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Solution of Generalized Optical Bloch Equations by the Method of Matrix Continued Fraction

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A numerical method is developed for solving the optical Bloch equations in the center-of-mass momentum space for a closed V system in a counterpropagating field configuration. The method consists of an iterative procedure based on the matrix continued fraction and a transformation by which the optical Bloch equations can be organized into the tridiagonal matrix recurrence form.

Key Words: laser cooling; atom optics; quantum optics; matrix continued fraction; continued fraction.

A variety of laser cooling and trapping techniques have been developed during the past two decades in an effort to push the atomic temperature to its theoretical limit $T = 0$; see for example, [1]. These advances eventually led to the recent spectacular display of Bose–Einstein condensation of alkali atoms [2–4]. In this paper, we present a numerical method for studying the cooling features of a closed V system in a counterpropagating field configuration as shown in Fig. 1. Here, the 1–3 transition is dipole-forbidden while the 1–2 and 3–2 transitions are characterized by the same spontaneous decay rate Γ. In addition, the latter two transitions are driven, independently, by laser fields of the same frequency ω, wave number k, and Rabi frequency E. This model can be realized, in real atoms, by driving a $J = 0$ (ground level) to $J = 1$ (excited level) atomic transition with counterpropagating laser fields of σ_+ and σ_- polarizations. An in-depth analysis of the cooling force was given by Dalibard, Reynaud, and Cohen-Tannoudji [5] and later by Cai and Bigelow [6] in a semiclassical approach in which the motion of the atoms is described by means of the Fokker–Planck equations. The Doppler effect is identified as the underlying physical mechanism leading to cooling in this model. As a result, the average kinetic energy $\bar{K}$ is limited to the energy width of the excited levels, that is,

$$\bar{K} \equiv \frac{\overline{\Delta p}^2}{2M} \simeq \frac{\hbar\Gamma}{4}, \tag{1}$$

where M is the atomic mass and $\overline{\Delta p}$ is the momentum width. Let $\omega_r \equiv \hbar k^2/2M$ be the

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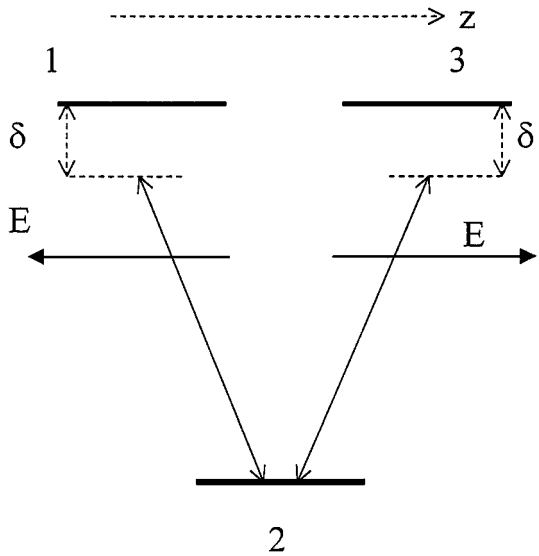

FIG. 1. A graphical representation of three-level V-type atoms interacting with two counterpropagating laser fields.

photon recoil frequency shift. For atoms of narrow line, $\Gamma \leq \omega_r$ and the momentum width can be narrower than $\hbar k$ according to Eq. (1). In such a circumstance, the de Broglie matter wavelength of the atoms exceeds the optical wavelength of the laser fields. No longer can atoms be considered particles moving classically under the influence of the electromagnetic fields. Hence, the results obtained from the semiclassical approach may no longer hold.

This consideration led Castin, Wallis, and Dalibard [7] (also Wallis and Ertmer [8]) to a quantum mechanical treatment in which both the internal and external degrees of the atomic freedom are treated quantum mechanically. The V system, compared to others, forbids a photon of one direction to be transferred, via the stimulated process, to a photon of the opposite direction, a phenomenon known as the coherent photon redistribution. As a result, atoms initially residing at $|2, p\rangle$ can only recycle among the three members, $(|2, p\rangle, |1, p-\hbar k\rangle, |3, p+\hbar k\rangle)$, of a momentum family $\mathcal{L}(p)$ as far as the stimulated process is concerned. The coupling among the members of different momentum families is accomplished through the momentum redistribution by the spontaneous emission. Due to the randomness in the spontaneous emission, an excited atom of momentum $p+q$ with $|q| \leq \hbar k$ has the $N(q)$ probability of becoming a ground atom of momentum p, where

$$N(q) = \frac{3}{8\hbar k}\left[1 + \left(\frac{q}{\hbar k}\right)^2\right],$$

assuming the emitted photons are circularly polarized. Following the notion of the momentum family [10, 11] along with the momentum redistribution by the spontaneous emission, Castin, Wallis, and Dalibard [7] constructed, for each momentum family $\mathcal{L}(p)$, nine equations corresponding to each density-matrix element in $\mathcal{L}(p)$. These equations are known as the generalized optical Bloch (GOB) equations that are both differential (with respect

to time) and integral (over the center-of-mass momentum). Recently, we have developed a matrix continued fraction method to solve the GOB equations for the purpose of studying the effect of atomic recoil on the absorption spectrum of driven V-type atoms [9]. In that work, the V-system is open and the focus of the work is on the spectrum calculation. In this paper, we extend this method to the closed V-system and focus our attention on the atomic momentum distribution which determines the temperature of the atoms.

To obtain the steady state solution, we set all the time derivatives in the GOB equations to zero. This leads to nine coupled integral equations. A straightforward method in dealing with the coupled equations is to first reduce the coupled equations to one equation involving one unknown by forward substitution, and then to obtain all the unknowns by backward substitution, starting from the solution to the equation for one unknown. Let $\rho_{22}(p) = \langle p, 2|\rho|2, p\rangle$, $\rho_{11}(p) = \langle p - \hbar k, 1|\rho|1, p - \hbar k\rangle$, and $\rho_{33}(p) = \langle p + \hbar k, 3|\rho|3, p + \hbar k\rangle$, where ρ is the density-matrix operator and p is the eigenvalue of the center-of-mass momentum operator. Our derivation (not shown for simplicity) leads to an integral equation for $\rho_{22}(p)$ in the form of

$$\begin{aligned}\Lambda(p)\rho_{22}(p) = \Gamma \int_{-\hbar k}^{+\hbar k} dq\, N(q) c_{32}(p - \hbar k + q)\rho_{22}(p - \hbar k + q) \\ + \Gamma \int_{-\hbar k}^{+\hbar k} dq\, N(q) c_{12}(p + \hbar k + q)\rho_{22}(p + \hbar k + q),\end{aligned} \tag{2}$$

where

$$\Lambda(p) = \Gamma c_{12}(p) + \Gamma c_{32}(p),$$

and $c_{12}(p)$ and $c_{32}(p)$ are coefficients defined through the relations between the excited and ground populations

$$\rho_{11}(p) = c_{12}(p)\rho_{22}(p) \quad \text{and} \quad \rho_{33}(p) = c_{32}(p)\rho_{22}(p). \tag{3}$$

The explicit expressions for these $c_{ij}(p)$ functions are too complex to present here. For the purpose of this paper, it seems sufficient to know that they are determined by various single- and two-photon absorption rates, which are themselves functions of various decay rates, the Rabi frequency, and laser detunings. Physically, Eq. (2) is a result of detailed balance among the populations in momentum space. In addition to Eq. (2), $\rho_{22}(p)$ is constrained by the closure condition, which, with the help of Eqs. (3), leads to the normalization condition for $\rho_{22}(p)$,

$$\int_{-\infty}^{+\infty} [1 + c_{12}(p) + c_{32}(p)]\, \rho_{22}(p)\, dp = 1. \tag{4}$$

Evidently, the key to the total atomic momentum distribution is to develop efficient algorithms for solving Eq. (2) subject to the normalization condition (4). In what follows, we show that Eq. (2) can be cast into a tridiagonal matrix recurrence equation, and solve it by the method of matrix continued fraction [12, 13]. To begin with, we divide q between $-\hbar k$ and $+\hbar k$ into L divisions and replace the integrals in Eq. (2) with Simpson's rule [14]. This

process turns Eq. (2) into

$$-\Gamma\frac{\Delta p}{3}\sum_{l=-L}^{0} b_{l+L}N(\hbar k+p_l)c_{32}(p_{n+l})\rho_{22}(p_{n+l})+\Lambda(p_n)\rho_{22}(p_n)$$
$$-\Gamma\frac{\Delta p}{3}\sum_{l=0}^{L} b_l N(-\hbar k+p_l)c_{12}(p_{n+l})\rho_{22}(p_{n+l})=0, \tag{5}$$

where $p_n = n\Delta p$ and $b_l = 4$ or 2 depending on whether l is odd or even with the exception of $b_0 = b_L = 1$. Note that in arriving at the form for the first sum in Eq. (5), we have made the transformation $l - L \to l$ along with the condition $L\Delta p = 2\hbar k$. Equation (5) can be further organized into

$$\sum_{l=-L}^{L} A_n^l \rho_{22}(p_{n+l}) = 0, \tag{6}$$

where

$$A_n^0 = \Lambda(p_n) - \Gamma\frac{\Delta p}{3}N(-\hbar k)c_{12}(p_n) - \Gamma\frac{\Delta p}{3}N(\hbar k)c_{32}(p_n),$$
$$A_n^l = -\Gamma\frac{\Delta p}{3}b_l N(-\hbar k+p_l)c_{12}(p_{n+l}) \quad \text{if } l>0,$$
$$A_n^l = -\Gamma\frac{\Delta p}{3}b_{l+L} N(\hbar k+p_l)c_{12}(p_{n+l}) \quad \text{if } l<0.$$

Next, we follow a standard procedure [14] and transform Eq. (6) into a tridiagonal matrix recurrence equation

$$\mathbf{Q}_n^-\vec{c}_{n-1} + \mathbf{Q}_n\vec{c}_n + \mathbf{Q}_n^+\vec{c}_{n+1} = 0, \tag{7}$$

where c_n is a vector of dimension L defined as

$$\vec{c}_n = \begin{pmatrix} \rho_{22}(p_{Ln}) \\ \rho_{22}(p_{Ln+1}) \\ \vdots \\ \rho_{22}(p_{Ln+L-1}) \end{pmatrix},$$

while $\mathbf{Q}_n$'s are matrices of $L \times L$ defined as

$$(\mathbf{Q}_n^+)_{ij} = A_{Ln+i-1}^{j-i+L}, \quad (\mathbf{Q}_n^-)_{ij} = A_{Ln+i-1}^{j-i-L}, \quad (\mathbf{Q}_n)_{ij} = A_{Ln+i-1}^{j-i},$$

where $A_n^l = 0$ if $|l| > L$. Let the entire momentum space, ranging from $p_{\min}$ to $p_{\max}$ be divided into (max − min) number of $2\hbar k$ blocks, where $\max - \min = (p_{\max} - p_{\min})/2\hbar k$. (In this paper, $p_{\min} = -p_{\max}$ since our model is symmetric.) As long as $p_{\min}$ and $p_{\max}$ remain far away from the center, the elements in both $\vec{c}_{\max+1}$ and $\vec{c}_{\min-1}$ remain fairly constant. For technical reasons, we first assume this constant to be 1 and set all the elements in $\vec{c}_{\max+1}$ and $\vec{c}_{\min-1}$ to 1. (This constant will later be fixed by the normalization condition.)

To solve Eq. (7) under this assumption, we first require that the solution to Eq. (7) follow a backward ansatz

$$\vec{c}_{n-1} = -\mathbf{S}_{n-1}\mathbf{Q}^{+}_{n-1}\vec{c}_n - \vec{a}_{n-1}, \tag{8}$$

where $\mathbf{S}_n$ is a matrix of dimension $L \times L$, and $\vec{a}_n$ is a vector of dimension L. $\mathbf{S}_n$ and $\vec{a}_n$ are found, after Eq. (8) is inserted into Eq. (7), to obey

$$\begin{aligned} \mathbf{S}_n &= (\mathbf{Q}_n - \mathbf{Q}^{-}_n\mathbf{S}_{n-1}\mathbf{Q}^{+}_{n-1})^{-1}, \\ \vec{a}_n &= -\mathbf{S}_n\mathbf{Q}^{-}_n\vec{a}_{n-1}, \end{aligned} \tag{9}$$

for $n >$ min, and to be equal to

$$\begin{aligned} \mathbf{S}_{\min} &= (\mathbf{Q}_{\min})^{-1}, \\ \vec{a}_{\min} &= \mathbf{S}_{\min}\mathbf{Q}^{-}_{\min}\vec{c}_{\min-1}, \end{aligned} \tag{10}$$

for $n =$ min. The numerical procedures are summarized as follows. First, obtain all the $\mathbf{S}_n$ and $\vec{a}_n$ from Eq. (9) by forward iteration starting from Eq. (10). Second, solve for all the $\vec{c}_n$ from Eq. (8) by backward iteration starting from $\vec{c}_{\max+1}$. Finally, divide the solution by the normalization factor, $\int_{-\infty}^{+\infty}[1 + c_{12}(p) + c_{32}(p)]\,\rho_{22}(p)\,dp$, to obtain the true excited momentum distribution $\rho_{22}(p)$.

Items of interest in our study include the total momentum distribution

$$\rho_{total}(p) = \rho_{11}(p + \hbar k) + \rho_{22}(p) + \rho_{33}(p - \hbar k), \tag{11}$$

and the average kinetic energy

$$\bar{K} = \int_{-\infty}^{+\infty} \frac{p^2}{2M}\rho_{total}(p)\,dp, \tag{12}$$

which is a direct measure of the atomic temperature. In the simulation bellow, $\hbar k$ is chosen to be the unit for the momentum, Γ to be the unit for any rates and frequencies, and the momentum is sampled at a rate of about 10 divisions per $\hbar k$. Figure 2 displays a sequence of atomic momentum distributions that distinguish themselves by their Rabi frequencies. It is produced for atoms with relatively narrow atomic transition lines of $\omega_r\,(\equiv E_r/\hbar) = \Gamma$ subject to lasers of red detuning of $\delta = -2.5\Gamma$. It clearly shows that for atoms of narrow line, the atomic distribution can be nonMaxwellian if the lasers are sufficiently weak. Figure 3 shows how the average kinetic energy $\bar{K}$ changes with the laser detuning δ for different Rabi frequencies E. It indicates that for a given E, the average kinetic energy reaches a minimum $\bar{K}_{\min}$ at a certain laser detuning $\delta_{\min}$. It deserves mention that curve (a) of Fig. 3 is produced under the limit of narrow atomic line ($\omega_r/\Gamma = 10 \gg 1$) and low laser intensity ($E_L/\Gamma = 0.1 \ll 1$). From curve (a), we find that $\bar{K}_{\min} \simeq 0.513\hbar\omega_r$ and $\delta_{\min} \simeq -43.10\Gamma = -4.31\omega_r$. These values are in close agreement with analytical results $\bar{K}_{\min} \simeq 0.53\hbar k$ and $\delta_{\min} \simeq -4.5\omega_r$ under the same limit [7]. In addition, we find (not shown) that as δ increases beyond $\delta_{\min}$ (that is, δ is on the right side of $\delta_{\min}$), first the average kinetic energy [Eq. (12)] fails to converge, and then the steady state atomic momentum distribution [Eq. (11)] ceases to exist. Numerically, $\bar{K}$ [Eq. (12)] is recognized as being divergent if

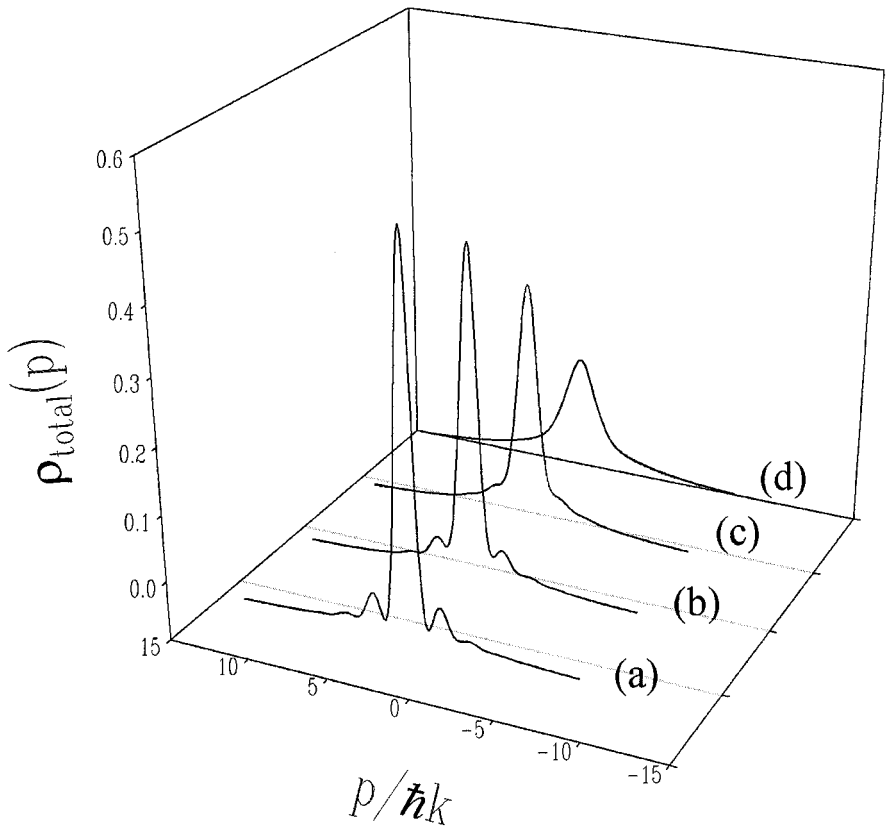

FIG. 2. A sequence of total atomic momentum distributions $\rho_{total}(p)$ consisting of (a) $E = 0.05\Gamma$, (b) $E = 0.5\Gamma$, (c) $E = 1.0\Gamma$, and (d) $E = 2.5\Gamma$. Other parameters are $\omega_r = \Gamma$ and $\delta = -2.5\Gamma$.

it always increases with the increase in the momentum space (meaning large $|p_{\min}|$ and $p_{\max}$). Similarly, a solution is considered unphysical if the momentum distribution [Eq. (11)] always broadens with the momentum space. All these results match those found by Castin, Wallis, and Dalibard [7].

In this paper, we have applied the method of matrix continued fraction to solve steady state GOB equations obtained by a full quantum mechanical approach. It is worthwhile to compare this method with other numerical approaches. One way to obtain the steady state momentum distribution is to propagate the GOB equations along time, either by direct integration or by Monte–Carlo simulation, until the solution does not change with time. However, this method is time consuming. Another method is to treat the steady state GOB equations as linearly coupled equations consisting of $(N_{\max} - N_{\min})L$ number of unknowns per atomic variable in momentum space. But, since the dimension of the matrix to be inverted can be very large, this method requires a long time and much memory space. In comparison, the matrix inverse operations in our method are all performed on matrices of $L \times L$ dimension, where L is typically much smaller than the total number of divisions in the momentum space. That is why our method is efficient in terms of both computing time and memory storage. This work, to our knowledge, represents the first application of the method of matrix continued fraction in laser cooling problems where the center-of-mass motion is quantized. We expect that this method will find its use in many other

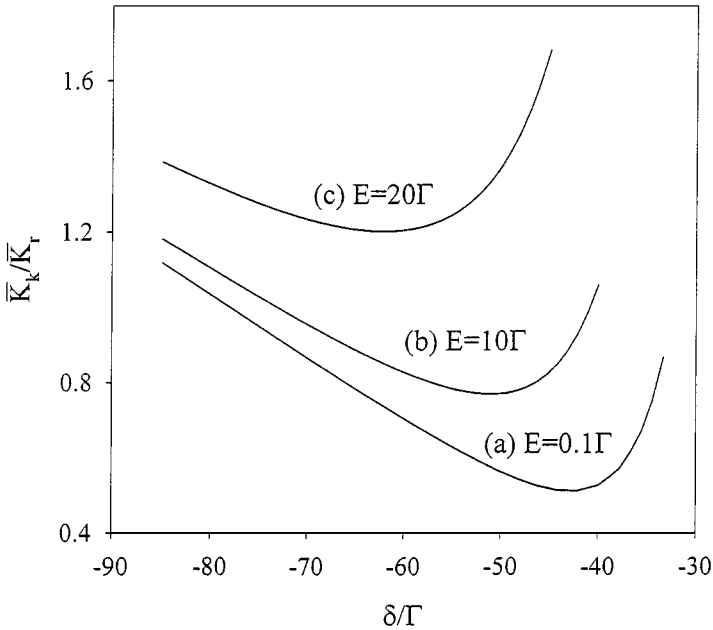

FIG. 3. The dependence of the average kinetic energy on the laser detuning for (a) $E = 0.1\Gamma$, (b) $E = 10\Gamma$, and (c) $E = 20\Gamma$. Other parameters are $\omega_r = 10\Gamma$ and $\delta = -38\Gamma$. The average kinetic energy is called to the photon recoil kinetic energy: $\bar{K}_r = \hbar\omega_r$.

problems, especially in problems where subrecoil cooling features can emerge from a broad background in momentum space [15, 16].

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