EUROPHYSICS LETTERS 15 October 2006

Europhys. Lett., **76** (2), pp. 196–202 (2006)
DOI: 10.1209/epl/i2006-10260-0

How different are multiatom quantum solitons from mean-field solitons?

I. E. MAZETS[1,2] and G. KURIZKI[1]

[1] *Department of Chemical Physics, Weizmann Institute of Science Rehovot 76100, Israel*
[2] *Ioffe Physico-Technical Institute - St. Petersburg 194021, Russia*

received 29 April 2006; accepted in final form 25 August 2006
published online 13 September 2006

PACS. 03.75.-b – Matter waves.
PACS. 05.30.Jp – Boson systems.
PACS. 42.65.Tg – Optical solitons; nonlinear guided waves.

Abstract. – We theoretically investigate the free dispersion, scattering and disintegration of an N-particle quantum soliton by Bragg light pulses, comparing the exact quantum result with its quasiclassical (mean-field) limit. Remarkably, we find that the correlation properties of a quantum soliton approach the (mean-field) limit very rapidly as the particle number N grows. A modest discrepancy between the classical and quantum results is observed for $N = 3$.

Thus far, most of the work related to solitons has dealt with their nonlinear wave properties [1], along with quantum noise (squeezing) corrections to their mean-amplitude ("mean-field") dynamics [2]. Second quantized solitons whose mean-field description breaks down have been studied to a much lesser extent, notwithstanding notable recent achievements [3,4]. Perhaps the most powerful tool of the theory of quantum solitons is the Bethe ansatz solution [5], providing an exact quantum-mechanical solution for a one-dimensional (1D) quantum system of pairwise interacting N particles [6]. This solution has been extended to a two-band periodic nonlinear structure [7].

Intuitively, it is clear that for $N \gg 1$ the intrinsic correlation properties of a quantum soliton will approach the quasiclassical (mean-field) limit. Conversely, one may expect that for a relatively low N a quatum soliton still exhibits genuinely quantum properties. The quest for such properties may be regarded as a part of a broader effort to understand multipartite correlations in complex quantum systems, particularly trapped BECs [8–11]. In the present letter we demonstrate that, surprisingly, the correlation properties of a quantum soliton consisting of more than 3 particles are hardly distinguishable from the properties of its quasiclassical counterpart.

The Hamiltonian under consideration describes N atoms coupled by attractive contact interactions, propagating along the x-axis and scattered by an external x-dependent potential. Such a system is realizable [8–14] when ultracold bosonic atoms are confined in the transverse (y, z)-plane, so as to render their motion effectively one-dimensional (1D). The Hamiltonian then reads

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} - \frac{2\hbar^2\kappa}{m}\sum_{j=1}^{N}\sum_{j'=1}^{j-1}\delta(x_j - x_{j'})\,. \tag{1}$$

Here κ is the inverse size of a two-atom bound state, henceforth dubbed "dimer". We assume attractive interactions with $\kappa > 0$. When the transverse (y,z) confinement is not too tight, *i.e.* its radius w_r is larger than the absolute value of the scattering length $|a|$, then the general expression for κ [14] reduces to $\kappa = |a|/w_r^2$.

Here we do not consider excitation of the transverse degrees of freedom, *i.e.* oscillations of the atoms in the (y,z)-plane in the radial confining potential. Such a breakdown of a purely 1D model leads to effects such as damping of the center-of-mass motion of a soliton [13]. We, however, focus on the intrinsic properties of a 1D quantum soliton.

The general eigenfunction of the Hamiltonian (1) is given by the Bethe ansatz [6]:

$$\psi(x_1,\ldots,x_N) = \mathcal{A}\sum_P\prod_{j=1}^{N}\prod_{j'=1}^{j-1}\left[1+\frac{2i\kappa\,\mathrm{sgn}\,(x_j-x_{j'})}{k_j-k_{j'}}\right]\exp\left[i\sum_{j=1}^{N}k_jx_j\right]. \tag{2}$$

The sum is here taken over all the permutations P of $\{x_1,\ldots,x_N\}$ and $\mathcal{A}$ is the normalization factor. If we set $k_j = K - iQ_j$, where $Q_j = -2\kappa j + \kappa(N+1)$, $j = 1,2,\ldots,N$, we get the N-atom bound state

$$|\psi_b(N,K)\rangle = \mathcal{A}\exp\left[-\kappa\sum_{j=1}^{N}\sum_{j'=1}^{j-1}|x_j - x_{j'}| + iK\sum_{l=1}^{N}x_l\right] \tag{3}$$

with the energy $E_b(N,K) = N\hbar^2K^2/(2m) + \varepsilon_b(N)$, the internal energy of the N-atom bound state being $\varepsilon_b(N) = -N(N^2-1)\hbar^2\kappa^2/(6m)$. This bound state is the ground state of the *relative* motion of the atoms. The center-of-mass motion in eq. (3) is described by a plane wave, hence this state is correlated but delocalized. A localized N-atom wave packet is a superposition of the states $|\psi_b(N,K)\rangle$ with a suitable choice (*e.g.*, Gaussian) of probability amplitudes for different K's [2].

The fact that the eqs. (2), (3) are eigenstates of the Hamiltonian (1) can be easily checked by their substitution in the appropriate Schrödinger equation. The contact interactions in (1) cause discontinuities in the wave function derivatives $[(\partial/(\partial x_1) - (\partial/\partial x_2)]\,\psi|_{x_1=x_2+0} - [(\partial/(\partial x_1) - (\partial/\partial x_2)]\,\psi|_{x_1=x_2-0} = -4\kappa\psi|_{x_1=x_2}$. Repulsive interactions ($\kappa < 0$) admit only continuum states of the relative motion, whereas attractive interactions with $\kappa > 0$ considered here admit also bound multiatom states [3,6].

A possible manifestation of the quantum nature of a soliton may be the dispersion of its center-of-mass free 1D motion as opposed to the invariance of the interparticle distances [2]. When the effects of dispersion are negligible, a quantum soliton consisting of atoms with attractive interactions becomes a classical (mean-field) bright soliton. Note that the superselection rule prohibiting quantum superposition of states with different N's holds for atomic ensembles [15] and is supposed to be true even for laser-emitted photons [16]. Hence, a quantum soliton propagates as a single quantum entity of the mass Nm. In fig. 1 we show its broadening δX, namely, the r.m.s. deviation of the center-of-mass of a quantum soliton from the quasiclassical (dispersionless) trajectory, *vs.* the propagation time t. The center-of-mass coordinate uncertainty can be estimated as $\delta X \sim \sqrt{\hbar t/(Nm)}$. Suppose the quantum soliton consists of $N \sim 10$ atoms, $m \sim 10^{-22}$ g and $t \sim 10^{-3}$ s. Then $\delta X \sim 10^{-5}$ cm. Such a length scale is of the order of the radial trapping size w_r for an experimentally attainable radial

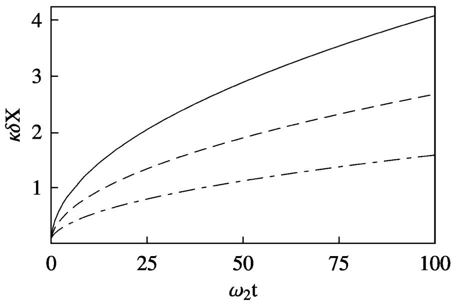

Fig. 1 – The r.m.s. deviation of the center-of-mass of a quantum soliton *vs.* propagation time. The inverse dimer size κ and the dimer binding frequency $\omega_2 = |\varepsilon_b(2)|/\hbar = \hbar\kappa^2/m$ are used for normalization on the vertical and horizontal axes, respectively. The initial uncertainty of the center-of-mass position is $0.1/\kappa$. $N = 3$ (solid line), 7 (dashed line) and 20 (dot-dashed line).

confinement (by an optical potential) characterized by the fundamental frequency of about 10 kHz [17]. If the absolute value of the 3D atomic scattering length exceeds w_r (by means of Feshbach resonance), the effective 1D contact interaction is attractive and $\kappa \sim w_r^{-1}$ [14, 17]. In other words, for such a choice of parameters δX reaches the dimer size κ^{-1} at relatively short propagation times (see fig. 1). This uncertainty of the quantum soliton position is quite appreciable, since it is much larger than $(N\kappa)^{-1}$, which is the typical deviation of the coordinate of an individual atom from the center-of-mass coordinate. Further increase of κ (beyond w_r^{-1}) is impossible, since in this case the 1D approximation breaks down.

Our quest for more conspicuous signatures of a 1D quantum soliton leads us to consider its scattering by an external potential $U(x)$. Such scattering may either leave the soliton intact or decouple atoms from the bound state. Setting $k_j = K' - iQ'_j$, where $Q'_j = -2\kappa j + \kappa N$, $j = 1, 2, \ldots, N-1$, and $k_N = K' + k$, we get a solution $|\psi_d(N-1, 1, K', k)\rangle$ describing $N-1$ atoms in the bound state and one atom decoupled from the bound core (asymptotically free).

Suppose that the potential is an optically-induced Bragg grating [18] imparting a momentum $\hbar q$ (along the x-axis) and an energy $\hbar\omega$ to the N-atom bound state. Lengthy calculations give an expression for the matrix element of the N-atom operator of the momentum shift, whose general form is

$$\langle\psi_d(N-1, 1, K', k)| \sum_{j=1}^{N} \exp[iqx_j] \, |\psi_b(N, K)\rangle = \delta_{NK+q,\, NK'+k} \, (L\kappa)^{-1/2} M(q, k) e^{i\Phi(q,k)}, \quad (4)$$

$M(q, k)$ and $\Phi(q, k)$ being the normalized modulus and the phase, respectively, of the matrix element and L being the quantization length.

Momentum and energy conservation yields $K' - K = (q - k)/N$ and

$$\frac{\hbar^2 k^2}{2m} \left(1 - \frac{1}{N}\right) = \hbar \left(\omega - \frac{\hbar K q}{m}\right) - \Delta\varepsilon(N), \quad (5)$$

$$\Delta\varepsilon(N) \equiv \varepsilon_b(N-1) - \varepsilon_b(N) = \frac{\hbar^2 N\kappa^2 \,(N-1)}{2m}. \quad (6)$$

Here $\Delta\varepsilon(N)$ is the difference of the binding energies of the $(N-1)$- and N-atom bound states. Thus, given ω, q, and the Rabi frequency Ω_R of the Bragg excitation, we can find, from the

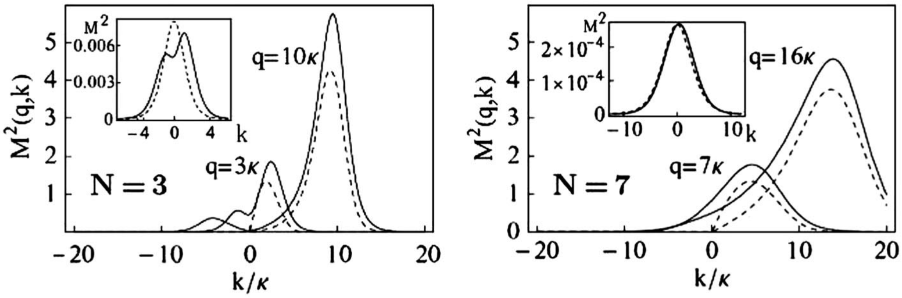

Fig. 2 – The values of $M^2(q,k)$ *vs.* normalized k for particular values of q for $N = 3$ and 7 (solid lines). Dashed lines: quasiclassical approximation (quasiclassical motion of a decoupled atom in a potential generated by a classical soliton). Insets: plots for the case $q = 0.6\kappa$. Units on the axes are dimensionless.

Fermi Golden Rule, the spectrum of the excitation rate Γ_B leading to the decoupling of a single atom from an N-atom quantum soliton:

$$\Gamma_B(\omega, q, N) = \Omega_R^2 \int \frac{\mathrm{d}k}{\kappa}\, M^2(q,k)\, \delta\left[\frac{\hbar k^2(N-1)}{2Nm} - \left(\omega - \frac{\hbar K q}{m}\right) + \frac{\Delta\varepsilon(N)}{\hbar}\right]. \tag{7}$$

We find that

$$\begin{aligned} M(q,k)e^{i\Phi(q,k)} &= 2\delta_{NK+q,\,NK'+k}(2\kappa)^{N-1/2}(N-2)!(N-1)! \times \\ &\times \sum_{\alpha=1}^{N}\sum_{\beta=1}^{N} \Xi_\alpha^* \left[\prod_{j=1}^{N-1}\sum_{l=1}^{j}\left(\tilde{Q}_l^\alpha + Q_l^\beta\right)\right]^{-1}, \end{aligned} \tag{8}$$

where

$$\Xi_1 = 1, \qquad \Xi_\alpha = \prod_{j=1}^{\alpha-1}\left(\frac{-iQ'_j - k - 2i\kappa}{-iQ'_j - k + 2i\kappa}\right), \qquad \alpha > 1, \tag{9}$$

$$Q_j^\beta = Q_j + q\delta_{j\beta}, \qquad \tilde{Q}_j^\alpha = \begin{cases} Q'_j - i(K'-K), & j < \alpha, \\ -ik - i(K'-K), & j = \alpha, \\ Q'_{j-1} - i(K'-K), & j > \alpha. \end{cases} \tag{10}$$

In fig. 2 we show the squared modulus of the matrix element $M^2(q,k)$ calculated from eq. (8). The dashed line shows the squared quasiclassical matrix elements

$$M^{qcl}(q,k) = \sqrt{N\kappa}\left|\int_{-\infty}^{+\infty} \mathrm{d}x\, \psi_k^{qcl\,*}(x)\exp[iqx]\phi_0(x)\right|, \tag{11}$$

where $\psi_0(x) = \sqrt{N\kappa/2}\cosh^{-1} N\kappa x$ is the well-known mean-field solution [1,3] of the nonlinear Schrödinger equation (with attraction), normalized to 1, and

$$\psi_k^{qcl}(x) = \frac{\exp\left[ik\int_{-\infty}^{x}\mathrm{d}x'\sqrt{1 + 4(N\kappa/k)^2\cosh^{-2} N\kappa x'}\right]}{[1 + 4(N\kappa/k)^2\cosh^{-2} N\kappa x]^{1/4}} \tag{12}$$

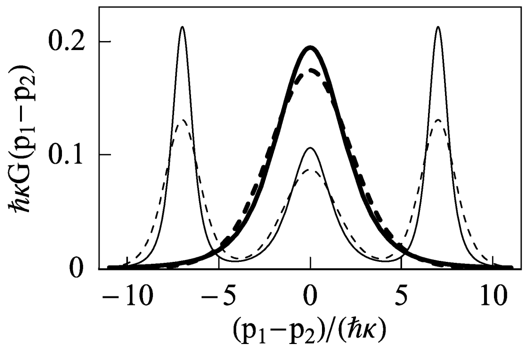

Fig. 3 – The two-atom momentum correlation function for states with $N = 3$: $|\psi_b(3, K)\rangle$ (thick lines) and $|\psi_d(2, 1, K', k)\rangle$ with $k = 7\kappa$ (thin lines). The exact quantum and quasiclassical results are shown by solid and dashed lines, respectively. Units on the axes are dimensionless.

is the quasiclassical wave function of a decoupled atom in the field of N-particle quantum soliton with the asymptotics $\exp[ikx]$ for $x \to -\infty$ (here we neglect terms of the order of N^{-1}).

The small peak at the values of k directed opposite to q for $N = 3$, which is *not reproduced* by the quasiclassical approximation, represents an atomic dimer that carries away most of the transferred momentum $\hbar q$, while the remaining (free) atom travels more slowly, in contrast to the more probable situation (the main peak at $k \approx q$) where the decoupled atom carries away nearly all the transferred momentum. The width of the main peak scales as $N\kappa$ for $N \geq 3$. It is noteworthy that the quasiclassical approximation works well for large momentum transfer $|q| \gtrsim N\kappa$, even for small N ($N \geq 3$).

In the opposite case of small transferred momentum, $|q| \lesssim N\kappa$, the matrix element can be fit by the expression $M^2(q, k) \approx 5[q/(N\kappa)]^4 \cosh^{-2}[2k/(N\kappa)]$. This fitting is satisfactory for $N = 3$ and *excellent* for $N > 3$ (see insets in fig. 2).

To compare further the quantum and quasiclassical results, we calculate the two-particle correlation function $G(p_1 - p_2)$ in momentum space for $N = 3$. We assume the following normalization: $\int_{-\infty}^{\infty} \mathrm{d}p\, G(p) = 1$. We obtain the following *exact* quantum result for the bound state $|\psi_b(N, K)\rangle$ with $N = 3$:

$$G_{quant}(p_1 - p_2) = [3\pi\hbar\kappa(4 + \tilde{p}^2)^3(9 + \tilde{p}^2)]^{-1}(1056 + 204\tilde{p}^2 + 5\tilde{p}^4)\,, \tag{13}$$

where $\tilde{p} = (p_1 - p_2)/(2\hbar\kappa)$. The quasiclassical expression, calculated from the atomic wave function $\prod_j \phi_0(x_j)$, yields for $N = 3$

$$G_{qcl}(p_1 - p_2) = \pi(3\hbar\kappa)^{-1} F[\pi\tilde{p}/3]\,, \tag{14}$$

where $F(y) = \frac{1}{4}\int_{-\infty}^{+\infty} \mathrm{d}x \cosh^{-2}(x + y)\cosh^{-2} x$. As one can see from fig. 3, the agreement between eqs. (13) and (14) is unexpectedly good even for $N = 3$. In other words, the mean-field approach predicts the atomic correlation properties of quantum solitons quite precisely. The difference between the quantum and quasiclassical results is mainly in the asymptotics for large $|p_1 - p_2|$: eq. (13) decreases as $(p_1 - p_2)^{-4}$, whereas eq. (14) decreases exponentially.

The power law decrease of these *distinctly quantum* (non-mean-field) "tails" is due to non-analyticity of the wave function $|\psi_b(N, K)\rangle$ at $x_1 = x_2$, where its derivative is discontinuous. However, it is challenging to measure the "tail" of the correlation function experimentally.

By contrast, for the final state of two bound atoms and one atom decoupled, $|\psi_d(N-1,1,K',k)\rangle$, for $N=3$, the correlation functions (also displayed in fig. 3) are calculated to be

$$G_{quant}(p_1-p_2)=\frac{1}{24\pi\hbar\kappa}\sum_{\ell=1}^{3}\frac{a_\ell}{\left(\frac{1}{4}+\zeta_\ell^2\right)^2}\,, \tag{15}$$

where $a_1=1$, $a_2=a_3=2$, $\zeta_1=\tilde{p}/2$, $\zeta_2=\tilde{p}+\tilde{k}$, $\zeta_3=\tilde{p}-\tilde{k}$, $\tilde{k}=k/(2\kappa)$, as opposed to its quasiclassical counterpart:

$$G_{qcl}(p_1-p_2)=\frac{1}{3\hbar\kappa}\left[\frac{\pi}{2}F(\pi\zeta_1)+\sum_{\ell=2}^{3}\frac{\pi}{4\cosh^2(\pi\zeta_\ell/2)}\right]. \tag{16}$$

As seen from fig. 3, the two correlation functions (15) and (16) are quite close to each other. The sidebands calculated by the quasiclassical eq. (16) for $N=3$ are lower by the factor $\pi/2$ than their quantum counterparts (the peak areas are the same in both the cases). However, such a difference may be easily masked by various broadening mechanisms that are present in a real experiment. The difference between the quasiclassical and quantum correlation functions is found to be practically negligible for $N>3$.

The flux of outcoupled atoms will be proportional to the product of the number of N-atomic quantum solitons in the system and $|M(q,k)|^2$ with k determined from energy conservation. The system containing many bound complexes of atoms can be created in a bunch of 1D waveguides formed in a 2D optical lattice [17]. One may apply an additional optical lattice along the waveguide axis, so that few atoms are trapped in each potential minimum. Sudden switching-off of this additional lattice will project these trapped states on the states of free motion. By proper choice of the lattice parameters one may attain significant probability of creation multiatom bound states, which then will be subject to Bragg spectroscopic studies.

The momentum correlation functions can be measured experimentally using the technique developed to study the Mott insulator phase of rubidium atoms in an optical lattice [19]. For quantum solitons, time-of-flight measurements after releasing atoms from a trap will reflect the underlying spatial correlations in the multiatom bound state. Bragg spectroscopy [18] will directly yield the value of matrix elements $M(q,k)$, since both the transferred energy and momentum are controllable experimental parameters in this case.

It is reasonable to assume that approximately 4000 individual waveguides formed by a 2D optical lattice are filled with $N_{tot}\sim 10^5$ atoms, with the characteristic length of the atomic sample in the x-direction $\ell\approx 50\,\mu$m. We assume that the sample is prepared in such a way that bound states with $N>3$ are practically absent. Initially the atomic velocities are small compared to the final ones, *e.g.* $q=10\,\kappa$. To ensure such transferred momentum detection by Bragg spectroscopy, we take $\kappa\approx 10^4\,\text{cm}^{-1}$. To distinguish by time-of-flight measurement atoms outcoupled from atomic bound states with $N=3$ and $N=2$ the Bragg pulse duration T_p has to be longer than the typical time scale $m/(\hbar\kappa^2)$, which means, for $m\sim 10^{-22}\,$g, $T_p\gg 1\,$ms. Let us choose the two-photon Bragg detuning such that we are at resonance with outcoupling an atom at $k=2.5\,q$ from a 3-atom bound state. Energy and momentum conservation results in the velocities of the outcoupled atom and the remaining dimer equal to $5\,\hbar\kappa/m$ and $1.25\,\hbar\kappa/m$, respectively. The resonant condition is not fulfilled for single atoms and dimers, so that they are not affected by the Bragg pulse. After free propagation during the time-of-flight interval $T_f=50\,$ms, part of the sample that remains intact, the outcoupled atoms and the newly produced (recoiled) dimers become spatially resolved. Each fast outcoupled atom is correlated with a respective recoiled dimer. If 30% of all the atoms are bound into trimers, and almost all the trimers are dissociated by the Bragg pulse, the signal consists of $\sim 10^4$ atoms, a detectable number [18].

To conclude, we have studied the free propagation of a 1D N-atom quantum soliton and its response to Bragg excitations. We find an unexpected degree of quasiclassicality of quantum solitons with particle numbers as small as $N = 3$ in terms of Bragg excitation probabilities and momentum correlation functions. Such a property is surprising because 1D systems usually exhibit prominent quantum correlations and fluctuations. The free propagation broadening remains significant for $N < 10$.

* * *

We thank Prof. M. Oberthaler for helpful discussions. The support of the EC (the QUACS RTN and SCALA NOE), and ISF is acknowledged. IEM also thanks the program Russian Leading Scientific Schools (grant 9879.2006.2).

REFERENCES

[1] Boyd R. W., *Nonlinear Optics* (Academic Press, New York) 1992, §6.5.
[2] Lai Y. and Haus H. A., *Phys. Rev. A*, **40** (1989) 844; 854.
[3] Drummond P. D., Kheruntsyan K. V. and He H., *J. Opt. B: Quantum Semiclass. Opt.*, **1** (1999) 387; Bullough R. K. and Wadati M., *J. Opt. B: Quantum Semiclass. Opt.*, **6** (2004) S205.
[4] Kanamoto R., Saito H. and Ueda M., *Phys. Rev. Lett.*, **94** (2005) 090404.
[5] Bethe H. A., *Z. Phys.*, **71** (1931) 205.
[6] Girardeau M., *J. Math. Phys.*, **1** (1960) 516; Lieb E. H. and Liniger W., *Phys. Rev.*, **130** (1963) 1605; McGuire J. B., *J. Math. Phys.*, **5** (1964) 622; Thacker H. B., *Rev. Mod. Phys.*, **53** (1981) 253.
[7] Cheng Z. and Kurizki G., *Phys. Rev. Lett.*, **75** (1995) 3430; *Phys. Rev. A*, **54** (1996) 3576.
[8] Morgan S. A., Ballagh R. K. and Burnett K., *Phys. Rev. A*, **55** (1997) 4338; Khaykovich L. *et al.*, *Science*, **296** (2002) 1290.
[9] Machholm M., Pethick C. J. and Smith H., *Phys. Rev. A*, **67** (2003) 053613.
[10] Greiner M. *et al.*, *Nature*, **415** (2002) 39.
[11] Louis P. J. Y., Ostrovskaya E. A. and Kivshar Yu. S., *Phys. Rev. A*, **71** (2005) 023612.
[12] Anker Th. *et al.*, *Phys. Rev. Lett.*, **94** (2005) 020403.
[13] Sinha S., Cherny A. Yu., Kovrizhin D. and Brand J., *Phys. Rev. Lett.*, **96** (2006) 030406.
[14] Olshanii M., *Phys. Rev. Lett.*, **81** (1998) 938.
[15] Cohen-Tannoudji C. and Robillard C., *C. R. Acad. Sci. Ser. IV*, **2** (2001) 445.
[16] Mølmer K., *Phys. Rev. A*, **55** (1997) 3195.
[17] Moritz H. *et al.*, *Phys. Rev. Lett.*, **94** (2005) 210401.
[18] Kozuma M. *et al.*, *Phys. Rev. Lett.*, **82** (1999) 871; Stenger J. *et al.*, *Phys. Rev. Lett.*, **82** (1999) 4569; Steinhauer J., Ozeri R., Katz N. and Davidson N., *Phys. Rev. Lett.*, **88** (2002) 120407.
[19] Fölling S. *et al.*, *Nature*, **434** (2005) 481.