Nonlinear Atom Optics

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We study an ensemble of N bosonic atoms coupled by dipole-dipole interaction and also interacting with an electromagnetic field. Effective single-atom nonlinear Schrödinger equations are derived. The implications of these equations are discussed in the context of some standard atom optics geometries, illustrating in particular how many-body effects modify the Pendellösung of Bragg scattering. In another regime, the problem is reduced to a classical massive Thirring model, with the possibility of generating atomic Thirring solitons.

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Atomic cooling has witnessed considerable progress due to the realization that the standard recoil limit of cooling can be circumvented by velocity-selective coherent population trapping [1], and it is clear that nano-kelvin and sub-nano-kelvin temperatures are now within reach. The availability of such ultracold atoms opens up exciting new avenues of research in atomic physics and quantum optics. An obvious goal, actively pursued by several experimental groups, is to achieve Bose condensation of atoms [2]. However, there are a number of other fascinating facets to the physics of cold atoms which can best be put into perspective by mentioning just one number: The de Broglie wavelength $\lambda_{\rm dB}$ of an atom in the 100 K temperature range is of the order of a few microns, that is, it is comparable to or larger than an optical wavelength λ.

This progress provides considerable impetus for studying the optics of very cold atoms, especially when the center-of-mass motion is quantized as is the case in atom optics. Atoms interact directly via a number of mechanisms, the simplest one being the "exchange force" resulting from quantum statistics. They are also subject to "ultracold collisions," which are unusual in that the atomic de Broglie wavelength $\lambda_{\rm dB}$ can be much larger than the scale of the interatomic potential. Indeed, ultracold collision cross sections between ground state alkali atoms can be as large as the resonant absorption cross section of light $\lambda^2/2\pi$ [3,4].

In this Letter, we consider the many-body description of an ensemble of N bosonic atoms coupled by dipole-dipole interaction. The atoms also interact with an electromagnetic field, e.g., a single standing-wave laser mode acting as a diffraction grating for atoms. We apply a standard Hartree approximation to derive effective nonlinear Schrödinger equations that govern the evolution of a single atom in the ensemble. We discuss the implications of these equations in some standard atom optics geometries, illustrating in particular how many-body effects modify the Pendellösung of Bragg scattering [5], and in another limit, reducing the problem to a massive classical Thirring model [6,7], with the possibility of generating atomic Thirring solitons.

The general many-body Hamiltonian including a two-body interaction can be expressed in a standard way as

$$\begin{aligned}\hat{\mathcal{H}} &= \int d1\, d2 \langle 1|H_0|2\rangle \hat{\psi}^\dagger(1)\hat{\psi}(2) \\ &\quad + \frac{1}{2}\int d1\, d2\, d3\, d4 \langle 1,2|V|3,4\rangle \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)\hat{\psi}(4)\hat{\psi}(3) \\ &= \hat{\mathcal{H}}_0 + \hat{\mathcal{V}}. \end{aligned} \tag{1}$$

Here, H_0 is the single-particle Schrödinger Hamiltonian, and includes the atom-field dipole interaction, the electromagnetic field being either classical or quantized, and V is the two-body dipole-dipole potential due to the exchange of transverse photons. In this paper, all kets $|\ell\rangle$ give a complete description of the single atom states, i.e., they include both the center of mass and the internal quantum numbers. We use numbers to indicate dummy variables and letters to label a specific state. The state $|\ell\rangle$ is obtained by application of the creation operator $\hat{\psi}^\dagger(\ell)$ to the vacuum $|0\rangle$, where $[\hat{\psi}(\ell), \hat{\psi}^\dagger(\ell')] = \delta(\ell - \ell')$ for bosons, and the δ function should be interpreted as a product of δ functions for continuous quantum numbers and Kronecker deltas for discrete ones. A normalized N-particle state $|\psi\rangle_N$ is obtained as

$$|\psi\rangle_N = \frac{1}{\sqrt{N!}}\int d1 \cdots dN f_N(1,2,\ldots,N)\hat{\psi}^\dagger(N)\cdots\hat{\psi}^\dagger(1)|0\rangle, \tag{2}$$

where the N-body wave function $f_N(1,2,\ldots,N)$ is totally symmetric in its arguments. With Eq. (2), the matrix elements of $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{V}}$ become

$${}_N\langle\psi|\hat{\mathcal{H}}_0|\psi\rangle_N = N\int d1\cdots d(N-1)\int d\ell\, d\ell' \langle\ell'|H_0|\ell\rangle f_N^\star(1,\ldots,N-1,\ell') f_N(1,\ldots,N-1,\ell) \tag{3}$$

and

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$$
{}_N\langle\psi|\hat{\mathcal{V}}|\psi\rangle_N = \frac{N(N-1)}{2}\int d1\cdots d(N-2)\int d\ell\, d\ell' dm\, dm' \langle \ell', m'|V|\ell, m\rangle \times f_N^\star(1,\ldots,N-2,\ell',m') f_N(1,\ldots,N-2,\ell,m). \quad (4)
$$

We now perform the Hartree approximation, in which the N-body wave function $f_N(1,\ldots,N)$ is written as a product of the form $f_N(1,\ldots,N)=\prod_{\ell=1}^N \phi_N(\ell)$. The effective single-particle states $\phi_N(\ell)$ are assumed normalized, $\int \phi_N^\star(\ell)\phi_N(\ell)d\ell = 1$, and are dependent on the internal quantum numbers implicit in the label ℓ. This trial ansatz therefore generalizes previous treatments to allow for the internal degrees of freedom. In the time-dependent Hartree approximation, the equations of motion for the effective single-particle wave states are determined from the variational principle [8]

$$
\frac{\delta}{\delta\phi_N^\star(\ell)}\left[{}_N\langle\psi|i\hbar\frac{\partial}{\partial t} - H|\psi\rangle_N\right] = 0. \quad (5)
$$

With the Hartree ansatz, this readily yields the system of effective single-particle nonlinear Schrödinger equations

$$
i\hbar\frac{\partial\phi_N(\ell)}{\partial t} = \int d2\langle\ell|H_0|2\rangle\phi_N(2) + (N-1)\int d1\, d2\, d3\langle\ell,1|V|2,3\rangle\phi_N^\star(1)\phi_N(2)\phi_N(3). \quad (6)
$$

All that remains is to evaluate the various matrix elements in this equation for the explicit problem at hand. For concreteness, we consider the situation of the near-resonant Kapitza-Dirac effect, where two-level atoms with lower electronic level $|g\rangle$ and upper electronic level $|e\rangle$ are diffracted by a standing-wave monochromatic classical laser field of frequency Ω and wave number q. The kets describing the system now take the form $|\ell\rangle \to |x,\mu\rangle$, where $\mu = e$ or g, and the interaction between an atom and the field is described by the Hamiltonian (see, e.g., [9])

$$
H_0 = \frac{\hat{\mathbf{p}}^2}{2M} - \hbar\delta\left(|e\rangle\langle e| - |g\rangle\langle g|\right) + \hbar\mathcal{R}\cos(\mathbf{q}\cdot\hat{\mathbf{x}})\left(|e\rangle\langle g| + |g\rangle\langle e|\right), \quad (7)
$$

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

To incorporate the two-body interaction, we proceed by eliminating the transverse vacuum field and replacing it by a phenomenological dipole-dipole interaction, which we assume to be a contact potential of the form

$$
\hat{V} = (V_0/2q)\int dx\, dy\delta(x-y) \times \left(|x,e\rangle|y,g\rangle\langle x,g|\langle y,e| + \text{H.c.}\right). \quad (8)
$$

In this way we approach the problem by replacing the dipole-dipole potential in Eq. (6) by its first moment. The coefficient $V_0/2q$ in Eq. (8) 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 $\hbar\gamma$, where γ is the spontaneous decay rate of the upper to lower electronic state transition. The length scale of the two-body potential indicates that its δ-function approximation is valid for very cold atoms of de Broglie wavelength large compared to λ. The actual dipole-dipole potential has the same spin-flip structure, but in coordinate space it is a linear combination of spherical Bessel functions of the second kind [10].

In the coordinate representation, we have $\phi_N(\ell) \to \phi_\mu(x)$, where we have dropped the index N for clarity and $\mu = e$ or g labels the electronic state. Combining Eqs. (7) and (8) in Eq. (6) then yields the pair of nonlinear Schrödinger equations for the effective single-particle states $\phi_{e,g}(x)$,

$$
i\hbar\frac{\partial\phi_e(x)}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}\phi_e(x) - \frac{1}{2}\hbar\delta\phi_e(x) + \hbar\mathcal{R}\cos(qx)\phi_g(x) + (N-1)(V_0/q)|\phi_g(x)|^2\phi_e(x), \quad (9)
$$

the equation for ϕ_g being obtained by the substitution $e \leftrightarrow g$, $\delta \to -\delta$.

These equations form the basis of nonlinear atom optics and are the central result of this Letter. In the limit $V_0 \to 0$, they reduce to the conventional single-particle equations of atoms optics. Furthermore, they show that, from the perspective of a single atom, the $N-1$ other bosonic atom 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 origin of the nonlinear behavior of the atoms is of course the dipole-dipole interaction, whose ultimate origin is the interaction of the atoms with the transverse vacuum field. When this field is traced over, as is the case in the effective Hamiltonian (8), 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 interaction potential (8) 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 individual components of the wave function (self-phase modulation.) Such a contribution would also appear here if the two-body interaction contained a spin-preserving contribution due to the exchange of longitudinal photons, e.g., the van der Waals interaction.

Equations (9) have direct analogies with nonlinear optics, in particular gap solitons in nonlinear periodic structures [11], and nonlinear focusing effects [12]. Furthermore, if these equations are transformed to momentum space they reveal a variety of four-wave-mixing terms including those responsible for phase conjugation. This raises the possibility of an atomic phase conjugator capable of reconstructing distorted atomic wave functions. These prospects, including the study of atomic gap solitons [13], shall be pursued in future work. In the remainder of this Letter, we reexamine the problem of atomic scattering from a standing-wave light field in light of the nonlinearity of Eqs. (9), and predict nonlinear Pendellösung oscillations as well as atomic Thirring solitons.

Consider a quasi-plane-wave atomic beam whose initial momentum along the longitudinal z direction is large enough to be treated classically, and restrict the quantum description of the atomic motion to the transverse x direction. The atoms are taken to be at resonance with the field, $\delta = 0$, and prepared in their ground electronic state $|g\rangle$, with initial momentum $p_x = \hbar q/2$. It is known from the theory of the near-resonant Kapitza-Dirac effect that such atoms can undergo Doppleron-type resonances [14,15] between electrotranslational states of momenta $+\hbar q/2$ and $-\hbar q/2$. To proceed we express the effective single-particle states $\phi_g(x,t)$ and $\phi_e(x,t)$ in the form $\phi_g(x,t) = G(x,t)\exp(iqx/2)\exp(-i\omega_r t/4)$, $\phi_e(x,t) = E(x,t)\exp(-iqx/2)\exp(-i\omega_r t/4)$, where $G(t)$ and $E(t)$ are assumed to be slowly varying functions of x, $q^2|G(x)| \gg q|\partial_x G(x)| \gg |\partial_x^2 G(x)|$ and $\omega_r = (\hbar q)^2/2m$ is the recoil frequency. Substituting these states into Eqs. (9) and dropping slowly varying terms yields the pair of equations

$$\begin{aligned} i\hbar\frac{\partial G(x,t)}{\partial t} &= -\frac{i\hbar^2 q}{2M}\frac{\partial G(x,t)}{\partial x} + \frac{\hbar\mathcal{R}}{2}E(x,t) \\ &\quad +(N-1)(V_0/q)|E(x,t)|^2 G(x,t), \\ i\hbar\frac{\partial E(x,t)}{\partial t} &= +\frac{i\hbar^2 q}{2M}\frac{\partial E(x,t)}{\partial x} + \frac{\hbar\mathcal{R}}{2}G(x,t) \\ &\quad +(N-1)(V_0/q)|G(x,t)|^2 E(x,t). \end{aligned} \tag{10}$$

These equations provide an accurate description of the Doppleron resonance of atom optics in the limits that the envelope wave functions G and E vary little over an optical wavelength and $\omega_r/\mathcal{R} \gg 1$, which restricts atomic scattering to the two selected electrotranslational states.

Consider first the case of a pure momentum-eigenstate input, so that the transverse derivatives may be dropped in Eqs. (10). The resulting pair of equations is easily solved with $|E(0)|^2 + |G(0)|^2 = 1/L$, and the initial condition $G(0) = L^{-1/2}$, $E(0) = 0$, where L is the quantization length, to give

$$|G(t)|^2 = \frac{1}{2L}\left[1 + \mathrm{cn}(\mathcal{R}t|\alpha)\right], \tag{11}$$

where cn is Jacobi elliptic function and $\alpha = [(N-1)/(N_c-1)]^2$, the critical number of atoms N_c being defined as $N_c = 1 + 2\hbar\mathcal{R}/|V_0|L \simeq 2qL(\mathcal{R}/\gamma)$. In the limit $\alpha = 0$ ($N = 1$ or alternatively $V_0 = 0$), the solution (11) reduces to the Pendellösung solution $|G(t)|^2 = (1 + \cos\mathcal{R}t)/2L$, which gives rise to periodic and complete transfer of population between the two states. The general solution (11) is also periodic, but with period $4K(\alpha)$, $K(\alpha)$ being the complete elliptic integral of the first kind. In the regime $0 < N < N_c$, the oscillations in population are still complete, but the period increases with increasing atom number N, and actually diverges for $N = N_c$. For $N > N_c$, the period decreases with increasing N, but the oscillations are no longer complete. This nonlinear Pendellösung solution is a dramatic manifestation of many-body effects in atom optics. Note that if the number N of atoms is fluctuating, Eq. (11) must be summed over the probability distribution $p(N)$, thereby leading to collapses and revivals of $|G(t)|^2$.

As a second example, we consider again Eqs. (10), but retaining the spatial derivatives. This system 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 $G \to \chi_2$ [7]. The MTM is an integrable classical field theory, and that it has exact soliton solutions. In particular, the MTM has 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 zero velocity atomic Thirring soliton takes the form

$$\begin{aligned} G_s(x,t) &= q^{1/2}\left(\frac{\hbar\mathcal{R}/2}{(N-1)|V_0|}\right)^{1/2}\sin Q e^{\mp i\nu t}\mathrm{sech}(x/x_0 \pm iQ/2), \\ E_s(x,t) &= \pm q^{1/2}\left(\frac{\hbar\mathcal{R}/2}{(N-1)|V_0|}\right)^{1/2}\sin Q e^{\mp i\nu t}\mathrm{sech}(x/x_0 \mp iQ/2), \end{aligned} \tag{12}$$

where $\nu = (\mathcal{R}/2)\cos Q$, $qx_0 = 2\omega_r/(\mathcal{R}\sin Q)$, $Q = (N-1)|V_0|/4\hbar\omega_r$, and the upper (lower) sign corresponds to V_0 negative (positive). Atomic Thirring solitons are therefore possible irrespective of the sign of the two-body interaction. Note also that in compliance with our assumptions, the width of the soliton is always broader than an optical wavelength since in Bragg-type diffraction $\omega_r/\mathcal{R} \gg 1$.

The atomic Thirring soliton corresponds to 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 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. More generally, soliton solutions are expected to play a central role in the dynamics of the system even in the presence of nonintegrable perturbations, since they correspond to stable, *coherent* excitations of the many-atom system [16].

The question remains to determine whether the effects outlined in this Letter are amenable to experimental verification. Nonlinear effects are expected to become noticeable as soon as the effective nonlinearity $(N-1)V_0|\phi|^2/q$ becomes comparable to the effects of linear diffraction, whose strength is of the order of $\hbar^2 q^2/2M$. This yields the critical linear density $\rho_L \simeq N/L \simeq \omega_r q/\beta\gamma$. Here β is a geometrical factor which reflects the fact that the effective strength of the dipole-dipole interaction is given by the fraction of spontaneously emitted photons that can be reabsorbed by atoms inside the laser beam. For the sodium D-line, we have $\rho_L \simeq 270/\beta$ cm^{-1}, which corresponds to acceptably low densities of $\rho \simeq 2 \times 10^{13}$ cm^{-3} for $\beta = 10^{-2}$. Of course, larger β's, and lower densities, could be achieved in cavity QED geometries.

While the competing effects of spontaneous emission are of course always of concern in atom optics, they can be circumvented to a large extent by working off resonance. Indeed, except for the density requirements just discussed, the conditions under which linear and nonlinear atom optics experiments can be carried out are essentially the same [9]. While the examples explicitly discussed in this Letter are on resonance, they can readily be extended to off-resonance situations. In this case, Thirring solitons, for example, degenerate into gap solitons [13].

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