Dynamics of Lieb-Liniger gases

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It is proved that the Lieb-Liniger (LL) cusp condition implementing the delta function interaction in one-dimensional Bose gases is dynamically conserved under phase imprinting by pulses of arbitrary spatial form and the subsequent many-body dynamics in the thermodynamic limit is expressed approximately in terms of solutions of the time-dependent single-particle Schrödinger equation for a set of time-dependent orbitals evolving from an initial LL-Fermi sea. As an illustrative application, generation of gray solitons in a LL gas on a ring by a phase imprinting pulse is studied.

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Recent advances and experiments on ultracold atomic vapors in atom waveguides \(1,2,3,4,5,6,7,8,9,10,11,12,13\) and potential applicability to atom interferometry \(14\) and integrated atom optics \(3,15\) create a need for accurate theoretical modelling of such systems, and this is underscored by recent experimental achievement of optical atom interferometer structures of Mach-Zehnder and Michelson type \(16\). At sufficiently low temperatures and densities and high transverse frequencies \(\omega_0\) the transverse degrees of freedom of a Bose-Einstein condensate (BEC) in an atom waveguide are frozen in the ground transverse mode and the dynamics is described by an effective 1D Hamiltonian with delta function interactions \(17\). In the spatially uniform case the exact ground state was found in 1963 by Lieb and Liniger (LL) \(19\). The properties of this LL gas are determined by a dimensionless parameter \(\gamma = m g_{1D}/\hbar^2\) where \(n\) is the 1D density and the effective 1D coupling constant \(g_{1D}\) is related to the 3D s-wave scattering length \(a\) by \(17\)

\[ g_{1D} = 2a\hbar^2/m\ell_0^2[1 - (C/\sqrt{2})(a/\ell_0)] \]

with \(\ell_0 = \sqrt{\hbar/m\omega_0}\) the transverse oscillator length and \(C = 1.4603\ldots\). If \(\gamma \gg 1\) the dynamics reduce to those of a 1D gas of hard core, or impenetrable, point bosons \(17,18\), the “TG gas” \(20,21,22,23,24,25\). This is a model for which exact many-body eigenstates and dynamics were found using a mapping from the Hilbert space of eigenstates of an ideal gas of spinless fermions to that of many-body eigenstates of hard core bosons \(20,24,27,28,29,30,31,32,33\). The TG regime is only a tiny part of the LL regime, most of the latter having already been reached experimentally \(3,3,10,12,13\), and it is desirable to extend the techniques applicable in the TG regime to the whole LL regime so as to reduce the many-body dynamics of free and trapped LL gases to solution of the time-dependent single-particle Schrödinger equation for a set of time-dependent orbitals evolving from initial orbitals comprising a LL-Fermi sea. It will be shown herein that although this cannot be done exactly for all values of \(\gamma\) and all time intervals, it can be done in good approximation for limited time intervals for all \(\gamma\), and exactly in some special cases.

**LL cusp condition and energy eigenstates:** The \(N\)-particle energy eigenstates satisfy

\[ \hat{H}_0 \psi_{B\alpha} = E_{\alpha} \psi_{B\alpha} \]

where \(\psi_{B\alpha}\) is symmetric (Bose). LL considered a uniform system and used dimensionless units such that \(\hbar = 2m = 1\), yielding a Hamiltonian

\[ \hat{H}_0 = \sum_{j=1}^{N} \left( -\frac{\partial^2}{\partial x_j^2} + 2c \sum_{1 \leq j < k \leq N} \delta(x_j - x_k) \right) \]  

where \(2c = g_{1D} = 2\gamma n\). They used periodic boundary conditions \(\psi_{B\alpha}(\cdots x_j \pm L \cdots) = \psi_{B\alpha}(\cdots x_j \cdots)\). The \(N\)-particle configuration space decomposes into \(N!\) permutation sectors, each defined by one particular ordering of numerical values of the \(x_1, \cdots, x_N\). In view of the Bose symmetry of the \(\psi_{B\alpha}\), it is sufficient to define them only in the fundamental permutation sector \(R_1\) wherein \(x_1 < x_2 < \cdots < x_N\), then extending to all \(N!\) sectors by symmetry. The cusp condition following from the \(\delta(x_j - x_k)\) interactions is

\[ \left( \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_k} \right) \psi_{B\alpha}|_{x_j = x_k + \epsilon} = c \psi_{B\alpha}|_{x_j = x_k + \epsilon} \]  

Define \(\hat{B}_j = \partial/\partial x_j + 1 - \partial/\partial x_j - c\hat{1}\) where \(\hat{1}\) is the unit operator. Then in \(R_1\)

\[ \hat{B}_j \psi_{B\alpha}|_{x_j = x_j + \epsilon} = 0 . \]  

In \(R_1\) the energy eigenstates satisfying this are

\[ \psi_{B\alpha}(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!L^N}} \sum_P a_P(K_\alpha) e^{i(P K_\alpha) \cdot X} \]  

and their energies are \(E_\alpha = \sum_k k^2\). Here \(K_\alpha\) is an \(N\)-dimensional vector \((k_1, k_2, \cdots, k_N)\) with \(k_1 < k_2 < \cdots < k_N\), the sum runs over the \(N!\) permutations \(P\) of this set, and \(X\) is the \(N\)-dimensional position vector \(X = (x_1, x_2, \cdots, x_N)\), assuming \(x_1 < x_2 < \cdots < x_N\). There are infinitely many such choices \(k_1, \cdots, k_N\), and \(\alpha\) labels each particular choice. The coefficients are

\[ a_P(K_\alpha) = \epsilon_P \prod_{1 \leq j < \ell \leq N} \frac{\gamma n + i(Pk_\ell - Pk_j)}{\sqrt{(\gamma n)^2 + (Pk_\ell - Pk_j)^2}} \]  

and
where \( P k_j \) is the image of \( k_j \) under \( P \) and \( \epsilon_P \) is the parity \( \pm 1 \) of \( P \). This differs from the \( \epsilon_P \) of LL Eqs. (2.12) ff. only by a constant phase.

Although the symmetrical extension of \( \psi_{Bo} \) to all permutation sectors is bosonic (totally symmetric under permutations of \( x_1, \ldots, x_N \)), it can be shown [28] that it is nevertheless antisymmetric under permutations of \( k_1, \ldots, k_N \). Thus \( \psi_{Bo} \) must be built from \( N \) singly-occupied orbitals. The ground state \( \psi_{Bo} \) is obtained by a particular choice \( k_0 \) consisting of the smallest \( N \) different \( k_j \) consistent with the periodic boundary condition on the \( \psi_{Bo} \) [19], a “LL-Fermi sea”.

**Thermodynamic limit:** The allowed \( k_j \) were determined in the LL paper by requiring that \( \psi_{Bo}(x_1, \ldots, x_N) \) be periodic in each \( x_j \) with periodicity length \( L \), leading to \((k_j+1-k_j)L = \sum_{j=1}^{N}(\theta_{s_j} - \theta_{s,j+1}) + 2\pi n_j\) where \( \theta_{s} = -2\tan^{-1}[(k_s - k_j)/\gamma n]\) and the \( n_j \) are any integers \( \geq 1 \), whose values distinguish between all the \( N \)-particle energy eigenstates [19, 22]. The ground state is given by \( n_j = 1 \) for all \( j \). It follows that the individual orbitals \( e^{ik_jx} \) in [19] are not \( L \)-periodic; the \( k_j \) are not actual particle momenta but rather nonuniformly spaced quasimomenta [19]. Since our goal is reduction of the many-particle time-dependent Schrödinger equation (MBTDSE) to the single-particle time-dependent Schrödinger equation (SPTDSE), this leads to difficulties related to nonhermiticity of the single-particle Hamiltonian and an ill-posed initial value problem for the orbital evolutes \( \phi_j(x,t) \) on the finite interval \(-\frac{L}{2} < x < \frac{L}{2}\).

These can be mitigated in the thermodynamic limit \( N \to \infty, L \to \infty, N/L \to \eta = \text{const} \), wherein both the quasimomenta \( k_j \) and the actual particle momenta \( k_\nu \) become dense and every quasimomentum can be approximated with arbitrary accuracy by the \( k_\nu = \nu 2\pi / L \) with \( \nu = 0, \pm 1, \pm 2, \cdots \), appropriate to periodic boundary conditions. The initial orbitals \( e^{ik_\nu x}/\sqrt{L} \) and their evolutes \( \phi_\nu(x,t) \) are then orthonormal on \(-\frac{L}{2} < x < \frac{L}{2}\). In this limit any thermodynamically intensive or extensive quantity expressible as a sum of contributions of “quasiorbitals” evolving from the quasimomentum plane waves \( e^{ik_\nu x} \) approaches a similar expression expressed in terms of contributions of \( L \)-periodic orbitals evolving from \( L \)-periodic plane waves \( e^{ik_\nu x} \). In doing this it is necessary to take into account the nontrivial density of states of the allowed quasimomenta. For example, the ground state energy in the thermodynamic limit is \( \sum_{\nu} \beta(k_\nu) C_{\nu}^2 \) where \( \beta(k_\nu) \) is the ratio of the LL ground state density of states to its limiting value \( 1/2\pi \) in the TG limit, and \( C_{\nu} = L k_{\nu,LLF}/2\pi \) where \( k_{\nu,LLF} \), the wave vector at the top of the LL-Fermi sea, is determined by the condition \( \int_{-k_{\nu,LLF}}^{k_{\nu,LLF}} \beta(k)dk = 2\pi n_\nu \) [19].

**Response to phase imprinting:** Solitons have been generated in experiments on cigar-shaped BECs by application of phase-imprinting pulses [28, 37]. We have recently studied [28] the exact dynamics of such a process in the TG limit, as well as phase-imprinting pulse generated interference effects in a TG gas on a ring [31, 33] and in a double-X atom interferometer [32]. A similar LL model will be studied here. Consider a LL gas on a ring of circumference \( L \) initially in its ground state, and represent the positions of the \( N \) atoms by a 1D coordinate \(-\frac{L}{2} < x < \frac{L}{2}\) measured around the circumference. Suppose that this system is subjected at \( t = 0 \) to a phase-imprinting pulse \( v(x,t) = -\delta(t)S(x) \). Denoting the orbitals of the LL solution by \( e^{ik_jx} \), the orbitals just after the pulse are \( \phi_j(x,t = 0+) = e^{iS(x)} e^{ik_jx} \), and by [41] just after the pulse \( \psi_B(x_1, \ldots, x_N; t = 0+) = \psi_{Bo}(x_1, \ldots, x_N) \exp(i \sum_{j=1}^{N} S(x_j)) \). Supposing that \( x_1 < x_2 < \cdots < x_N \), and using the \( B \) of Eqs. (2) and (3), one finds

\[
\hat{B}_j \psi_B(0+) = i \psi_B(0+) [\hat{S}'(x_{j+1}) - \hat{S}'(x_j)] + e^{iS} \hat{B}_j \psi_{Bo}
\]

(6) with \( S = \sum_{j} S(x_j) \). This vanishes as \( x_{j+1} \to x_j+ \). It follows that the cusp condition need not be imposed as a constraint during the pulse, being exactly valid at \( t = 0+ \) independently of the spatial form and strength of the pulse.

**Dynamics:** Consider next free propagation according to \( \hat{H}_0 \) following such a pulse. This is generated in \( \mathcal{R}_1 \) by the kinetic energy alone, i.e., by Eq. (11) with the delta function interactions omitted. Let \( \psi_B(x_1, \ldots, x_N; t) \) be a wave function differing from [41] only by replacement of the orbitals \( e^{ik_jx} \) by the solutions \( \phi_j(x,t) \) of the single-particle TDSE \( [i\partial/\partial t + \partial^2/\partial x^2] \phi_j(x,t) = 0 \) reducing to \( \phi_j(x,t = 0+) = 0 \) as \( t \to 0+ \). Then \( \psi_B(x_1, \ldots, x_N; t) \) satisfies the MBTDSE \( [i\hat{\partial}/\partial t - \hat{H}_0(t)] \psi_B = 0 \) in the interior of \( \mathcal{R}_1 \) for \( t > 0 \) and reduces to the previously discussed wave function \( \psi_B(x_1, \ldots, x_N; t = 0+ \) as \( t \to 0+ \). However, a subtle complication enters here: Although the derivative operators in \( \hat{B}_j \) of Eq. (2) commute with the kinetic energy, the ratio of third to second derivative of the wave function is different from the ratio of first to zeroth derivative required by the cusp condition [12, 29], so a wave function propagated as above does not in general satisfy the cusp condition for \( t > 0 \). However, it is satisfied trivially for \( \gamma \to 0 \), and also for \( \gamma \to \infty \) (TG limit). Furthermore, by temporal continuity of the solution of the TDSE it is satisfied in good approximation for a nonzero range of times \( t > 0 \) for all \( \gamma \), assuming as in [41] that \( \psi_B(\cdots; t = 0+) \) is an energy eigenstate [12, 40]. By a temporal phase mixing argument the length of this range should increase with decreasing values of \( \Delta E/E \), suggesting that constraint-free propagation as above is a reasonable approximation for \( \Delta E/E \ll 1 \) where \( E \) is the energy and \( \Delta E \) is its dispersion.

**Single particle density and soliton propagation:** Suppose now that the initial \( N \)-particle wave function \( \psi_B(\cdots; t = 0+) \) differs from the LL ground state \( \psi_{Bo} \) at most by multiplication of the LL orbitals \( e^{ik_jx}/\sqrt{L} \) by \( e^{iS(x)} \) as in the previously discussed case of phase im-
where the \( \phi_j(x,t) \) are evolved by the single-particle TDSE starting from \( \phi_j(x,0+) = e^{ik_j x}e^{i\theta_j(x)}/\sqrt{L} \). The single particle density at time \( t \) is

\[
\rho(x,t) = N \int |\psi_B(x,0+)|^2 dx \prod_{j} |\phi_j(x,t)|^2 \text{d}x
\]

and their phases oscillate as a function of \( j/t \) and their phases oscillate as a function of \( j - \ell \), and this phase variation is compounded by oscillation of the phases of the factors \( a_{\ell}^{P}(K_0)a_{\ell}^{P}(K_0) \) from Eq. 4. One therefore expects that in the thermodynamic limit the net off-diagonal contribution will be small compared with the diagonal ones and will be dropped, an approximation in the same spirit as the random phase approximation. The diagonal contributions \( P = P' \) behave very differently. Since Eq. 4 holds only in \( R_1 \) and is to be extended to other sectors by Bose symmetry, the integrations over \( x_2, \ldots, x_N \) have different limits for each different ordering of \( x, x_2, \ldots, x_N \). However, summing over all permutations, collecting coefficients of \( |\phi_j(x)|^2 \), and performing appropriate permutations of the names of integration variables, one finds that the integrations over \( x_2, \ldots, x_N \) sum to a multiple of

\[
\int_{-L/2}^{L/2} \prod_{j} |\phi_j(x_2)|^2 \prod_{\ell} |\phi_{\ell}(x_N)|^2 = 1,
\]

and the same holds for the coefficients of the other \( |\phi_j(x)|^2 \). Noting also that \( |a_{\ell}^{P}(K_0)|^2 = 1 \) by Eq. 6 and that there are \((N-1)!\) permutations \( P \) such that \( P1 = j \) for each \( j = 1, \ldots, N \), one finds that the final expression collapses simply to the sum of absolute squares of all \( N \) orbitals. Recalling that approximation of the nonperiodic LL exponentials \( e^{ik_{\ell} x} \) by the periodic exponentials \( e^{ik_{\ell} x} \) in the thermodynamic limit requires inclusion of a density of states factor, one obtains

\[
n(x,t) = \sum_{\nu=-\nu_0}^{\nu_0} \beta(k_{\nu})|\phi_{\nu}(x,t)|^2 \quad (8)
\]

where \( \nu_0 \) and \( \beta(k_{\nu}) \) were defined in the previous discussion of the thermodynamic limit.

To apply this to gray soliton generation consider a ring of circumference \( L \) with circumferential coordinate \( x \) with \(-L/2 \leq x \leq L/2 \) and impose a phase shift \( \pi \) on the left half \(-L/2 \leq x \leq 0 \). The density of states was determined by solution of Eqs. (3.18) and (3.20) of LL 10, 39, and the TDSE propagation was effected by FFT of the initial orbitals \( e^{ik_{\nu}x}e^{i\theta_j(x)} \) after which the resultant Fourier components have trivial time dependence \( e^{-ik_{\nu}t} \). The density functions showing soliton propagation are shown in Fig. 4 for the cases \( \gamma = \infty \) (TG limit), \( \gamma = 1 \) (intermediate regime), and \( \gamma = 0.05 \) (Bogoliubov regime) for \( \nu_0 = 32 \), corresponding to a LL-Fermi sea of 65 orbitals. The periodicity cell lengths \( L \) were adjusted to keep the mean density (65 in the units used) and hence the LL-Fermi momentum fixed, using Eqs. (3.14)-(3.21) of LL 19.

The shape of the density profile is quite insensitive to \( \gamma \) apart from the indicated scaling of the periodicity length \( L \) and observation time \( t \), in spite of strong peaking of the density of states about low momenta as \( \gamma \) varies from the TG regime \( \gamma \gg 1 \) to the Bogoliubov regime \( \gamma \ll 1 \). This insensitivity is consistent with scaling of the allowed momenta \( k_{\nu} = 2\pi/L \) inversely with \( L \) and scaling of observation times \( t \) in their propagation factors \( e^{-ik_{\nu}t} \) directly with \( L^2 \).

One can define a LL-Fermi sea quasimomentum distribution function \( f(k) \) as the absolute square of the Fourier transform of each orbital, weighted by the LL quasimomentum density of states and summed over all orbitals. This was evaluated with the aid of an FFT code and is shown in Fig. 2 for the case \( \gamma = 1 \) before and just after the \( \pi \) phase imprint. The perturbation promotes particles just under the LL-Fermi surface to states just above the
surface, indicating that Pauli blocking is still quite effective at \( \gamma = 1 \), to be expected since the density of states is still almost flat. The quasimomentum distribution is not the same as the true momentum distribution, which is peaked about \( k = 0 \) even in the TG limit \( [17] \) and becomes increasingly peaked as \( \gamma \) decreases \( [27] \). Nevertheless, the energy is given exactly by \( E = \sum_k k^2 f(k) \) both for the LL ground state \( [10] \) and the LL excited states \( [23] \). It is thus reasonable to approximate the energy of the phase-imprinted state by the same simple expression. Furthermore, since one starts from the ground state which has zero dispersion, the energy dispersion after the pulse should be of the same order as the mean excitation energy \( E_{\text{after}} - E_{\text{before}} \). The FFT evaluation yields \( (E_{\text{after}} - E_{\text{before}})/E_{\text{before}} = 0.083 \ll 1 \), suggesting that the soliton density profiles of Fig. 1 are good approximations to exact profiles which are not currently calculable.

Discussion: The LL solitons exhibit density ripples absent from Gross-Pitaevskii solitons even for \( \gamma \) as small as \( 0.05 \), being many-orbital features stemming from fermionization which is present for any nonzero \( \gamma \), no matter how small \( [14, 34] \). Even the ground state of a trapped LL gas is currently unknown, so it is not clear whether or not such ripples will be present in soliton-like dynamics of a trapped LL-gas, an important topic for future investigations. The approach used for \( \delta(t) \) pulses could be extended to arbitrary potentials \( v(x, t) \) by split-operator propagation of orbitals. Could it be extended to the trapped LL gas?

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