Nonlinear atom optics: General formalism and atomic solitons

G. Lenz, P. Meystre, and E. M. Wright
Optical Sciences Center, University of Arizona, Tucson, Arizona 85721
(Received 24 March 1994)

We present a many-body theory of nonlinear atom optics, and discuss some of its physical implications in the coherent regime. Considering a system of N identical two-level atoms interacting with classical and quantum-mechanical electromagnetic fields, we derive a Fock-space many-particle master equation. Introducing a Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy and a Hartree-Fock factorization to truncate this hierarchy, we obtain an effective nonlinear single-particle master equation that forms the basis of nonlinear atom optics. In the second part of the paper, we concentrate on the coherent part of that master equation, and derive an effective single-atom nonlinear Schrödinger equation. This equation leads to the prediction of a number of effects, and in particular, several kinds of atomic solitons. We discuss and numerically study two such kinds of solitons, Thirring solitons and gap solitons. Finally, the axial containment of an atomic gap soliton is illustrated.

PACS number(s): 42.50.Vk, 03.75.Be

I. INTRODUCTION

Considerable progress has recently been made towards the manipulation of trapped and cooled atoms in optical fields. One example is the observation of quantized atomic motion in one-, two-, and three-dimensional optical lattices [1–4]. More generally, the study of the physics of ultracold atoms in light fields opens up a broad new field of fundamental and applied research. It plays an essential role in understanding the fundamental limitations of atomic cooling, and hence of devices such as atomic clocks: The many-body effects that are expected to occur when the atomic temperature is near the recoil limit are bound to lead to shift and broadening mechanisms, and possibly nonlinear heating, thereby influencing the achievable performance of these devices. Many-body effects are also expected to be important in lithographic applications, whose basic principles are closely related to those of optical lattices: In order to achieve reasonable writing speeds, high atomic densities will clearly be required. In addition to these immediate practical concerns, the availability of ultracold atoms is of considerable interest in atom interferometry, since it naturally leads to the possibility of coherently splitting atomic wave functions with a large separation between the arms of the interferometer. Such macroscopic separations are highly desirable since most applications of atom interferometry require that the arms of the interferometer be placed in different environments and/or that large areas be covered by the interferometers, as, e.g., in gyroscopic applications.

This paper deals with the physics of ultracold atoms *in light fields*, in the regime where two-body interactions become important [5–8]. Here, the words "in light fields" are emphasized because it is important to realize the difference between the situation at hand and the closely related problem of Bose condensation of atomic vapors [9,10], where the understanding of many-body interactions is also of central importance: In Bose condensation, one needs to carefully balance the favorable effects of collisions, which are essential in rethermalizing the sample during evaporative cooling, and their detrimental effects, which are most importantly heating, as well as possibly a collapse of the Bose condensate for attractive interactions. Thus the presence of light fields is to be avoided in that situation, and the major source of many-body effects is the short-range van der Waals interaction between ground state atoms, which becomes important at the high densities necessary to reach Bose condensation. Our point of view is different, and complementary: We view many-body interactions as having a positive effect, which may lead to novel kinds of collective atomic behaviors in *optically driven*, relatively low density atomic systems. For this reason, we are interested in using the effects of the long-range dipole-dipole interaction between excited and ground state atoms. This interaction is second order in perturbation theory, while the van der Waals interaction is fourth order, hence the lower densities that we need to consider.

It is important at this point to give a note of caution about attractive versus repulsive interactions. In contrast to the free space situation, atoms in periodic light fields are characterized by a band structure, and can therefore have either positive or negative effective masses. Thus an interaction which might naively be thought of as, say, repulsive, becomes effectively attractive for a negative effective mass. Hence sweeping arguments based solely on the sign of the interaction are misleading at best. In particular, we shall see that an atomic sample in a light field can sustain many-atom bound state soliton solutions for both signs of the two-body potential.

The net effect of any two-body interaction $V_{12}(r)$ is given by its overlap with the atomic wave functions, properly symmetrized in the case of indistinguishable particles. As soon as this integral becomes significant, it becomes incorrect to treat the atoms in the sample as independent. We shall see that many-body effects can lead to an effective nonlinear behavior of the single atoms. This regime, that we call "nonlinear atom optics," is to de Broglie optics what nonlinear optics is to conventional

optics. It suggests that novel effects such as the generation of atomic solitons and solitary waves, atomic wave mixing, and atomic phase conjugation should be possible. In addition, sufficiently high atomic densities in optical lattices could lead to spontaneous pattern formation and the creation of other stable long-range structures, such as possibly superlattices. Even more intriguing perhaps, the combination of nonlinearities with dissipation, in the form of spontaneous emission and of a "pump" mechanism, suggests the possibility of a "coherent atomic beam generator," which could loosely be considered as the atom optics version of a laser.

The first part of this paper outlines the derivation of an effective single-atom master equation for nonlinear atom optics: In Sec. II we apply the Power-Zienau transformation to the minimal coupling Hamiltonian to go to the multipolar Hamiltonian [11]. This Hamiltonian has the advantage that the atom-field coupling is written in terms of the physical, retarded fields. Our model is then obtained by performing the dipole and rotating-wave approximations on the Power-Zienau Hamiltonian, and describing the atoms as two-level systems. The vacuum field is adiabatically eliminated in Sec. III in the Born-Markov approximation, thereby deriving a many-body master equation in the many-particle Fock space. The reduction of this master equation to an effective single-atom master equation involves two steps: First we develop a Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy for one-, two-, ..., N-atom density matrices, a step described in Sec. IV. This hierarchy is finally truncated in Sec. V by performing a Hartree-Fock approximation. The result of this development is an effective, nonlinear single-atom master equation including the effects of spontaneous emission as well as the long-range dipole-dipole interaction. In addition, an imaginary potential appears in this equation, which describes nonlocally confined excitation and decay processes.

In the second part of the paper, we concentrate on the *coherent* part of the effective single-atom master equation only. That is, we neglect dissipative effects as well as the imaginary potential. Both terms *together* are the single-particle equivalent of the many-body Lindblad-type Liouvillian [12] that describes the destruction of coherences. In this coherent case, the evolution of the system is described by a nonlinear Schrödinger equation, which is presented in Sec. VI. The remainder of the paper shows that these equations admit envelope solitons, and in Secs. VII and VIII, we discuss specifically two kinds of atomic solitons, Thirring solitons and gap solitons. The possibility of soliton oscillations in a focused laser beam is also analyzed. Finally, Sec. IX is a summary and conclusion.

II. MODEL

Since atom-atom interactions are mediated by the electromagnetic field, we seek to develop a model describing the dynamics of atoms in the vacuum field, as well as external laser fields that describe, e.g., cooling and trapping fields and atom optical elements, and that may be treated quantum mechanically or classically, depending upon the circumstances. Instead of the Coulomb gauge, we chose to work within the multipole expansion, in which the evaluation of atom-atom interactions is more conveniently carried out [11]. Specifically, we proceed by performing a Power-Zienau transformation on the minimal coupling Hamiltonian

$$\hat{H} = \sum_{i,\alpha_i} \frac{1}{2m_{\alpha_i}} \left(\hat{p}_{\alpha_i} - \frac{q_{\alpha_i}}{c}\hat{\mathcal{A}}(\hat{r}_{\alpha_i})\right)^2 + \frac{1}{8\pi}\int dr[\hat{\mathcal{B}}^2(r) + \hat{\mathcal{E}}_\perp^2(r)] + \frac{1}{2}\int dr d\acute{r}\frac{\hat{q}(r)\hat{q}(\acute{r})}{|r-\acute{r}|}, \tag{1}$$

where $\hat{\mathcal{E}}_\perp(r)$ is the conjugate momentum of the transverse part of the vector potential $\hat{\mathcal{A}}(r)$, $\hat{\mathcal{B}}(r)$ is the magnetic field, and the index i runs over the atoms and α_i over their constituents. The charge density is $\hat{q}(r) = \sum_{i,\alpha_i} q_{\alpha_i}\delta(r - \hat{r}_{\alpha_i})$. We assume charge neutrality, $\sum_{\alpha_i} q_{\alpha_i} = 0$, and furthermore that it is meaningful to consider individual atoms. Hence we ignore the effects of electron exchange.

When applied to the minimal coupling Hamiltonian (1), the Power-Zienau transformation yields the new Hamiltonian

$$\hat{H} = \sum_i (\hat{H}_i + \hat{V}_i) + \frac{1}{2}\sum_{i\neq j}\hat{V}_{ij} + \hat{\mathcal{H}}_f, \tag{2}$$

where

$$\hat{H}_i = \sum_{\alpha_i}\frac{1}{2m_{\alpha_i}}\left(\hat{p}_{\alpha_i} + \frac{q_{\alpha_i}}{c}\int_0^1 d\lambda\lambda(\hat{r}_{\alpha_i} - R_i) \times\hat{\mathcal{B}}(R_i + \lambda(\hat{r}_{\alpha_i} - R_i))\right)^2 + 2\pi\int dr\hat{P}_{\perp,i}^2(r) + \frac{1}{2}\int dr d\acute{r}\frac{\hat{q}_i(r)\hat{q}_i(\acute{r})}{|r-\acute{r}|}, \tag{3}$$

$$\hat{V}_i = -\int dr\hat{P}_i(r)\cdot\hat{\mathcal{E}}_\perp(r), \tag{4}$$

$$\hat{V}_{ij} = 4\pi\int dr\hat{P}_{\perp,i}(r)\cdot\hat{P}_{\perp,j}(r) + \int dr d\acute{r}\frac{\hat{q}_i(r)\hat{q}_j(\acute{r})}{|r-\acute{r}|} = 4\pi\int dr\hat{P}_i(r)\cdot\hat{P}_j(r), \tag{5}$$

and

$$\hat{\mathcal{H}}_f = \frac{1}{8\pi}\int dr[\hat{\mathcal{B}}^2(r) + \hat{\mathcal{E}}_\perp^2(r)], \tag{6}$$

where $\hat{P}_i(r)$ is the polarization of atom i. Note that in the new representation we still use the symbols $\hat{p}_{\alpha_i}/m_{\alpha_i}$ and $\hat{\mathcal{E}}_\perp(r)$, with the understanding that these operators belong to the conjugate momentum of x_{α_i} and $\mathcal{A}_\perp(r)$, respectively [and *not* to the velocity v_{α_i} and the electric field $E_\perp(r)$].

The Hamiltonian (2) is still exact. We now proceed to simplify it by dropping all magnetic terms and re-

placing the Hamiltonian (3) by that of a few-level atom, specifically a two-level system in this paper. The polarization of atom i is then replaced by $\hat{P}_i(r) = (\mathbf{d}_{12}\sigma^+ + \mathbf{d}_{12}^*\sigma^-)\delta(r-\hat{r}_i)$, so that the contact interaction (5) reads, for our two-level systems,

$$\hat{V}_{12} = 3\pi\hbar\gamma_0(\hat{\sigma}^+ \otimes \hat{\sigma}^- + \hat{\sigma}^- \otimes \hat{\sigma}^+)\delta(|k_0|(\hat{r}_1 - \hat{r}_2)). \quad (7)$$

In this equation, we have dropped nonresonant terms to be consistent with the rotating-wave approximation that will be performed later on, and have introduced the spontaneous decay rate $\hbar\gamma_0 = 4|d_{12}|^2k_0^3/3$. It is worth mentioning at this point that the only instantaneous coupling is the two-body contact interaction (5).

In the next section, we adiabatically eliminate the vacuum field, thereby introducing the dipole-dipole interaction between atoms. In preparation of this step, it is useful to split the dipole interaction term (4) into a contribution containing the vacuum modes of the field and a contribution due to the macroscopically populated external laser fields. Our model Hamiltonian reduces then to

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_s + \hat{\mathcal{H}}_f - \int dr\hat{\mathcal{P}}(r)\cdot\hat{\mathcal{E}}_\perp(r), \quad (8)$$

where in addition to the Hamiltonian (3), $\hat{\mathcal{H}}_s$ includes the contact term (5) as well as the part of the dipole interaction (4) due to macroscopic fields.

We conclude this section by introducing a few useful definitions and notations. First, we note that in the following, *single-* or *two-*particle operators in the Hilbert space of fixed-particle number are indicated by a hat, e.g., $\hat{a}, \hat{b}, \ldots, \hat{A}, \hat{B}, \ldots$. Calligraphic letters $\hat{\mathcal{A}}, \hat{\mathcal{B}}, \ldots$ are reserved for operators in Fock space. Also, we introduce the positive frequency component of the "electromagnetic field":

$$\hat{\mathcal{E}}_\perp^+(r) = \sum_{\{\kappa\}} i\epsilon(\kappa)\hat{a}_\kappa e^{ik\cdot r}, \quad (9)$$

where κ is a compound index labeling both the polarization i and wave vector k of a field mode, $\epsilon(\kappa) = [2\pi\hbar\omega_k/V]^{1/2}\epsilon_i(k), i = 1, 2$ and $\epsilon_i(k)$ are the usual polarization vectors. In second quantization, the dipole moment operator of the system is

$$\hat{\mathcal{P}}(r) = \int d\{i\}\langle 1|\hat{d}(r)|2\rangle\hat{\Psi}^\dagger(1)\hat{\Psi}(2)$$

$$\equiv \mathbf{d}_{12}\hat{\mathcal{S}}^+(r) + \mathbf{d}_{12}^*\hat{\mathcal{S}}^-(r), \quad (10)$$

where $\hat{d}(r) = (\mathbf{d}_{12}\hat{\sigma}^+ + \mathbf{d}_{12}^*\hat{\sigma}^-)\delta(r-\hat{r})$. Hence, in the rotating-wave approximation, the dipole interaction reduces to

$$\hat{\mathcal{H}}_{sf} = -\int dr \int d\{i\}\langle 1|\hat{\sigma}^+(r)|2\rangle \times\hat{\Psi}^\dagger(1)\hat{\Psi}(2)\hat{\mathcal{E}}_\perp^+(r) + \text{H.c.}, \quad (11)$$

where from here on the polarization vectors of $\hat{\mathcal{E}}_\perp^\pm$ are understood to be multiplied by the dipole moment $\mathbf{d}_{12}$ of the particles, and the operator $\hat{\sigma}^\pm(r)$ is given by $\hat{\sigma}^\pm \otimes \delta(r-\hat{r})$.

We finally recall that "integrating over numbers" such as $d1, d2$ means a summation over a complete set of quantum numbers for the single-particle system under consideration. In our case, this could be, e.g., a spin and coordinate, or a quasimomentum and band index. Formally stated, the dummy index r is the spectrum of $\hat{r}$, so it is a one-, two-, or three-dimensional vector depending on the experimental configuration. The wave vector k is of course always three dimensional.

III. MASTER EQUATION

Since we are only interested in the dynamics of the atoms coupled to the macroscopic fields described by the system Hamiltonian $\hat{\mathcal{H}}_s$, we now eliminate the vacuum modes of this system for the case of a bath at $T = 0$ in the Born-Markov approximation [13]. (More general results for the case of a reservoir at temperature $T \neq 0$ are given in Ref. [14].) In the interaction picture with respect to $\hat{\mathcal{H}}_s + \hat{\mathcal{H}}_f$ this procedure yields the Liouville equation for the system reduced density operator ϱ_s in Fock space,

$$\frac{\partial\hat{\varrho}_s(t)}{\partial t} = -\frac{1}{\hbar^2}\int_0^t d\tau \mathrm{Tr}_f\left\{[\hat{\mathcal{H}}_{sf}(t), [\hat{\mathcal{H}}_{sf}(\tau), \hat{\varrho}_{sf}(\tau)]]\right\}, \quad (12)$$

where the operators in $\hat{\mathcal{H}}_{sf}$ carry the time dependence of their free fields. We assume as usual the coarse-grained factorization of $\hat{\varrho}(\tau)_{sf}$ into $\hat{\varrho}_f^{\text{equi}}\otimes\hat{\varrho}_s(\tau)$, where $\hat{\varrho}_f^{\text{equi}}$ is the thermal equilibrium density operator of the bath, thereby being left with free-field expectation values.

Since the correlation functions of the reservoir decay over a time scale short compared to the characteristic time of the system dynamics, it is possible to extend the upper integration limit t to infinity on the right-hand side of Eq. (12). The evaluation of this integral then reduces to the evaluation of the half-sided Fourier transform of the field correlation

$$\hbar^2[\gamma(r_{12}) + i\delta\omega_0(r_{12})]$$

$$= \int_0^\infty d\tau\langle\hat{\mathcal{E}}^+(r_2, t-\tau)\hat{\mathcal{E}}^-(r_1, t)\rangle e^{-i\omega_0\tau}, \quad (13)$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ and ω_0 is the Bohr frequency of the atomic electronic transition. This frequency now appears since in reverting from the interaction representation we must account for the fact that the operators $\hat{\mathcal{S}}^\pm(r_{1/2})$ appearing in Eq. (12) are to be taken at different times t and $t-\tau$. The explicit forms of $\gamma(r_{12})$ and $\delta\omega_0(r_{12})$ are

$$\gamma(r_{12}) = \frac{\gamma_0}{2}\left[j_0(k_0|r_{12}|) - \frac{1}{2}\left\{1 - 3[e(r_{12})\cdot e(d_{12})]^2\right\}j_2(k_0|r_{12}|)\right] \quad (14)$$

and

$$\delta\omega_0(r_{12}) = \frac{\gamma_0}{2\pi}\int_0^\infty d\omega \mathrm{P}\left(\frac{1}{\omega-\omega_0}\right)\left(\frac{\omega}{\omega_0}\right)^3 \times\Bigg\{ j_0(\omega|r_{12}|/c) - \frac{1}{2}\left\{1-3\left[e(r_{12})\cdot e(d_{12})\right]^2\right\} \times j_2(\omega|r_{12}|/c)\Bigg\}. \quad (15)$$

Here the functions j_i are modified spherical Bessel functions of the first kind [15], $e(\mathbf{x})$ is the unit vector in direction $\mathbf{x}$, and $\mathrm{P}(1/x)$ stands for principal value.

In usual quantum optics, the imaginary part of the bath correlation functions is associated with an infinite "Lamb shift" that is normally ignored. More caution is needed in the present situation: $\delta\omega_0(r_{12})$ depends on the distance between two atoms. Hence it contains contributions involving the dipole operators of two atoms, in addition to the usual single-atom terms. It is possible to reorder the operators appearing in Eq. (12) so as to obtain a von Neumann equation which resembles a single-atom one. This reordering leads to the final form of the Fock-space master equation,

$$\begin{aligned}\frac{\partial\hat{\varrho}_s}{\partial t} &= -\frac{i}{\hbar}[\hat{\mathcal{H}}_s,\hat{\varrho}_s] - \frac{i}{2\hbar}\int dr_1 dr_2 V_{\mathrm{dip}}(r_{12})[\hat{\mathcal{S}}^+(r_1)\hat{\mathcal{S}}^-(r_2)+\hat{\mathcal{S}}^-(r_1)\hat{\mathcal{S}}^+(r_2),\hat{\varrho}] \\ &+\frac{i}{2\hbar}\int dr\hbar\delta\omega_0(0)[\hat{\Psi}^\dagger(r,e)\hat{\Psi}(r,e)-\hat{\Psi}^\dagger(r,g)\hat{\Psi}(r,g),\hat{\varrho}] \\ &-\int dr_1 dr_2\gamma(r_{12})[\hat{\mathcal{S}}^+(r_1)\hat{\mathcal{S}}^-(r_2)\hat{\varrho}+\hat{\varrho}\hat{\mathcal{S}}^+(r_1)\hat{\mathcal{S}}^-(r_2)-2\hat{\mathcal{S}}^-(r_2)\hat{\varrho}\hat{\mathcal{S}}^+(r_1)],\end{aligned} \quad (16)$$

where V_{dip} is the dipole-dipole potential between atoms,

$$V_{\mathrm{dip}}(r_{12}) = \frac{\hbar\gamma_0}{2}\left\{y_0(k_0|r_{12}|) - \frac{1}{2}\{1-3\left[e(r_{12})\cdot e(d_{12})\right]^2\}y_2(k_0|r_{12}|)\right\}, \quad (17)$$

the functions y_i being modified spherical Bessel functions of the second kind [15].

IV. BBGKY HIERARCHY

The Fock-space master equation (16) contains more information than necessary for most experimental measurements, which can normally access only a small subset of one- and two-particle observables. It is therefore meaningful to reduce Eq. (16) to a BBGKY hierarchy of reduced density operator equations for low particle number subspaces of the many-particle Fock space. We proceed by defining a normalized density operator in the N-particle subspace of the Fock space as

$$\hat{\varrho} = \int \frac{d^N\{i\}d^N\{i'\}}{N!}\rho_N(1,\ldots,N;1',\ldots,N')\prod_{i=N,\ldots,1}\hat{\Psi}^\dagger(i)|0\rangle\langle 0|\prod_{i'=1',\ldots,N'}\hat{\Psi}(i'), \quad (18)$$

with $\mathrm{Tr}\hat{\varrho} = \int d^N\{i\}\rho_N(1,\ldots,N;1,\ldots,N) = 1$. Expectation values of operator products are related in an obvious way to such reduced density matrices. For example, we have

$$\begin{aligned}\langle\hat{\Psi}^\dagger(b)\hat{\Psi}(a)\rangle &=: N\rho_1(a;b) \\ &= N\int d^{N-1}\{i\}\rho_N(1,\ldots,N-1,a;1,\ldots,N-1,b),\end{aligned} \quad (19)$$

$$\begin{aligned}\langle\hat{\Psi}^\dagger(d)\hat{\Psi}^\dagger(c)\hat{\Psi}(a)\hat{\Psi}(b)\rangle &=: N(N-1)\rho_2(a,b;c,d) \\ &= N(N-1)\int d^{N-2}\{i\}\rho_N(1,\ldots,N-2,a,b;1,\ldots,N-2,c,d).\end{aligned} \quad (20)$$

In this paper, we are primarily interested in deriving an equation of motion for the single-particle density matrix $\rho_1(a,b) =: \langle a|\hat{\rho}|b\rangle$. However, this equation is coupled to the two-particle density matrix $\rho_2(a,b;c,d)$, and so on. This coupled system of equations forms a BBGKY hierarchy analogous to a classical physics situation [16], with the addition of a damping part in the initial N-particle equation. Specifically, for $\rho_1(a;b)$ this yields the equation of motion

$$\begin{aligned}N\frac{\partial\rho_1(a;b)}{\partial t} &= +\frac{i}{\hbar}\mathrm{Tr}\{[\hat{\mathcal{H}},\hat{\Psi}^\dagger(b)\hat{\Psi}(a)]\hat{\varrho}\} \\ &+\frac{i}{\hbar}\mathrm{Tr}\{[\hat{\mathcal{V}},\hat{\Psi}^\dagger(b)\hat{\Psi}(a)]\hat{\varrho}\} \\ &+\mathrm{Tr}\{\hat{\Psi}^\dagger(b)\hat{\Psi}(a)\mathcal{L}\hat{\varrho}\}.\end{aligned} \quad (21)$$

In the first two terms on the right-hand side of this expression, we have separated the single-particle contributions from those originating from two-body interactions. The single-particle contribution to Eq. (21) is readily reexpressed as

$$\frac{i}{\hbar}\mathrm{Tr}\{[\hat{\mathcal{H}},\hat{\Psi}^\dagger(b)\hat{\Psi}(a)]\hat{\varrho}\} = -N\frac{i}{\hbar}\langle a|[\hat{H},\hat{\rho}_1]|b\rangle, \tag{22}$$

where $\hat{\rho}_1$ denotes the single-particle density operator. Here, $\hat{H}$ is the single-particle Hamiltonian and includes the coupling to cooling and trapping fields, atom optical elements, etc. However, it does not include the contact term, which is a two-body interaction included in the second term on the right-hand side of Eq. (21). This term requires some care in its evaluation, since as seen from Eq. (16), $\hat{\mathcal{V}}$ still contains self-interaction terms. These terms, which are infinite, must be identified and eliminated. This yields finally

$$\frac{i}{\hbar}\mathrm{Tr}\{[\hat{\mathcal{V}},\hat{\Psi}^\dagger(b)\hat{\Psi}(a)]\hat{\varrho}\} = -N(N-1)\frac{i}{\hbar}\langle a|\mathrm{Tr}_2\{[\hat{V},\hat{\rho}_2]\}|b\rangle, \tag{23}$$

where $\hat{V}$ is the sum of the dipole-dipole and contact interactions and $\hat{\rho}_2$ is the two-particle density matrix. The contribution of the Liouvillian $\hat{\mathcal{L}}\hat{\varrho}$ to Eq. (21) is best evaluated by expressing it in Fourier space as

$$\mathcal{L}\hat{\varrho} = -\frac{3\gamma_0}{4}\oint\frac{d\Omega(k)}{4\pi}[\hat{\mathcal{S}}^+(k)\hat{\mathcal{S}}^-(k)\hat{\varrho} + \hat{\varrho}\hat{\mathcal{S}}^+(k)\hat{\mathcal{S}}^-(k) - 2\hat{\mathcal{S}}^-(k)\hat{\varrho}\hat{\mathcal{S}}^+(k)], \tag{24}$$

where [see also Eq. (10)]

$$\hat{\mathcal{S}}(k) = \int d\{i\}\langle 1|\hat{\sigma}^\pm(k)|2\rangle\hat{\Psi}^\dagger(1)\hat{\Psi}(2), \tag{25}$$

with

$$\hat{\sigma}^\pm(k) = \sqrt{1-[e(k)\cdot e(d_{12})]^2}\int dr\hat{\sigma}^\pm(r)e^{\pm ik\cdot r}. \tag{26}$$

Separating the one- and two-particle contributions gives then

$$\mathrm{Tr}\{\hat{\Psi}^\dagger(b)\hat{\Psi}(a)\mathcal{L}\hat{\varrho}\} = -N\left\langle a\left|\left\{\frac{3\gamma_0}{4}\oint\frac{d\Omega(k)}{4\pi}\left[\hat{\sigma}^+(k)\hat{\sigma}^-(k)\hat{\rho}_1 + \hat{\rho}_1\hat{\sigma}^+(k)\hat{\sigma}^-(k) - 2\hat{\sigma}^-(k)\hat{\rho}_1\hat{\sigma}^+(k)\right] + (N-1)\frac{i}{\hbar}\mathrm{Tr}[\hat{V}_c,\hat{\rho}_2]\right\}\right|b\right\rangle, \tag{27}$$

where $\hat{V}_c$ is *not* to be taken as a symmetrized matrix element.

Surprisingly perhaps, the two-body effects of $\hat{\mathcal{L}}$ take the form of a Hamiltonian contribution, but with an *imaginary* potential

$$\hat{V}_c = \frac{i\hbar\gamma_0}{2}\left\{j_0(k_0|\hat{r}_{12}|) - \left(\frac{1}{2} - \frac{3[e(d_{12})\cdot e(r_{12})]^2}{2}\right)\times j_2(k_0|\hat{r}_{12}|)\right\}\{\hat{\sigma}^-\otimes\hat{\sigma}^+ - \hat{\sigma}^+\otimes\hat{\sigma}^-\}. \tag{28}$$

This Hermitian term describes excitation and decay processes which are not locally confined, and its physical origin lies in the fact that a particle that decays at x need not reappear in its lower electronic level at that same location. A similar term appears in the Heisenberg picture approach of Zhang *et al.* [8]

V. HARTREE-FOCK APPROXIMATION

The BBGKY hierarchy can be self-consistently truncated by different schemes of various degrees of sophistication, and whose appropriateness depends considerably on the physics involved. Here, we use the simplest such method, the Hartree-Fock approximation: We truncate the BBGKY hierarchy after the single-particle density matrix while keeping the influence of the particle statistics by introducing the ansatz

$$\rho_2(a,b;c,d) = \rho_1(a;c)\rho_1(b;d) - \eta\rho_1(a;d)\rho_1(b;c) + \Delta\rho_2(a,b;c,d), \tag{29}$$

where $\eta = \mp 1$ for bosons and fermions, respectively. It is assumed that $\Delta\rho_2$ remains negligible during the time evolution. Equation (29) also includes the Hartree approximation, by setting $\eta = 0$. Two-atom density operators appear in Eqs. (23) and (27). With the Hartree-Fock ansatz, the right-hand side of Eq. (23) becomes

$$-\left(\frac{i}{2\hbar}\right)N(N-1)[\{a:1|\hat{V}|2:3\}\rho_2(2,3;b,1) - \rho_2(a,3;1,2)\{1:2|\hat{V}|b:3\}]$$
$$= -\left(\frac{i}{\hbar}\right)N(N-1)\{\langle a:1|\hat{V}|2:3\rangle[\rho_1(2;b)\rho_1(3;1) - \eta\rho_1(3;b)\rho_1(2;1)] - [\rho_1(a;1)\rho_1(3;2) - \eta\rho_1(a;2)\rho_1(3;1)]\langle 1:2|\hat{V}|b:3\rangle\}, \tag{30}$$

where we have introduced the symmetrized matrix element $\{a:1|\hat{V}|2:3\} = \langle a:1|\hat{V}|2:3\rangle - \eta\langle a:1|\hat{V}|3:2\rangle$. The corresponding term in Eq. (27) may be expressed as

$$-\left(\frac{i}{\hbar}\right)N(N-1)[\langle a:1|\hat{V}_c|2:3\rangle\rho_2(2,3;b,1) - \rho_2(a,3;1,2)\langle 1:2|\hat{V}_c|b:3\rangle]$$
$$= -\left(\frac{i}{\hbar}\right)N(N-1)\{\langle a:1|\hat{V}_c|2:3\rangle\,[\rho_1(2;b)\rho_1(3;1) - \eta\rho_1(2;1)\rho_1(3;b)]$$
$$-[\rho_1(a;1)\rho_1(3;2) - \eta\rho_1(a;2)\rho_1(3;1)]\,\langle 1:2|\hat{V}_c|b:3\rangle\}. \tag{31}$$

Regrouping all terms yields the effective single-atom Hartree-Fock master equation of nonlinear atom optics

$$\frac{\partial\rho(a;b)}{\partial t} = -\frac{i}{\hbar}\langle a|[\hat{H},\hat{\rho}_1]|b\rangle$$
$$-\left(\frac{i}{\hbar}\right)(N-1)\int d\{i\}\{\langle a:1|(\hat{V}+\hat{V}_c)|2:3\rangle\,[\rho(2;b)\rho(3;1) - \eta\rho(3;b)\rho(2;1)]$$
$$-[\rho(a;1)\rho(3;2) - \eta\rho(a;2)\rho(3;1)]\,\langle 1:2|(\hat{V}+\hat{V}_c/2)|b:3\rangle\}$$
$$-\frac{3\gamma_0}{4}\left\langle a\left|\oint\frac{d\Omega(k)}{4\pi}\left[\hat{\sigma}^+(k)\hat{\sigma}^-(k)\hat{\rho}_1 + \hat{\rho}_1\hat{\sigma}^+(k)\hat{\sigma}^-(k) - 2\hat{\sigma}^-(k)\hat{\rho}_1\hat{\sigma}^+(k)\right]\right|b\right\rangle, \tag{32}$$

where we have changed the notation from ρ_1 to ρ since no ambiguity is possible from now on. This equation is the central result of this paper: It is the basis for studying atom optics in the presence of a two-body dipole-dipole interaction and of spontaneous emission.

VI. COHERENT REGIME

In the remainder of this paper we isolate the coherent part of the master equation (32), which entails neglecting spontaneous emission and the imaginary potential V_c. Neglecting both of these terms is consistent since they both have the same origin and do not conserve $\mathrm{Tr}(\rho^2)$, that is, the purity of the state, in contrast to the dipole-dipole potential. In the coherent regime, which neglects dissipative processes, we are then left with the single-particle Hamiltonian H and the two-body potential V, which includes both the dipole-dipole and the contact terms. In that case, and for bosonic atoms, the master equation (32) is equivalent to the nonlinear Schrödinger equation

$$i\hbar\frac{\partial\phi(\ell)}{\partial t} = \int d2\langle\ell|\hat{H}|2\rangle\phi(2)$$
$$+(N-1)\int d1d2d3\langle\ell,1|\hat{V}|2,3\rangle$$
$$\times\phi^\star(1)\phi(2)\phi(3), \tag{33}$$

with the identification $\rho(a;b) = [\phi(a)]^\star\phi(b)$. This equation is equivalent to that previously obtained in the Hartree approximation which is appropriate for bosons [7].

We now specialize to the case of a system of two-level atoms with lower electronic level $|g\rangle$ and upper electronic level $|e\rangle$, which is interacting with a standing-wave, monochromatic classical laser field of frequency ω and wave number q. The single-particle Hamiltonian for this system is (see, e.g., [17])

$$\hat{H} = \frac{\hat{p}^2}{2M} - \hbar\delta\hat{\sigma}_3 + \hbar\mathcal{R}\cos(q\hat{r})\left(\hat{\sigma}^+ + \hat{\sigma}^-\right), \tag{34}$$

where M is the atomic mass, $\delta = \omega - \omega_0$ is the detuning between the laser frequency and the electronic transition frequency ω_0, and $\mathcal{R}$ is the field Rabi frequency.

In addition, we assume that the two-body interaction may be adequately described by a contact potential of the form

$$\hat{V} = (V_0/2q)\delta(\hat{r}_{12})\left(\sigma^+\otimes\hat{\sigma}^- + \sigma^-\otimes\hat{\sigma}^+\right). \tag{35}$$

The coefficient $V_0/2q$ in Eq. (35) then reflects the fact that the range of the dipole-dipole interaction is of the order of an optical wavelength $\lambda = 2\pi/q$, and V_0 is of the order of $\hbar\gamma_0$.

Though not essential, this approximation, which replaces the full potential by its first moment, provides considerable physical insight into the many-body atomic bound states discussed in Secs. VII and VIII. It is important to realize that the approximation (35) is not valid in general, but should be quite good for ultracold atoms. Specifically, the problem is characterized by three length scales. The first one is determined by the contact potential appearing in the Power-Zienau Hamiltonian and is of the order of the Bohr radius a_0. The second one, of the order of an optical wavelength, is given by the range of the dipole-dipole interaction. The third one is the thermal de Broglie wavelength λ_d of the atoms. The approximation of the dipole-dipole potential by a contact interaction is expected to be valid provided that $\lambda_d \gg \lambda$, i.e., for temperatures well below the recoil limit. Note also that at the moderate atomic densities we are considering, we are justified in ignoring the effects of the "true"

contact potential (7).

In coordinate representation, we have $\phi(\ell) \to \phi_\mu(x)$, where $\mu = e$ or g labels the electronic state. Combining Eqs. (34) and (35) with Eq. (33) then yields the pair of nonlinear Schrödinger equations for the effective single-particle states $\phi_{e,g}(x)$ [7],

$$\begin{aligned} i\hbar\frac{\partial\phi_e(x)}{\partial t} &= -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}\phi_e(x) - \frac{1}{2}\hbar\delta\phi_e(x) \\ &\quad +\hbar\mathcal{R}\cos(qx)\phi_g(x) \\ &\quad +(N-1)(V_0/q)|\phi_g(x)|^2\phi_e(x), \\ i\hbar\frac{\partial\phi_g(x)}{\partial t} &= -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}\phi_g(x) + \frac{1}{2}\hbar\delta\phi_g(x) \\ &\quad +\hbar\mathcal{R}\cos(qx)\phi_e(x) \\ &\quad +(N-1)(V_0/q)|\phi_e(x)|^2\phi_g(x). \end{aligned} \tag{36}$$

These equations show that, from the perspective of a single atom, the $N-1$ other bosonic atoms effectively act as a nonlinear medium. This is analogous to the situation in conventional nonlinear optics, where the presence of a medium can lead to an effective nonlinear behavior of the light field when the medium dynamics is traced over. In the present case, the ultimate origin of the nonlinear behavior of the atoms is their interaction with the vacuum field. Hence the reversal of the roles of light and matter between the situations of conventional and atom optics is carried over into the nonlinear regime. We note, however, that the dipole-dipole interaction leads only to a modulation of the upper state wave function due to the presence of a lower state population and vice versa (cross-phase modulation.) This is in contrast to a third-order optical nonlinearity, which generally also includes a term corresponding to the self-interaction of the invidual components of the wave function (self-phase modulation.)

As pointed out in Ref. [7], the dynamical effects described by Eqs. (36) include matter-wave phase conjugation, soliton solutions, and nonlinear focusing effects. This work also showed how nonlinear effects modify the usual Pendellösung of atomic Bragg scattering. In the next two sections, we investigate numerically the generation of Thirring solitons and gap solitons. A different class of soliton solutions has also been predicted in Ref. [8] for atoms diffracted off resonance by a traveling wave field.

VII. THIRRING SOLITONS

First we consider atomic Thirring solitons, which occur for an ensemble of ultracold atoms interacting with a resonant standing-wave light field. Specifically, we assume that the effective single-particle states $\phi_g(x,t)$ and $\phi_e(x,t)$ can be expressed as

$$\phi_g(x,t) = G(x,t)\exp(iqx/2)\exp(-i\omega_r t/4), \tag{37}$$

$$\phi_e(x,t) = E(x,t)\exp(-iqx/2)\exp(-i\omega_r t/4), \tag{38}$$

where the envelopes $G(x,t)$ and $E(x,t)$ are assumed to vary slowly over an optical wavelength, $q^2|G(x,t)| \gg q|\partial_x G(x,t)| \gg |\partial_x^2 G(x,t)|$, and $\omega_r = \hbar q^2/2m$ is the recoil frequency. Equation (37) describes a quasi plane wave corresponding to an electrotranslational state with the atom in its ground electronic state and momentum $\hbar q/2$, while Eq. (38) corresponds to an atom in its excited electronic state and momentum $-\hbar q/2$. We may confine our attention to these two states in the limit $\omega_r/\mathcal{R} \gg 1$. Substituting Eqs. (37) and (38) into Eq. (36) and dropping nonslowly varying terms yields the pair of equations

$$\begin{aligned} i\hbar\frac{\partial G(x,t)}{\partial t} &= -\frac{i\hbar^2 q}{2M}\frac{\partial G(x,t)}{\partial x} + \frac{\hbar\mathcal{R}}{2}E(x,t) \\ &\quad +(N-1)(V_0/q)|E(x,t)|^2 G(x,t), \\ i\hbar\frac{\partial E(x,t)}{\partial t} &= +\frac{i\hbar^2 q}{2M}\frac{\partial E(x,t)}{\partial x} + \frac{\hbar\mathcal{R}}{2}G(x,t) \\ &\quad +(N-1)(V_0/q)|G(x,t)|^2 E(x,t). \end{aligned} \tag{39}$$

In the plane-wave limit where G and E are independent of x, these equations describe the velocity-tuned (Doppleron) resonance between the two electrotranslational states.

The pair of envelope equations (39) can be converted to the canonical form of the classical massive Thirring model (MTM) of field theory by making the substitutions $qx \to X$, $\omega_r t \to T$, $\mathcal{R}/2\omega_r \to m$, $(N-1)V_0/2\hbar\omega_r \to -g$, $E \to \chi_1$, and $G \to \chi_2$ [18]. The MTM is an integrable classical field theory with soliton solutions. In particular, it possesses a two-parameter family of fundamental soliton solutions whose parameters control the velocity and charge of the soliton. The same soliton solutions apply to the present problem, where the velocity corresponds to a transverse velocity and the charge is fixed by the normalization of the atomic wave function. Then, the atomic Thirring soliton takes the form

$$\begin{aligned} G_s(x,t) &= q^{1/2}\left(\frac{\hbar\mathcal{R}/2}{(N-1)|V_0|}\right)^{1/2}\sin Q\left(\frac{1-\beta}{1+\beta}\right)^{1/4} \\ &\quad \times\operatorname{sech}\left[\frac{\mathcal{R}\sin Q}{2\omega_r}\gamma(qx-\beta\omega_r t) \pm iQ/2\right] \\ &\quad \times\exp\left[\pm i\left\{\frac{\mathcal{R}\cos Q}{2\omega_r}\gamma(\beta qx-\omega_r t)+\sigma_0\right\}\right], \\ E_s(x,t) &= \pm q^{1/2}\left(\frac{\hbar\mathcal{R}/2}{(N-1)|V_0|}\right)^{1/2}\sin Q\left(\frac{1+\beta}{1-\beta}\right)^{1/4} \\ &\quad \times\operatorname{sech}\left[\frac{\mathcal{R}\sin Q}{2\omega_r}\gamma(qx-\beta\omega_r t) \mp iQ/2\right] \\ &\quad \times\exp\left[\pm i\left\{\frac{\mathcal{R}\cos Q}{2\omega_r}\gamma(\beta qx-\omega_r t)+\sigma_0\right\}\right], \end{aligned} \tag{40}$$

where $Q = (N-1)|V_0|/4\hbar\omega_r$, $\beta = 2Mv/\hbar q$ is the atomic momentum in units of $\hbar q$, v being the soliton velocity, and $\gamma = (1-\beta^2)^{-1/2}$. The parameter β is constrained between -1 and 1, and the Thirring soliton velocity is therefore constrained between $\pm\hbar q/2M$, that is, less than half the recoil limit. Using the solution Eq. (40), we may also introduce the soliton width x_0 as $x_0 = 2\omega_r/\gamma\mathcal{R}q\sin Q$.

This width is broad compared with an optical wavelength if $\omega_r/\mathcal{R} \gg \gamma$. Since $\gamma \geq 1$, the conditions on the soliton width are in keeping with our original assumption based on the ansatz in Eqs. (37) and (38).

An important feature of the Thirring soliton (40) is that the upper (lower) sign corresponds to an attractive (repulsive) potential. Thus Thirring solitons are possible irrespective of the sign of the two-body interaction. The atomic Thirring soliton is a coherent superposition of the two electrotranslational states participating in the Doppleron resonance. This combination has the property that it does not distort under the combined effects of the diffracting standing-wave light field and of the nonlinearity due to many-body effects. In contrast, without the nonlinearity the standing wave acts as a dispersive element which causes any input of finite spatial extent to broaden and also generally leads to diffraction into other scattering orders. The atomic Thirring soliton is immune to both of these processes.

The key property of atomic solitons is that they represent many-atom bound states which are immune to wave-packet spreading. To verify the nonspreading nature of the approximate Thirring solitons we have performed a number of numerical simulations of the original Eqs. (36) using Eqs. (40) as initial conditions. The numerical simulations employed the split-step method using a fast Fourier transform applied to Eqs. (36). (This numerical method is well known in the field of nonlinear optics.) We have found that the atomic Thirring solitons propagate over long times without spreading for a large range of parameters, and we have verified the limited range of validity, $\omega_r/\mathcal{R} \gg 1$. Figure 1 shows an example of our numerical results where we have used parameters $(N-1)V_0 = -1.6\hbar\omega_r$ (attractive interaction), $\omega_r/\mathcal{R} = 1.1$, and $\beta = 0.25$. For comparison, in Fig. 2 we have neglected many-body effects, $V_0 = 0$, and wave-packet spreading is evident (the packet travels at an angle due to the finite velocity). The solitonic

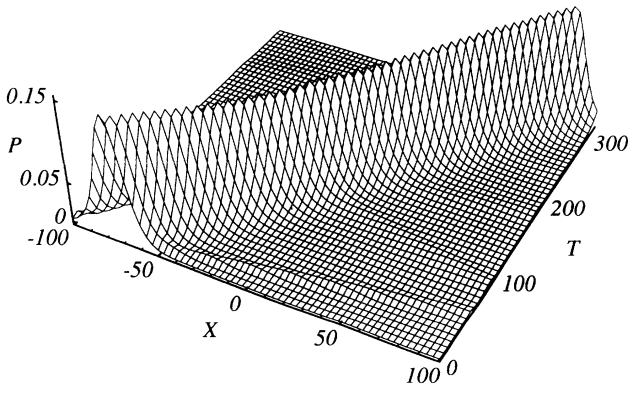

FIG. 1. A traveling solitary wave solution of Eq. (36). A Thirring soliton with the parameters $(N-1)V_0 = -0.9\hbar\omega_r$, $\beta = 0.25\hbar\omega_r/q$, $\mathcal{R} = 0.9\hbar\omega_r$ was used as initial condition. In the dynamics $(N-1)V_0$ was set to $(N-1)V_0 = -1.6\hbar\omega_r$. Plotted is P, the probability density to find a particle at x independent of its electronic state, averaged over one wavelength, as a function of the dimensionless coordinates $X = qx$, $T = \omega_r t$.

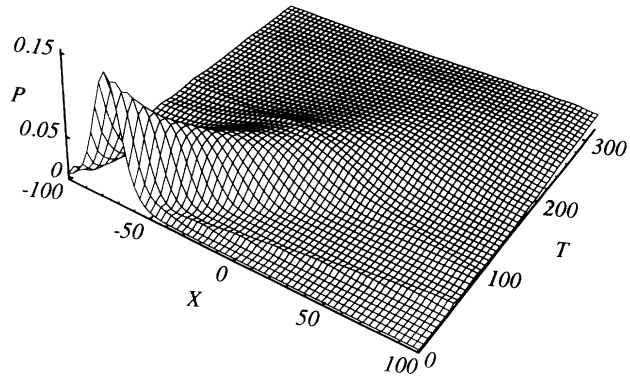

FIG. 2. Same initial condition as in Fig. 1 but $V_0 = 0.0$ in Eq. (36). The dispersion destroys the inital soliton shape very fast.

nature of the solution is demonstrated in Fig. 3 where two identical solitons with opposite velocities $\beta = \pm 0.25$ are collided: In keeping with their solitonic nature the wave packets emerge relatively unscathed from the collision. (Radiation components are also present after the collision, showing that these solutions are more properly referred to as solitary waves.) However, the approximate soliton solution (40) predicts soliton propagation for $(N-1)V_0 = -0.9\hbar\omega_r$, in apparent contradiction with the numerics. The result in Fig. 1 is actually a testimony to the robustness of the soliton solution even beyond its apparent regime of validity since we have used $\omega_r/\mathcal{R} = 1.1$ in the simulation. The simulation therefore shows that soliton solutions appear for a broader range of parameters, but with renormalized soliton parameters. Similar results were obtained for a repulsive two-body interaction.

VIII. GAP SOLITONS

Atomic Thirring solitons present two major restrictions, namely, that they occur on resonance and have low transverse velocities $|v| < \hbar q/2M$. While Thirring

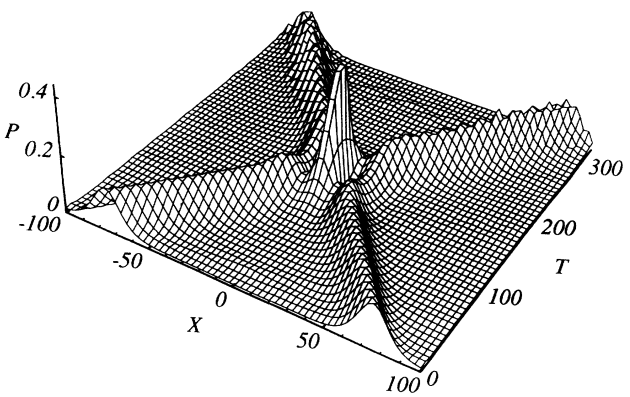

FIG. 3. With the same settings as in Fig. 1, two counterpropagating Thirring solitons were used as initial condition for Eq. (36). The solitary wave character is clearly shown by the almost unperturbed shape of the single wave packets.

solitons may still be relevant in cavity QED geometries where spontaneous emission is inhibited, avoiding the detrimental effects of spontaneous emission generally requires working off resonance. For the present problem of atomic motion in a standing-wave field, atomic gap solitons are the appropriate generalization which may also be used for off-resonance operation. In addition, gap solitons allow for a broader range of velocities. In this section, we discuss atomic gap solitons and numerically illustrate them without going into many of the mathematical details, since they follow from a rather straightforward generalization of the theory developed in great detail by Sipe and Windful and de Sterke and Sipe in the context of nonlinear optical propagation in periodic structures [19–21]. A systematic derivation of atomic gap solitons starting from Eqs. (36), using the Floquet-Bloch theorem and a multiple scales analysis, can be transcribed in a one-to-one manner from those papers.

To proceed we first consider the effective single-particle Eqs. (36) without the nonlinear terms proportional to V_0. It is well known that these linear equations have eigensolutions of the Floquet-Bloch form

$$\phi_\mu(x,t) = \frac{1}{\sqrt{L}} e^{i(\kappa x - \Omega_\mu t)} \mathbf{u}_\mu(x), \tag{41}$$

where $\phi_\mu(x,t)$ is a 2-spinor with components $\phi_{e,\mu}(x,t)$ and $\phi_{g,\mu}(x,t)$, and $\mathbf{u}_\mu(x)$ is a 2-spinor with components $u_{e,\mu}(x)$ and $u_{g,\mu}(x)$, κ is the quasimomentum, restricted to the first Brillouin zone, the eigenstates are labeled by the index $\mu = \{n,\kappa\}$, and $E_n(\kappa) = \hbar\Omega_\mu$ is the corresponding eigenenergy. Previous studies of the near-resonant Kapitza-Dirac effect have discussed how the dispersion relation $E_n(\kappa)$ can be interpreted in terms of energy bands, n being the band index. An example of band structure is shown in Fig. 4. We assume periodic boundary conditions with period L, so that strictly speaking, the quasimomentum κ takes on discrete values only, but for all practical purposes it can be treated as a continuous variable. The eigenfunctions $\mathbf{u}_\mu(x)$ are scaled to obey the orthogonality condition

$$\frac{1}{L}\int_0^L dx \mathbf{u}_\mu^\dagger(x)\cdot\mathbf{u}_{\mu'}(x) e^{i(\kappa'-\kappa)x} = \delta_{\mu,\mu'}. \tag{42}$$

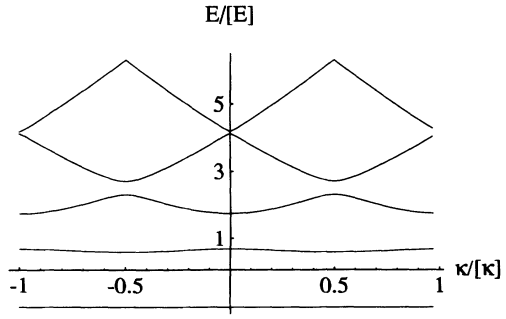

FIG. 4. The first five energy bands of the single-particle Hamiltonian Eq. (34) for $\mathcal{R} = 2.1\hbar\omega_r$ and $\delta = 0.0$. The energy is plotted in units of $\hbar\omega_r$. The quasimomentum κ is plotted in units of $\hbar q$, and the energy is in units of the recoil energy $\hbar^2 q^2/2M$.

To each point on the band structure we can associate a group velocity $v_n(\kappa) = (\partial\Omega_\mu/\partial\kappa)$ as well as an effective mass $m_n(\kappa) = \hbar(\partial^2\Omega_\mu/\partial\kappa^2)^{-1}$ which may be either positive or negative. Consider then a wave packet consisting of a slow modulation of the μth eigenstate,

$$\psi(x,t) = A_\mu(x,t)\phi_\mu(x,t), \tag{43}$$

the envelope $A_\mu(x,t)$ varies slowly on the length scale of q^{-1} as well as on the temporal scale of Ω_μ^{-1}. Within the effective mass approximation, the equation of motion for $A_\mu(x,t)$ is

$$i\hbar\left(\frac{\partial}{\partial t} + v_\mu\frac{\partial}{\partial x}\right)A_\mu = -\frac{\hbar^2}{2m_\mu}\frac{\partial^2 A_\mu}{\partial x^2}. \tag{44}$$

The normalization of the atomic wave function requires that the envelope $A_\mu(t)$ be likewise normalized to unity. It is important to realize that despite the scalar nature of Eq. (44), our description still retains the two-state nature of the atomic system, as evident from Eq. (43).

We now need to include the nonlinear terms arising from nonlinear effects. Our basic assumption is that these terms can be treated perturbatively and do not significantly modify the underlying band structure. (For a more precise discussion of these notions, see Ref. [20].) The many-body effects then lead to a nonlinear modification of Eq. (44). From Eq. (36), the effects of the nonlinearity may be expressed in matrix form as

$$\hat{V}\phi = (N-1)(V_0/q)\begin{pmatrix} |\phi_g|^2 & 0 \\ 0 & |\phi_e|^2 \end{pmatrix}\phi. \tag{45}$$

Consider first the case where $A_\mu(x,t)$ is independent of x. Substituting the ansatz (43) into Eq. (45) and taking the dot product with $\exp[-i(\kappa x - \Omega_\mu t)]\mathbf{u}_\mu^\dagger(x)$ to obtain the projection onto the envelope A_μ then yields the nonlinear term

$$e^{-i(\kappa x-\Omega_\mu t)}\mathbf{u}_\mu^\dagger\hat{V}\phi \to (N-1)(V_0/q)\Gamma_\mu|A_\mu|^2 A_\mu, \tag{46}$$

where the dimensionless parameter Γ_μ is

$$\Gamma_\mu = \frac{1}{L}\int_0^L dx|u_{e,\mu}(x)|^2|u_{g,\mu}(x)|^2, \tag{47}$$

which is independent of the quantization length L. It is important to note at this point that the form (46) is retained even when A_μ depends on x. The justification for this fact rests on the method of multiple scales, where the envelope A_μ formally varies with a different spatial variable (the slow variable) than the modulated eigenfunction (the fast variable).

Combining the nonlinear term (46) with Eq. (44) yields the nonlinear Schrödinger equation

$$i\hbar\left(\frac{\partial}{\partial t} + v_\mu\frac{\partial}{\partial x}\right)A_\mu = -\frac{\hbar^2}{2m_\mu}\frac{\partial^2 A_\mu}{\partial x^2} + (N-1)(V_0/q)\Gamma_\mu|A_\mu|^2 A_\mu. \tag{48}$$

Atomic gap solitons arise from the balance between the linear dispersion due to the standing-wave light field [the kinetic energy term in Eq. (48)] and the potential provided by the many-body effects [the nonlinear term in Eq. (48)]. For the case $\mathrm{sgn}(m_\mu V_0) = -1$, the nonlinear Schrödinger equation has a fundamental bright soliton solution, the atomic gap soliton, of the form

$$A_\mu(x,t) = \frac{1}{\sqrt{2w_\mu}}\mathrm{sech}\left[(x - x_0 - v_\mu t)/w_\mu\right] e^{-i\epsilon_\mu t/\hbar}, \quad (49)$$

where the soliton width w_μ is given by

$$w_\mu = \frac{4}{q\Gamma_\mu}\left|\frac{M}{m_\mu}\right|\left|\frac{\hbar\omega_r}{(N-1)V_0}\right| \quad (50)$$

and

$$\epsilon_\mu = -\frac{\hbar^2}{2m_\mu w_\mu^2}. \quad (51)$$

The total energy of the atomic gap soliton is $W_\mu = E_\mu + \epsilon_\mu$, with E_μ being the energy derived from the band structure.

Equation (48) also admits dark atomic gap solitons when $\mathrm{sgn}(m_\mu V_0) = 1$. In this case the finite quantization length L is essential to normalize the wave function. In the limit that $q^{-1} \ll w_\mu \ll L$, the basic dark soliton may be approximated by Eq. (49) with sech replaced by tanh.

We have performed a broad range of numerical simulations of Eqs. (36) combined with Eq. (43) as initial condition. The parameters m_μ, v_μ, and Γ_μ for the atomic gap soliton were obtained from band structure calculations. The soliton (or at least solitary wave) nature of the approximate envelope solutions was established by their invariance under propagation and their robustness against collisions. The numerical simulations yielded plots analogous to Fig. 1 for atomic Thirring solitons.

Rather than dwelling on the numerical validation of the atomic gap solitons, we conclude by demonstrating numerically how they can be contained axially in a focused laser beam. Realizable standing-wave laser fields have a beam profile of the form $\cos(qx)f(x/x_R)$ along the laser axis, where $x_R = qw_0^2$ is the Rayleigh range, w_0 is the transverse spot size at the beam waist $x = 0$, and $f(0) = 1$. For the purposes of illustration, we assume $f(x/x_R) = 1-(x/x_R)^2$. This is a good approximation for the situation that we are interested in, where the Rayleigh range is much greater than the predicted size of the atomic gap soliton, $x_R \gg x_\mu$. The question we wish to address is whether the slow axial variation of the laser field destabilizes the gap soliton, causing it to fall out of the laser focus, or whether it leads to axial confinement.

We proceed by substituting $\cos(qx)$ by $[1-(x/x_R)^2]\cos(qx)$ in Eqs. (36). This introduces in each equation a new term $-\hbar\mathcal{R}(x/x_R)^2\cos(qx)\phi_{e,g}$, which we treat as a perturbation. The effect of this linear perturbation on the gap soliton envelope A_μ may be found in a manner analogous to that of the nonlinear terms: The axial field variation adds a harmonic potential $m_\mu\omega_\mu^2 x^2/2$ to Eq. (48), where

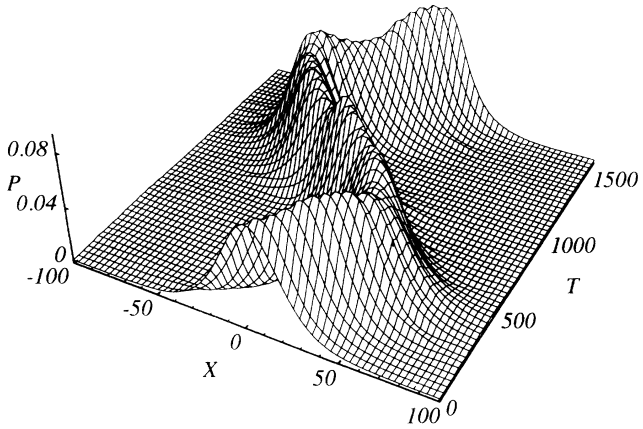

FIG. 5. A gap soliton oscillating in an inhomogeneous laser beam. As initial condition for Eq. (36) we chose a traveling soliton solution (49) of Eq. (48) with the initial velocity $c = 0.05$ in dimensionless units $X = qx$ and $T = \omega_r t$. The initial width and the nonlinearity were adjusted to allow a soliton solution in the unperturbed case. Plotted is the probability averaged over one wavelength as a function of the dimensionless coordinates $X = qx$, $T = \omega_r t$. The carrier solution was the Bloch-wave function in the first doppleron resonance at the upper band gap $-\phi_{0,1}-$ at a detuning $\delta/\omega_r = 1.5$ and a Rabi frequency $\mathcal{R}/\omega_r = 1.7$.

$$\omega_\mu^2 = -\frac{2\hbar\mathcal{R}\alpha_\mu}{m_\mu x_R^2} \quad (52)$$

and

$$\alpha_\mu = \frac{1}{L}\int_0^L dx \mathbf{u}_\mu^\dagger(x)\cdot\sigma_1\cdot\mathbf{u}_\mu(x)\cos(qx). \quad (53)$$

From Eq. (52) we see that for $\mathrm{sgn}(m_\mu\alpha_\mu) = -1$, the axial variation of the laser field provides a confining potential, while the gap soliton will fall out of the laser focus in the other case. Figure 5 shows a numerical simulation which verifies that gap solitons can be axially confined, thereby undergoing oscillations around the laser focus while maintaining their basic sech profile.

IX. SUMMARY AND CONCLUSION

In this paper, we have presented a formal development of the theory of nonlinear atom optics. Starting from an ensemble of N atoms interacting with the vacuum electromagnetic field as well as an arbitrary number of classical laser fields required, e.g., for cooling, trapping, and/or atom optics, we derived a Fock state master equation by adiabatically eliminating the vacuum modes. An effective single-atom master equation was then obtained by constructing a BBGKY hierarchy and introducing a Hartree-Fock ansatz. In future work, we will apply this master equation to the study of a number of problems in atom optics. For instance, we demonstrated in the second part of the paper how nonlinear atom optics leads to the prediction of atomic solitons, provided that only the coherent part of the dynamics is retained. The nonlin-

ear master equation will permit us to assess the effects of spontaneous emission on these solitons. In addition, a number of other problems can be addressed within this formalism. We have mentioned that the effective nonlinearity provided by the dipole-dipole interaction between ground and excited levels may lead to intriguing effects such as atomic wave mixing and phase conjugation of matter waves. Again, the understanding of the role of spontaneous emission is necessary in order to assess the practicality of these ideas. In addition, the extension of this work to multilevel atoms will permit us to address a number of further problems: For instance, sufficiently high atomic densities in optical lattices could lead to spontaneous pattern formation and the creation of other stable long-range structures, such as possibly superlattices. Even more intriguing perhaps, the combination of nonlinearities with dissipation, in the form of spontaneous emission, and of a "pump" mechanism suggests the possibility of a "coherent atomic beam generator," which could loosely be considered as the atom optics equivalent of a laser. These, and other problems in nonlinear atom optics, will be the subject of future investigations.

Turning now to the more formal aspects of our theory, it is important to emphasize that the Hartree-Fock approximation is not without its difficulties and shortcomings. While linear master equations of the Lindblad type [12], usually encountered in quantum and atom optics, have a built-in conversation of norm, Hermiticity, and positivity, only the first two of these properties are obvious for the time-dependent Hartree-Fock approximation. Hence improvements past this ansatz must be attempted. The obvious direction is to generalize the ansatz (18) to a full Fock-space density operator that is not diagonal and pure in number space.

Also, due to its intrinsic nonlinear character, it does not appear that the effective master equation is amenable to numerical solutions by Monte Carlo wave function simulations. Yet, the theory that we developed was of course linear at the onset. Hence one intriguing line of investigation would consist in attempting to first cast the theory in the framework of the Monte Carlo wave functions formalism, and then perform a Hartree-Fock ansatz. It is not at all obvious that such an approach will give the same result as the present one, but their comparison might help shed new light on the Hartree-Fock approximation.

ACKNOWLEDGMENTS

This work is funded by the U.S. Office of Naval Research Contract No. N00014-91-J1205, by the National Science Foundation Grant No. PHY92-13762, and by the Joint Services Optics Program. Discussions with P. Jessen and M. Wilkens are gratefully acknowledged.

[1] P. Verkerk, B. Lounis, C. Salomon, C. Cohen-Tannoudji, J.-Y. Courtois, and G. Grynberg, Phys. Rev. Lett. **68**, 3861 (1992).
[2] P. S. Jessen, C. Gerz, P. D. Lett, W. D. Phillips, S. L. Rolston, R. J. C. Spreeuw, and C. I. Westbrook, Phys. Rev. Lett. **69**, 49 (1992).
[3] A. Hemmrich and T. W. Hänsch, Phys. Rev. Lett. **70**, 410 (1993).
[4] G. Grynberg, B. Lounis, P. Verkerk, J.-Y. Courtois, and C. Salomon, Phys. Rev. Lett. **70**, 2249 (1993).
[5] Weiping Zhang, Phys. Lett. A **176**, 225 (1993).
[6] Weiping Zhang and D. F. Walls, Quantum Opt. **5**, 9 (1993).
[7] G. Lenz, P. Meystre, and E. W. Wright, Phys. Rev. Lett. **71**, 3271 (1993).
[8] W. Zhang, D. F. Walls, and B. C. Sanders, Phys. Rev. Lett. **72**, 60 (1994).
[9] M. Lewenstein and L. You, Phys. Rev. Lett. **71**, 1339 (1993).
[10] H. D. Politzer, Phys. Rev. A **43**, 6444 (1991).
[11] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, *Photons and Atoms, Introduction to Quantum Electrodynamics* (Wiley, New York, 1989).
[12] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).
[13] R. Graham and F. Haake, *Quantum Statistics in Optics and Solid-State Physics*, edited by G. Höhler, Springer Tracts in Modern Physics Vol. 66 (Springer, Berlin, 1973).
[14] G. Lenz and P. Meystre in *Quantum Optics VI*, edited by J. D. Harvey and D. F. Walls (Springer, Berlin, 1994).
[15] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).
[16] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).
[17] E. Schumacher, M. Wilkens, P. Meystre, and S. Glasgow, Appl. Phys. B **54**, 451 (1992).
[18] D. J. Kaup and A. C. Newell, Lett. Nuovo Cimento **20**, 325 (1977).
[19] J. E. Sipe and H. G. Winful, Opt. Lett. **13**, 132 (1988).
[20] C. M. de Sterke and J. E. Sipe, Phys. Rev. A **38**, 5149 (1988).
[21] C. M. de Sterke and J. E. Sipe, Phys. Rev. A **39**, 5163 (1989).