(\Omega + \delta)/c \approx 2\hbar k\) adding a recoil energy to the mechanical state of the atom

\[
\approx \frac{2\hbar^2 \Omega^2}{m} \approx \frac{2\hbar^2 k^2}{m}
\]

The detuning of the counter-propagating lasers, \(\delta\), is chosen to match the recoil frequency of the atom

\[
\delta \approx \frac{2\hbar \Omega^2}{mc^2} \approx \frac{2\hbar k^2}{m} \quad \text{where} \quad \delta \ll \Omega
\]

which then satisfies the Bragg condition since the field exchange leaves the field with an energy difference of \(\hbar \delta (\hbar \Omega - \hbar(\Omega + \delta))\), exactly canceling the energy gained by...
scattering as the energy is conserved as well as the momentum, and it is a virtual two-photon Raleigh scattering as the virutally absorbed photon and stimulated emitted photon have the same frequency.

By contrast, the Doppler-shifted Laue geometry virtually absorbs a photon of greater frequency than the emitted photon. The energy gained by the atom in the form of transverse kinetic energy is equal to the energy lost in the field by the unequal exchange of the field photons whose energies differ by $\hbar \delta$. From the spectroscopic point of view, the atom is involved in a virtual two-photon Raman scattering event as the absorbed photon has a larger frequency than the photon stimulating the emission. The deflected atom gains a transverse velocity proportional to the change of momentum arising from the collision of the photon scattered $\pi$ radians by the recoil of the atom. The scattering of the photon from the atom is a two-photon virtual process since the field frequencies are far from resonance with the virtually excited electronic state of the atom. The virtually absorbed photon is essentially reflected; however, its energy is decreased by $\hbar \delta$ in a Raman scattering that imparts energy to the mechanical state of the atom while energy in the field is diminished by $\hbar \delta$. As this occurs, the atom’s initial 0 transverse momentum is increased by two photons of momentum and although the internal electronic energy of the atom is left unaltered, the direct product state is increased as the mechanical energy is increased. It is also important to note that the frequency of the field opposing the atom’s motion must be off-resonant with an internal electronic transition $\omega$ labeled $\Delta = \omega - \Omega$. This detuning is distinct from the detuning of the fields with respect to each other. The relative field detuning in the counter-propagating beams $\delta$ determines the outgoing angle of the atom. The atom’s direct product state of electronic and mechanical energies is altered between the deflected and incoming beam:

- **Undeflected (Incoming):** $|g.s. \rangle \otimes |p_\perp = 0 \rangle$
- **Deflected (Diffracted):** $|g.s. \rangle \otimes |p_\perp = \sqrt{2m\hbar \delta} \rangle$

### IV. EQUATIONS

Off-resonant stimulated Raman scattering describes an exchange of energy from one field to the field counter-propagating with the incident atomic beam as the intermediary where adiabatic elimination of virtual transitions leads to a semi-classical formulation of the equations of motion. The fields are both far detuned from the ground-to-excited-state difference, $\omega - \Omega$. The counter-propagating fields are detuned from each other such that their frequency difference, $\delta$, will later define a new set of direct product ground states for the atom in which electronically, the atom is in the ground state while mechanically, it has momentum 0 or $2\hbar k$. 

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**FIG. 4.** In the ring configuration, it is easy to measure the gain from each mode separately: $\Omega$ and $\Omega + \delta$ each have different angles at each mirror and the differential gain is easy to observe.

the Bragg-diffracted atom. This geometry allows the experimentalist to change the order of resonant Bragg scattering without adjusting the angle of incidence.

In the counter-propagating ring cavity depicted in Fig. 4, it is possible to measure the relative gain from the outgoing rays from each vertex while correlating the population of deflected atoms. In order to insure that the final atomic states of the atomic beam are two-photon transitions, the fields are far off-resonance with respect to the internal states of the atoms. The lowest-order scattering is a two-photon process and the virtual upper state is never populated. Note, we have defined two resonances, one of the electronic state of each atom and the other of the mechanical state of the atom. Given the two features of the system which can be considered resonant or off-resonant and the fact that the internal electronic transitions are always off-resonant, we use the term resonant to refer to the outgoing momentum states of the atomic beam. For intermediate states which are not energy conserving, we use the term off-resonant.

### III. VIRTUAL TWO-PHOTON RAMAN SCATTERING

In the symmetric or standard Laue geometry, the frequency of each atomic beam is identical. The incoming atom has a transverse momentum that is reversed after virtual excitation and stimulated emission. This process conserves momentum as the photon opposing the transverse velocity of the atom is virtually absorbed far from electronic resonance and then virtually stimulated by a photon in the direction of the transverse velocity of the atom. Afterwards, the atom experiences a recoil momentum equivalent to two photons of momentum and the photon initially counter to the direction of the atom is essentially reflected backward so the momentum of the field is changed by two photons of momentum. Here momentum is conserved, and the energy of the atom has not changed nor has the energy of the field. Energy conservation is assured by the time in the field and only occurs if the initial transverse momentum of the atom is equal to the momentum of the photon momentum. It is a Bragg
In the event of very short interaction time, the atom can exchange \( N2\hbar k \), where \( N \) is any integer, momentum in either field direction, and this defines the Raman-Nath regime where energy is not conserved. The regime where the interaction time is large with respect to the energy action is labeled the Bragg regime which indicates that both momentum and energy are conserved. In the adiabatic limit, the Bragg regime leads to only one pair of resonant states. Here the atom’s transverse momentum is either 0 or \( 2\hbar k \). For large detuning from the Bragg resonance, we expect non-zero off-resonant final states due to the non-adiabatic components of the Hamiltonian; however, these states are negligible in the limit of large detuning and low event number. Further, the off-resonant final states are also accessible in the Raman-Nath regime where the time the atom spends in the field is small with respect to the decay width associated with the excited state; however, this regime is easily suppressed by low beam speed and large laser beam width.

\[ \hbar |\alpha\rangle = -\frac{\hbar^2}{2m} \nabla^2 |\alpha\rangle + \frac{1}{2} \hbar \omega \sigma_z |\alpha\rangle - \hbar (r_1 e^{i\Omega t} e^{\ik x} + r_2 e^{i(\Omega+\delta) t} e^{-\ik x} + c.c.) \sigma_x |\alpha\rangle \]  

Expanding the equations in terms of the population amplitudes of the two internal states we have:

\[ \begin{align*}
\hbar \dot{a}_1(t) &= -\frac{\hbar^2}{2m} \nabla^2 a_1(t) + \frac{1}{2} \hbar \omega a_1(t) - \hbar (r_1 e^{i\Omega t} e^{\ik x} + r_2 e^{i(\Omega+\delta) t} e^{-\ik x} + c.c.) a_2(t) \\
\hbar \dot{a}_2(t) &= -\frac{\hbar^2}{2m} \nabla^2 a_2(t) + \frac{1}{2} \hbar \omega a_2(t) - \hbar (r_1 e^{i\Omega t} e^{\ik x} + r_2 e^{i(\Omega+\delta) t} e^{-\ik x} + c.c.) a_1(t)
\end{align*} \]  

After a Fourier Transform and a change of basis in which we are in an interaction-momentum picture where the phase contains information about the field and the mechanical state of the atom, we have the following recurrence form for the various momentum state amplitudes,

\[ \hbar \dot{a}(p, t) = -\imath S a(p, t) - \imath \beta f(t) e^{i(\frac{2\hbar k}{m} - \omega_\kappa - \delta) t} a(p - 2\hbar k, t) - \imath \beta f(t) e^{i(-\frac{2\hbar k}{m} - \omega_\kappa + \delta) t} a(p + 2\hbar k, t) \]  

as follows with \( \tilde{\alpha}_n = \tilde{\alpha}(n\hbar k, t) \):

\[ \begin{align*}
-\imath \dot{\tilde{\alpha}}_0 &= \beta f(t) \tilde{\alpha}_2 \\
-\imath \dot{\tilde{\alpha}}_2 &= \beta f(t) \tilde{\alpha}_0
\end{align*} \]  

Including the next-order Bragg processes, the states \( \tilde{\alpha}_{-2} \) and \( \tilde{\alpha}_4 \),

\[ \begin{align*}
-\imath \dot{\tilde{\alpha}}_{-2} &= \beta f(t) e^{2\delta t} \tilde{\alpha}_0 \\
-\imath \dot{\tilde{\alpha}}_0 &= \beta f(t) e^{-2\delta t} \tilde{\alpha}_{-2} + \beta f(t) \tilde{\alpha}_2 \\
-\imath \dot{\tilde{\alpha}}_2 &= \beta f(t) e^{-2\delta t} \tilde{\alpha}_4 + \beta f(t) \tilde{\alpha}_0 \\
-\imath \dot{\tilde{\alpha}}_4 &= \beta f(t) e^{2\delta t} \tilde{\alpha}_2
\end{align*} \]  

These equations clearly couple an infinite number of states; however, for the following we retain only two off-resonant states. The resonant states are those without phase factors and represent the states and couplings which arise from energy conservation between mechanical states of the atom and the field. The resonant equations where all higher-order Bragg processes are neglected are
$$\dot{d} = \begin{pmatrix}
2\delta & \beta f(t) & 0 & 0 \\
\beta f(t) & 0 & \beta f(t) & 0 \\
0 & \beta f(t) & 0 & \beta f(t) \\
0 & 0 & \beta f(t) & 2\delta 
\end{pmatrix} \cdot d \quad (8)$$

## B. Extended Dressed Basis and its Consequence

It is important to remember that the solution to the equations of motion requires solving the countably infinite number of equations denoted by Eq. (10) below. When the methods of approximation for the reduced 4-level problem no longer suffice, we shall find that Eq. (10) gives arbitrarily precise solutions provided the dimensionless detuning is not too small and the number of equations is sufficient. Where n is the even number of states included in the calculation, the coupling is given by

$$\frac{n^2 - 2n}{4} \delta$$

and the equations of motion are given by the countably infinite coupled differential equations inferred by the following expression

$$i \begin{pmatrix}
\vdots \\
d_{-8} \\
d_{-6} \\
d_{-4} \\
d_{-2} \\
d_0 \\
d_2 \\
d_4 \\
d_6 \\
d_8 \\
d_{10} \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\vdots \\
2\delta & \beta f(t) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\
\beta f(t) & 12\delta & \beta f(t) & 0 & 0 & 0 & 0 & 0 & 0 & \vdots \\
0 & \beta f(t) & 6\delta & \beta f(t) & 0 & 0 & 0 & 0 & 0 & \vdots \\
0 & 0 & \beta f(t) & 2\delta & \beta f(t) & 0 & 0 & 0 & 0 & \vdots \\
0 & 0 & 0 & \beta f(t) & 0 & \beta f(t) & 0 & 0 & 0 & \vdots \\
0 & 0 & 0 & 0 & \beta f(t) & 0 & \beta f(t) & 0 & 0 & \vdots \\
0 & 0 & 0 & 0 & 0 & \beta f(t) & 2\delta & \beta f(t) & 0 & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \beta f(t) & 12\delta & \beta f(t) & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta f(t) & 20\delta & \vdots \\
\vdots
\end{pmatrix} \cdot d_{-8} \quad (10)$$

## V. NUMERICAL SOLUTIONS

### A. Solutions to the bare 4-state equations

The exact numerical solution of the bare state equations (7) are plotted for $f(t) = \frac{1}{2} \text{sech}(\frac{\pi t}{4})$. All values for time and frequency, $t$, $\delta$, and $\beta$ are dimensionless where $t$ is in units of the pulse width and $\delta$ and $\beta$ are in units of the inverse pulse width. The initial states are unpopulated except for $a_0(-\infty)$. Although the final states are resonant in the limit of large detuning, the off-resonant states are strongly populated during the pulse. See Fig. [0]. It is clear that the off-resonant states are in fact contributing to the dynamics during the pulse. Although the off-resonant states die off long before the pulse has, neglecting to calculate off-resonant states during the interaction [7] would clearly introduce error.

We seek the populations for $t = \infty$ after the atom passes the light crystal when off-resonant states no longer play a role in the dynamics of the system. These two resonant states are designated by $|a_{0,2}(\infty)|^2$ where $\delta$’s and $\beta$’s are varied. Plotting the off-resonant probabilities, $|d_4(\infty)|^2$ with $f(t) = \beta \frac{1}{2} \text{sech}(\frac{\pi t}{4})$ against $\delta$ and $\beta$ we see evidence of the non-adiabaticity of higher-order states; see Fig. [8]. It is clear that the system exhibits Pendel röungen as well, analogous to what is observed for changing the thickness of crystal sample. We shall demonstrate that the frequencies of these oscillations are strongly dependent on off-resonant states. However, if the detuning $\delta$ is too small, the Pendel röungen is washed out as the outgoing states become indistinguishable as the corresponding spatial quantization tends toward a continuum of momentum states.
FIG. 5. Bare state probabilities with $\delta = 5$: The solid black line represents $|a_0|^2$ and the solid gray line $|a_2|^2$ while the dotted lines are $|a_{-2}|^2$ and $|a_4|^2$. The dashed gray line shows the curve of the pulse $f(t) = \frac{1}{2} \text{sech}(\frac{\pi t}{2})$. Time is zeroed at the pulse maximum.

FIG. 6. Here the final dressed state population, $|a_4(\infty)|^2$, is plotted against detuning and field strength. Note: we see evidence of Pendell"osung.

B. Exact solutions for the dressed states

Looking at the dressed states for $f(t) = \frac{1}{2} \text{sech}(\frac{\pi t}{2})$ we see a symmetry that is not so clear in the bare states. Plotting the final probabilities for $f(t) = \frac{1}{2} \text{sech}(\frac{\pi t}{2})$ against $\delta$ and $\beta$ we can see the non-adiabaticity of the problem with only four states included. Plotting the final dressed off-resonant probabilities, $|d_4(\infty)|^2$ for $f(t) = \frac{1}{2} \text{sech}(\frac{\pi t}{2})$ against $\delta$ and $\beta$, Pendell"osung is clearly observed along with the non-adiabaticity clear in the bare picture plot. What must be determined is the number of states required to get adequate precision in predicting the final resonant-state probabilities.

VI. THE NEED FOR MANY STATES: PHYSICALLY CORRECT SOLUTIONS

If the non-adiabatic contributions were small, the various methods of approximation which only depend upon the resonant states and one pair of off-resonant states would suffice, but we now demonstrate that unless the field strength is small, these approximations yield imprecise predictions. For large enough detuning, the off-resonant populations can be made exponentially small; however, the effects of the higher order momentum states are in fact necessary for correctly predicting the Pendell"osung frequencies of the resonant states and, therefore, the probabilities of finding atoms which are deflected as a function of field strength. The equations of motion are coupled, term by term, to higher off-resonant momentum states whose number are countably infinite. We seek the dependence of the number of states with respect to field strength for a given detuning.

As the field strength increases, the frequency of the Pendell"osung oscillations decreases. Although the detuning insures that the final population of off-resonant states is negligible, the effects of high order off-resonant states during the pulse interaction are not. Using a hyperbolic secant pulse calculating for the resonant two-state problem, we have the Rosen-Zener solution,

$$ p_{2RZ}(t) = \text{sech}(\delta) \sin(\beta) $$

where $\delta$, the detuning, is usually kept fixed and $\beta$, the field strength or pulse area, indicates the frequency of Rabi oscillations. When compared with the four-state solution for the Kapitza-Dirac system we are analyzing, this solution is inadequate. At low field strengths and large detuning, the frequency is identical; however, as the field strength is increased, the frequency drops precipitously.

In Fig. 7 we have plotted the solutions to $|p_{2RZ}(\infty)|^2$ and $|p_{2\text{-state}}(\infty)|^2$ to show the variation of phase and
The dimensionless field strength ranges from 100 to 150, a region where both Pendellösung frequencies are seemingly constant. Notice the Pendellösung frequency of the 14-state solution is roughly $1/4$ the frequency of the two-state Rosen-Zener solution. For the same range of field intensity, the solutions calculated with fewer states are in fact monotonically greater in frequency until the two-state solution is reached. For 16-state solutions and greater, for field intensities in the same range, the frequency is stable. This represents the physical solution of the resonant momentum states, i.e., the correct Pendellösung frequency and phase.

In order to find the number of coupled equations which must be solved to find a physical solution, it is important to compare the probability of the resonant state $|a_0(\infty)|^2$ calculated with a range of states included over a range of dimensionless field intensities. As we add states to the calculation at a given field intensity and detuning, if the probabilities remain constant, it is reasonable to assume that we have found a physical solution. In Fig. 8, the cosine of the absolute value of adjacent pairwise calculated probabilities is plotted against field intensity.

$$|\cos(|p_{2n-\text{states}}(\infty)|^2 - |p_{2(n+2)-\text{states}}(\infty)|^2)| \quad (12)$$

The phase of Eq. (12) goes to zero as the probabilities calculated for greater $n$ agree. The plateau in Fig. 8 therefore represents the domain of physical solutions and the curve created by the precipice of this plateau, clearly a function of dimensionless field intensity and number of states, indicates the boundary between physical and incorrect solutions. Immediately obvious is the breakdown of the Rosen-Zener solution for field intensities much larger than one.

The dependence of Pendellösung frequency and phase on field strength and order of calculation is easier to discern in Fig. 9. Here are a series of two dimensional graphs plotted above each other where the resonant population $|a_0(\infty)|^2$ is plotted against field strength (all plots are for a dimensionless detuning of 5). The bottom curve represents the exact solution for the 2-state system of equations and each ascending sequential graph represents the addition of 2 states. At first glance, the various Pendellösung frequencies seem similar with only changes of phase, but at a given range of field strength, it is clear that the variations are dramatic. As in the previous example, Fig. 7 Pendellösung periods get larger as more states are considered.

Another important feature of Fig. 9 is the lack of variation of the populations of $|p_0(\infty)|^2$ for small field intensity. In other words, the Rosen-Zener solution which is the exact solution of the 2-state system with $f(t) = \frac{1}{\sqrt{\pi}} \text{sech}(\frac{\pi t}{2})$ gives the correct solution to the Bragg equations for all order provided the detuning is large enough ($\delta > 1$) and the field intensity is small.

Although we do not vary the detuning in these plots, it should be noted that the detuning $\delta$ cannot be too small which would lead to large coupling to higher-order states. In fact, if the detuning is small, it may be impossible to
predict the population of any state. Looking at Fig. 10 where the dimensionless detuning is 1/10, the numerical solutions quickly become chaotic for field intensities of almost any magnitude and final states may not be resonant implying energy nonconservation similar to the Raman-Nath regime. This is only speculative as computational solutions for $\delta \ll 1$ are practically impossible to find. In the Raman-Nath regime where the interaction time is small compared to the decay width, uncertainty leads to energy nonconservation. When $\delta$ is small, the corresponding recoil momentum is small and so the spatial quantization is smeared back to spatial continuum. Therefore, to observe atomic KDE, the detuning $\delta$ and the interaction time must both be large enough to allow for spatial quantization and energy conservation.

Here, we posit an upper limit of the number of states necessary to include in calculations to get a physically correct solution for a given $\beta$ and suggest that since the coupling between states is given by Eq. (9)

$$n \propto \sqrt{\frac{\beta}{\delta}}$$  \hspace{1cm} (13)

To test Eq. (13), in Fig. 11 we plot Eq. (13) over a set of graphs whose characteristics are similar to Fig. 9 and Fig. 10 in that each successively higher graph represents a higher order of Bragg scattering included in the calculation and the horizontal axis represents the dimensionless field amplitude. However, instead of graphing the population, the graphs measure the following,

$$\left| |p_{0}n+2-state(\infty)|^{2} - |p_{0-n-state}(\infty)|^{2}\right|$$  \hspace{1cm} (14)

where $n$ is the order of the Bragg scattering included in the calculation and is therefore always even. The lowest graph in Fig. 11 consequently represents the difference between the 2-state solution and numerical 4-state solution. It is clear from this plot that as the dimensionless field amplitude increases, the Rosen-Zener solution fails. The region of Fig. 11 above the curve of Eq. (13) clearly represents the physical solution because the variation from each higher and adjacent order of calculation yields the same result at a given dimensionless field amplitude.

In Fig. 11 the graphs represent the differences between adjacent orders of final resonant populations, $|p_{0}(\infty)|^{2}$; however, with large detuning, $\delta = 5$, the populations of the resonant states sum to one.

$$|p_{0}(\infty)|^{2} + |p_{2}(\infty)|^{2} \cong 1$$  \hspace{1cm} (15)

In other words, with a detuning large enough that far less than 1/1000 of the atoms passing the light grating travel with transverse momentum greater than $2\hbar$ or less than 0, the Rosen-Zener solution fails to predict the correct and physical Pendellösung frequency and phase. This is a consequence of the mixing of off-resonant states with resonant states temporally near the center of the pulse. Although the resonant states are the only ones observed after passing the light crystal, many states may be necessary in calculating phase and frequency of the deflected and undeflected. Analogous to multiple reflections within a crystal of the X-ray before leaving the sample, here, we can imagine a similar picture in which many momenta are experienced, primarily the resonant ones, leaving only one of two at the end of the pulse. With this more correct physical picture, it seems reasonable to ask how many states are enough in calculating the resonant ones at $t = \infty$.

If we look for asymptotic analytic solutions to the behavior of the Pendellösung for large field strength of the higher-order calculations, i.e. 4-state, 6-state, etc. solutions, we can neglect the detuning. The integral

$$\int e^{\int (\phi_{1} - \phi_{2}) dt}$$
is the solution for the dressed populations without the non-adiabatic contributions. The frequency predicted for the 4-state problem is \( \frac{1}{2} \) Rosen-Zener frequency. To compare the numerical data to this asymptotic value of the Pendellösung frequency, in Fig. 13 we plot

\[
|p_{4\text{-state, } \beta + f_{\text{asymptotic}}(\infty)}|^2 - |p_{4\text{-state, } \beta}(\infty)|^2
\]

for a range of \( \beta \) where \( \beta \) is the dimensionless field intensity and \( f_{\text{asymptotic}} \) is the frequency predicted from the non-adiabatic asymptotic prediction with no detuning. Numerical solutions of the eigenvalues of the dressed Hamiltonian matrices where the detuning is zero give the correct asymptotic Pendellösung frequencies. Although the frequency does not seem to decrease strictly monotonically, on average the frequency decreases monotonically and asymptotically to the value of the frequency predicted in the absence of detuning. If the asymptotic solutions are correct, plotting the variations must tend toward zero and indeed this is true for Fig. 13 which is in fact based on the 4-state numerical populations where

\[
f_{\text{asymptotic}} = \frac{1}{2} f_{\text{Rosen-Zener}}
\]

is the frequency used to plot the envelope of convergence. These calculations have been performed on equations with up to 12 terms and they all exhibit monotonic convergence on the predicted asymptotic Pendellösung frequency.

This still leaves open the question of detuning with regard to the asymptotic solutions of the Pendellösung frequency. Computing the frequency as a function of \( \beta \) is non-trivial so again we look at the numerical solutions where we plot \( |p_{4\text{-state, } \beta + f_{\text{asymptotic}}(\infty)}|^2 - |p_{4\text{-state, } \beta}(\infty)|^2 \) for several detunings. In Fig. 13 detunings of \( \delta = 20 \), \( \delta = 10 \) and \( \delta = 5 \) are plotted. It is clear that they all converge to the asymptotic value of the Pendellösung frequency and in fact the larger the detuning, the slower the convergence.

Remarkably, the asymptotic behavior is always in the region of figure 11 where the solutions are not physical. Because the asymptotic solutions expect a large field amplitude

\[
\beta \gg \delta
\]

the only way to achieve this for a given number of states is to pass the boundary condition for physical solutions into the unphysical solution space. Therefore, at a given dimensionless field amplitude, one cannot analytically determine the population of the resonant states even though there are no off-resonant states.

Essentially, one can break Fig. 12 into three regions, the numerical, the unphysical and the Rosen-Zener region. The asymptotic solutions all fit in the unphysical region and may therefore only be of interest theoretically. The numerical and Rosen-Zener regions are both physical and therefore if one wishes to work with large dimensionless field amplitudes, one can always find the number of states required in the calculation from Eq. (9). However, the Rosen-Zener region can be calculated analytically or quasi-analytically for symmetric pulses. In the case of the hyperbolic secant pulse, \( f(t) = \frac{1}{2} \text{sech}(\frac{t}{\sqrt{2}}) \), the solution is given by Eq. (11). However, in this Rosen-Zener region, the 2-state calculation is sufficient for predicting the resonant states.

VII. CONCLUSIONS

Figure 11 clearly indicates that unless the field strength is very low, the values for the final-state am-
FIG. 15. The solid line is the solution to the 2-state solution for the pulse \( f(t) = \frac{1}{\sqrt{\pi}} e^{-t^2} \). The thick dashed line is the absolute difference between the 4-state and 2-state solutions. Clearly, one period of Pendellösung is almost perfectly described without including off-resonant states.

The amplitudes predicted by the Rosen-Zener solutions will be wrong. However, this can be useful in that one can design an experiment in which the dimensionless field amplitudes are small and the detuning large enough that the quasi-analytic 2-state solutions are physical, that is they properly predict the outgoing resonant state populations. If one needs to work in a regime of large field amplitude, one can use Eq. (13) to insure that enough off-resonant states are included in the calculation to find physical solutions.

In the decades that have passed since Pritchard’s \(^{[4]}\) pioneering experiments, momenta transfers as high as \(10^2 \hbar k\) have been achieved by Kasevich, et. al. \(^{[7]}\). High resolution interferometry based on Bragg diffraction is being carried out by groups such as Muller, et. al. \(^{[8]}\) in which a greater knowledge of the final-state populations of the atom beam is critical. Work by Leeuwen, et. al. \(^{[9]}\), in large angle Bragg interferometers shows the utility of spatial quantization in the slow atomic beam physics where again, precise knowledge of the calculation of the resulting Pendellösung is critical to understanding system dynamics.

Given the precise knowledge gained in the populations of the resonant outgoing momentum states it is useful if one works in the Bragg regime to do atom interferometry, recoil-induced resonance lasing, and with multiple laser fields, correlation experiments between spatial quantization and gain. With an apparatus as depicted in Fig. \(^{[4]}\) it is easy to measure the gain and final beam trajectory.

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