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The dynamics of the one-dimensional delta-function Bose gas

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Abstract

We give a method to solve the time-dependent Schrödinger equation for a system of one-dimensional bosons interacting via a repulsive delta function potential. The method uses the ideas of Bethe Ansatz but does not use the spectral theory of the associated Hamiltonian.

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1. Introduction

In this paper we give an alternative approach to solve the time-dependent Schrödinger equation for a system of one-dimensional bosons interacting via a delta function potential. This quantum many-body model, called the *Lieb–Liniger model* [6, 7], is 'exactly solvable' by means of Bethe Ansatz [2] in the sense that the ground-state energy [7], the excitation spectrum [6] as well as equilibrium thermodynamics [13] are known. (See [5, 10] for textbook treatments.) Current widespread interest in the Lieb–Liniger model has arisen because of its connection to ultracold gases confined in a quasi one-dimensional trap. Indeed, it has been recently shown that the Lieb–Liniger model for one-dimensional bosons 'can be rigorously derived via a scaling limit from a dilute three-dimensional Bose gas with arbitrary repulsive interaction potential of finite scattering length' [8]. These applications focus interest on the time-dependent solutions. For a review of these developments see [3].

Recall that the Lieb–Liniger δ -function (*N*-particle) Bose gas Hamiltonian is

$$H = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2c \sum_{j < k} \delta(x_j - x_k)$$
⁽¹⁾

where c > 0 (the repulsive case) and $x_j \in \mathbb{R}^3$ Most work [1, 4, 6, 7, 9, 12] focuses on the eigenfunctions and eigenvalues of *H* from which, in principle, any solution $\Psi(x; t)$ of the

³ We choose units where 2m = 1 and $\hbar = 1$.

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time-dependent Schrödinger equation

$$H\Psi = i\frac{\partial\Psi}{\partial t},\tag{2}$$

subject to the initial condition

$$\Psi(x;0) = \Psi(x_1, \dots, x_N; 0) = \psi_0(x_1, \dots, x_N), \tag{3}$$

may be constructed⁴. In practice, due to the complexity of the Bethe eigenfunctions and the nonlinear Bethe equations, it is difficult to analyze time-dependent solutions whose initial conditions are not eigenfunctions. We give here an alternative to the spectral method for solving (2).

Since different physical conditions require different choices of the initial wavefunction ψ_0 , we develop here a flexible mathematical structure to incorporate these different choices. Suppose we solve (2) with the initial condition

$$\psi_{\delta}(x) = \psi_{\delta}(x_1, \dots, x_N) = \frac{1}{N!} \sum_{\sigma \in \mathbb{S}_N} \prod_{j=1}^N \delta(x_{\sigma(j)} - y_j)$$
(4)

where \mathbb{S}_N is the permutation group acting on $\{1, \ldots, N\}$. Here $y_j \in \mathbb{R}$ are fixed and without loss of generality we may assume

$$y_1 < y_2 < \dots < y_N. \tag{5}$$

If $\Psi_{\delta}(x, y; t)$ denotes this solution, then the solution to (2) satisfying (3) is

$$\Psi(x;t) = \int_{\mathbb{R}^N} \Psi_{\delta}(x,y;t) \psi_0(y) \,\mathrm{d}y$$

 $(dy = dy_1 \cdots dy_N)$. The subject of this paper is Ψ_{δ} , a Green's function for (2).

We remark that there are two natural choices for the initial wavefunction ψ_0 . The free particle Gaussian wavefunction localized at y is⁵

$$\varphi_a(x; y, p) = \frac{1}{(2\pi)^{1/4}\sqrt{a}} e^{-(x-y)^2/(4a^2)} e^{ipx}.$$

Thus an initial condition where the particles are separated and free is

$$\psi_{\text{free}}(x) = c_N \sum_{\sigma \in \mathbb{S}_N} \prod_{j=1}^N \varphi_a(x_{\sigma(j)}; y_j, p_j)$$

where c_N is a normalization constant.

A second choice is for the Bose gas to be initially confined to a subset of \mathbb{R} and in its ground state. Solving (2) with this initial condition corresponds to the confined Bose gas freely expanding into all of \mathbb{R} . The ground-state wavefunction for confinement to \mathbb{R}^+ has been computed by Gaudin [4] and confinement to a hard wall box by Batchelor *et al* [1].

We now recall a well-known [7, 10] reformulation of the problem. Since we seek symmetric solutions, it is sufficient to solve (2) in the region

$$\mathcal{R}: -\infty < x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N < \infty. \tag{6}$$

In the interior of \mathcal{R} , e.g. \mathcal{R}^o : $x_1 < x_2 < \cdots < x_N$, the δ -functions are zero and we have the free Schrödinger equation

$$-\sum_{i} \frac{\partial^2 \Psi_{\delta}}{\partial x_i^2} = \mathbf{i} \frac{\partial \Psi_{\delta}}{\partial t}.$$
(7)

⁴ ψ_0 is a given symmetric function of the coordinates x_j .

⁵ Thus $|\varphi_a(x; y, p)|^2$ is the Gaussian distribution centered at y with variance a^2 . Solving the time-dependent free Schrödinger equation shows that $\langle x \rangle = 2pt$; and hence, 2p is the classical velocity. (Recall 2m = 1.)

That is the effect of the δ -functions are confined to the boundary of \mathcal{R} , e.g. on the hyperplanes $x_j = x_{j+1}$, and their effect can be formulated as a boundary condition on the hyperplanes (we also use the fact that Ψ_{δ} is a symmetric function):

$$\left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j}\right) \Psi_{\delta}\Big|_{x_{j+1} = x_j} = c \Psi_{\delta}|_{x_{j+1} = x_j}.$$
(8)

Thus the problem is to solve (7) in \mathcal{R}^o subject to the boundary conditions (8) and the initial condition in \mathcal{R}

$$\Psi_{\delta}(x;0) = \prod_{j=1}^{N} \delta(x_j - y_j) \tag{9}$$

where y_j satisfy (5) and we have dropped the normalization constant N! since it can be incorporated at the end. The solution Ψ_{δ} is given below in (14).

2. Bethe Ansatz

We now explain how the ideas of Bethe Ansatz [2, 7] can be employed to solve the timedependent problem without using the spectral theory of the operator *H*. Since we avoid the eigenvalue problem, there are no *Bethe equations* in this approach⁶. To set the notation and to see the argument in its simplest form, we first solve N = 2.

2.1.
$$N = 2$$

It is elementary to verify that

$$\int_{\mathbb{R}} \int_{\mathbb{R}} A(k_1, k_2) e^{i(k_1 x_1 + k_2 x_2)} e^{-i(\varepsilon(k_1) + \varepsilon(k_2))t} dk_1 dk_2$$

with

$$\varepsilon(k) = k^2$$

solves (7) in $x_1 < x_2$. The insight from Bethe Ansatz is to add to this solution another solution with the integration variables permuted,

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \left[A_{12}(k_1, k_2) \, \mathrm{e}^{\mathrm{i}(k_1 x_1 + k_2 x_2)} + A_{21}(k_1, k_2) \, \mathrm{e}^{\mathrm{i}(k_2 x_1 + k_1 x_2)} \right] \, \mathrm{e}^{-\mathrm{i}(\varepsilon(k_1) + \varepsilon(k_2))t} \, \mathrm{d}k_1 \, \mathrm{d}k_2,$$

so that the boundary condition (8) can be applied pointwise to the above integrand. The result is the condition

$$ik_2A_{12} + ik_1A_{21} - ik_1A_{12} - ik_2A_{21} = c(A_{12} + A_{21}),$$

or equivalently,

$$A_{21} = -\frac{c - i(k_2 - k_1)}{c + i(k_2 - k_1)} A_{12}.$$

We set

$$S_{\alpha\beta} = S_{\alpha\beta}(k_{\alpha} - k_{\beta}) = -\frac{c - i(k_{\alpha} - k_{\beta})}{c + i(k_{\alpha} - k_{\beta})}$$
(10)

so that the above reads $A_{21} = S_{21}A_{12}$. It is also convenient to set

$$S(k) = -\frac{c - \mathrm{i}k}{c + \mathrm{i}k}.\tag{11}$$

 6 The methods here are an adaptation of the methods of [11].

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Observe that S(k) extends to a holomorphic function in the lower half-plane and so its Fourier transform, $\hat{S}(z)$, is supported in $[0, \infty)$.

With the initial condition (9) in mind, we choose

$$A_{12}(k_1, k_2) = e^{-i(k_1y_1 + k_2y_2)}$$

so the above solution becomes

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \left[e^{i(k_1(x_1-y_1)+k_2(x_2-y_2))} + S_{21}(k_2,k_1) e^{i(k_2(x_1-y_2)+k_1(x_2-y_1))} \right] e^{-i(\varepsilon_{k_1}+\varepsilon_{k_2})t} dk_1 dk_2$$
(12)

where from now on $dk_j \rightarrow dk_j/2\pi$.

At t = 0 the first term evaluates to $\delta(x_1 - y_1)\delta(x_2 - y_2)$. Thus we must show

$$\int_{\mathbb{R}} \int_{\mathbb{R}} S(k_2 - k_1) e^{ik_1(x_2 - y_1) + ik_2(x_1 - y_2)} dk_1 dk_2 = 0$$

for $y_1 < y_2$ and $x_1 \le x_2$ for the solution (12) to satisfy the initial condition (9). Making the change of variables $k_2 \rightarrow k_2 + k_1$ and $k_1 \rightarrow k_1$ in the above integral, we have (after performing the resulting integration over k_1)

$$\delta(x_1 + x_2 - y_1 - y_2) \int_{\mathbb{R}} S(k_2) \, \mathrm{e}^{\mathrm{i}k_2(x_1 - y_2)} \, \mathrm{d}k_2 = \delta(x_1 + x_2 - y_1 - y_2) \, \hat{S}(x_1 - y_2).$$

Now $\hat{S}(x_1 - y_2)$ is nonzero only in the region

$$x_1 - y_2 \ge 0$$

and the delta function requires that $x_1 + x_2 = y_1 + y_2$ for a nonzero contribution. But in \mathcal{R}

$$2x_1 \leqslant x_1 + x_2 = y_1 + y_2 < 2y_2,$$

i.e. $x_1 < y_2$. Hence the integral in the region \mathcal{R} is zero, and thus, we conclude (12) is the sought after solution $\Psi_{\delta}(x)$ for N = 2.

2.2. General N

Let $\sigma \in S_N$ be a permutation of $\{1, ..., N\}$. Recall that an inversion in a permutation σ is an ordered pair $\{\sigma(i), \sigma(j)\}$ in which i < j and $\sigma(i) > \sigma(j)$. We set

$$A_{\sigma} = \prod \{ S_{\alpha\beta} : \{\alpha, \beta\} \text{ is an inversion in } \sigma \}$$
(13)

where $S_{\alpha\beta}$ is defined by (10). Thus, for example, $A_{231} = S_{21}S_{31}$ and $A_{id} = 1$. We claim the solution that satisfies (7) with boundary conditions (8) and the initial condition (9) is

$$\Psi_{\delta}(x;t) = \sum_{\sigma \in \mathcal{S}_N} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} A_{\sigma} \prod_{j=1}^{N} e^{ik_{\sigma(j)}(x_j - y_{\sigma(j)})} e^{-it\sum_{j} \varepsilon(k_j)} dk_1 \cdots dk_N.$$
(14)

First, it is clear that (14) satisfies (7) in \mathcal{R}^o . As demonstrated in [7], if $T_i\sigma$ denotes σ with the entries $\sigma(i)$ and $\sigma(i + 1)$ interchanged, the boundary conditions will be satisfied provided that

$$A_{T_i\sigma} = S_{\sigma(i+1)\sigma(i)}A_{\sigma}$$

for all σ . Let us see why this relation holds. Let $\alpha = \sigma(i)$, $\beta = \sigma(i+1)$, and suppose $\alpha > \beta$. Then $\{\alpha, \beta\}$ is an inversion for σ but not for $T_i\sigma$, so $S_{\alpha\beta}$ is a factor in A_{σ} but not in $A_{T_i\sigma}$, and all other factors are the same. Therefore, using $S_{\alpha\beta}S_{\beta\alpha} = 1$, we have

$$A_{T_i\sigma} = S_{\beta\alpha}A_{\sigma} = S_{\sigma(i+1)\sigma(i)}A_{\sigma}.$$

The same identity holds immediately if $\beta > \alpha$, since $\{\beta, \alpha\}$ is an inversion for $T_i \sigma$ but not for σ .

As in the N = 2 case, the term corresponding to the identity permutation in (14) satisfies the initial condition (9). Thus to complete the proof we must show

$$\sum_{\sigma \in \mathcal{S}_N, \sigma \neq id} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} A_{\sigma} \prod_{j=1}^N e^{ik_{\sigma(j)}(x_j - y_{\sigma(j)})} dk_1 \cdots dk_N = 0.$$

Let $I(\sigma)$ denote the integral corresponding to σ term in the above sum. Recalling the definition (11) of *S*, the integrand for $I(\sigma)$ becomes

$$\prod_{j=1}^{N} e^{ik_{\sigma(j)}(x_j - y_{\sigma(j)})} \prod \{ S(k_{\alpha} - k_{\beta}) : \{\alpha, \beta\} \text{ is an inversion in } \sigma \}.$$

We again use the fact that S(k) extends analytically into the lower half-plane.

If a number γ appears on the left side of an inversion and never on the right side then in the integrand it appears only in factors of the form $S(k_{\gamma} - k_{\beta})$ and so integrating with respect to k_{γ} shows that the integrand is zero unless

$$x_{\sigma^{-1}(\gamma)} \geqslant y_{\gamma}. \tag{15}$$

Similarly, if a number δ appears on the right side of an inversion and never on the left side then in the integrand it appears only in factors of the form $S(k_{\alpha} - k_{\delta})$ and so integrating with respect to k_{δ} shows that the resulting integrand is zero unless

$$x_{\sigma^{-1}(\delta)} \leqslant y_{\delta}.$$
 (16)

We show $I(\sigma) = 0$ by induction on *N*. If $\sigma(1) = 1$ then 1 does not appear in an inversion, we can integrate with respect to k_1 , and we are reduced to the case N - 1. So assume $\sigma(1) = \gamma > 1$. Then $(\gamma, 1)$ is an inversion and there is no inversion of the form (α, γ) because γ appears in slot 1. So we can apply (15) with this γ and get the resulting integrand is zero unless

$$x_1 \ge y_{\gamma}$$
.

Next we observe as before that $(\gamma, 1)$ is an inversion, but now that 1, which appears on the right side of the inversion, cannot appear on the left side of an inversion (obviously). So we can apply (16) with $\delta = 1$ and get

$$x_{\sigma^{-1}(1)} \leq y_1.$$

Since $y_1 < y_{\gamma}$ the two inequalities give $x_{\sigma^{-1}(1)} < x_1$, which cannot happen. This completes the proof of (14).

The limit of impenetrable bosons is the limit $c \to \infty$. In this limit $S_{\alpha\beta} \to -1$ and $A_{\sigma} \to (-1)^{inv(\sigma)}$ where $inv(\sigma)$ is the number of inversions in σ . Thus in \mathcal{R}

$$\Psi_{\delta}(x;t) \to \Psi_{\infty}(x;t) = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \det(\mathrm{e}^{ik_{\alpha}(x_{\beta}-y_{\alpha})-it\varepsilon_{k_{\alpha}}}) \,\mathrm{d}k_{1} \cdots \,\mathrm{d}k_{N}$$
(17)

and the extension to \mathbb{R}^N follows by requiring Ψ_∞ to be a symmetric function of x_i .

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