

Supplementary Material for “Engineering momentum profiles of cold-atom beams”

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IMPURITY IN A BOSE GAS

To model one impurity atom that moves through a one-dimensional environment made of N cold bosonic atoms, we employ the following Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial y^2} + \lambda \sum_{i>j=1}^N \delta(x_i - x_j) + g \sum_{i=1}^N \delta(x_i - y), \quad (1)$$

where M is the mass of the impurity atom, and m is the mass of a bosonic particle. The position of the impurity is y , bosons are at the coordinates $\{x_i\}$. We assume that the realistic boson-boson and boson-impurity interactions are well-described by the zero-range potentials of strengths λ and g , respectively. The environment is large by assumption. To describe it, the periodic boundary conditions are used: The particles move in a ring of the circumference L , such that $0 < x_i < L$ and $0 < y < L$. We are interested in the thermodynamic limit: $N, L \rightarrow \infty$ with a fixed value of the density $\rho = \frac{N}{L}$.

If the system is non-interacting ($\lambda = g = 0$), the eigenstates are written as $e^{2\pi i \frac{n_1 x_1 + \dots + n_N x_N + m y}{L}}$, where n_1, \dots, n_N and m are arbitrary integers. For non-vanishing interactions we use these functions to write an eigenfunction of the Hamiltonian as $\Psi = \sum_{\{n_j\}, m} a_{\{n_j\}, m} e^{2\pi i \frac{\sum n_j x_j + m y}{L}}$. Because all interactions are pairwise, the total (angular) momentum of the system must be conserved, and we write it as $\mathcal{P} = \frac{2\pi\hbar}{L} \left(\sum_j n_j + m \right)$. A conserved quantity (\mathcal{P}) allows us to exclude one variable from the consideration. We write the function Ψ as $\Psi = e^{i \frac{\mathcal{P} y}{\hbar}} \sum_{\{n_j\}, m} a_{\{n_j\}, m} e^{2\pi i \frac{\sum n_j z_j}{L}} \equiv e^{i \frac{\mathcal{P} y}{\hbar}} \psi(z_1, \dots, z_N)$ with $z_i = L\theta(y - x_i) + x_i - y$, where $\theta(x)$ is the Heaviside step function, i.e., $\theta(x > 0) = 1$ and zero otherwise. The variables z_i are defined such that $0 \leq z_i \leq L$ and the impurity is placed at $z = 0$ ($z = L$). Now if we insert this function into the Schrödinger equation, $H\Psi = E\Psi$, we obtain the following equation for ψ ($0 < z_i < L$)

$$-\frac{\hbar^2}{2m} \sum_i \frac{\partial^2 \psi}{\partial z_i^2} - \frac{\hbar^2}{2M} \left(\sum_i \frac{\partial}{\partial z_i} \right)^2 \psi + i \frac{\hbar \mathcal{P}}{M} \sum_i \frac{\partial \psi}{\partial z_i} + \lambda \sum_{i>j} \delta(z_i - z_j) \psi = \left(E - \frac{\mathcal{P}^2}{2M} \right) \psi, \quad (2)$$

which must be supplemented with the boundary conditions:

$$\psi(z_i = 0) = \psi(z_i = L); \quad \frac{\partial \psi}{\partial z_i} \Big|_{z_i=L^-}^{z_i=0^+} = \frac{2g\kappa}{\hbar^2} \psi(z_i = 0), \quad (3)$$

where $\kappa = mM/(m + M)$ is the reduced mass.

By assumption the bosons interact weakly, such that the ansatz $\psi = \prod_i \Phi(z_i)$ can be used to approximate the system. To minimize the expectation value of the Hamiltonian the function $\Phi(z)$ must satisfy the following non-linear Schrödinger equation

$$-\frac{\hbar^2}{2\kappa} \frac{\partial^2 \Phi}{\partial z^2} + i \frac{\hbar \mathcal{P}}{M} \frac{\partial \Phi}{\partial z} - i \frac{\hbar^2 (N-1) A}{M} \frac{\partial \Phi}{\partial z} + \lambda (N-1) |\Phi|^2 \Phi = \mu \Phi, \quad (4)$$

where $A = -i \int \Phi(x)^* \frac{\partial}{\partial x} \Phi(x) dx$ defines the momentum of a boson, and μ is the Lagrange multiplier. We rewrite this equation as

$$-\frac{\partial^2 \Phi}{\partial z^2} + i v \frac{\partial \Phi}{\partial z} + \tilde{\lambda} (N-1) |\Phi|^2 \Phi = \tilde{\mu} \Phi, \quad (5)$$

where $\tilde{\mu} = \frac{2\kappa\mu}{\hbar^2}$, $\tilde{\lambda} = \frac{2\kappa\lambda}{\hbar^2}$, and $v = \frac{2\kappa P}{M\hbar}$ with $P = \mathcal{P} - \hbar A(N-1)$. P defines the momentum of the impurity in the thermodynamic limit; note that A is determined by P , and there is a unique value of \mathcal{P} for a given P . The boundary conditions for Eq. (5) read

$$\Phi(z = 0) = \Phi(z = L); \quad \frac{\partial \Phi}{\partial z} \Big|_{z=L^-}^{z=0^+} = \tilde{g} \Phi(0), \quad (6)$$

where $\tilde{g} = \frac{2\kappa g}{\hbar^2}$. The non-linear equation (5) has an analytic steady solution [1], which determines the properties of the dressed impurity in our problem. Let us first consider the non-interacting impurity $g = 0$. In this case the solution

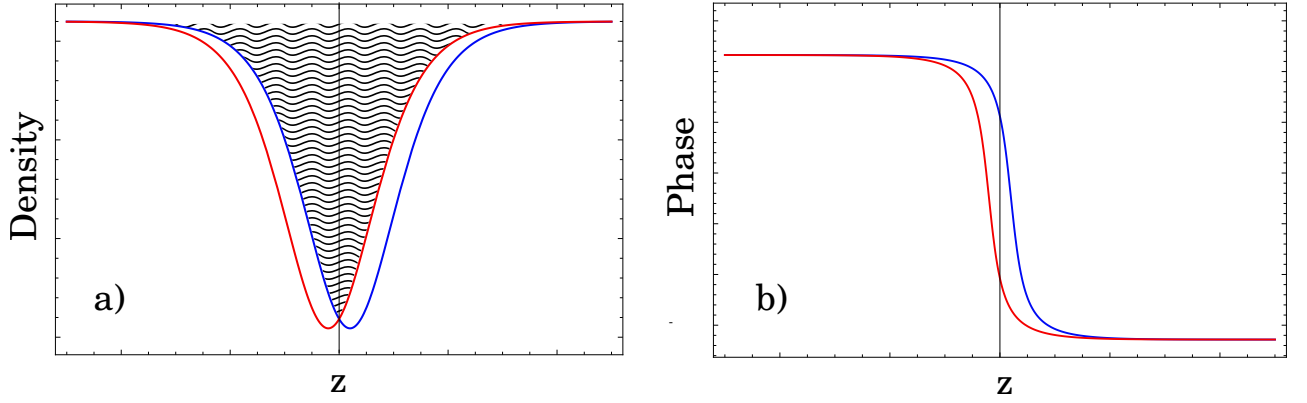


FIG. 1. Panel **a)**: The density, $|\Phi|^2 N$, of the Bose gas for $z_0 = a$ (red curve), $z_0 = -a$ (blue curve) ($a > 0$, the exact value of a is not important for our discussion). Note that the minimum of the density is at $-a$. The shaded area is a combination of the two solutions with the singularity at $z = 0$. Panel **b)**: The phase, ϕ , of the Bose gas for the densities from **a)**.

for $v > 0$ is [2, 3]

$$\Phi = \sqrt{\frac{\tilde{\mu}}{\tilde{\lambda}(N-1)}} \left(1 - \beta \operatorname{sech}^2 \left[\sqrt{\frac{\tilde{\mu}\beta}{2}}(z + z_0) \right] \right)^{\frac{1}{2}} e^{i\phi(z)}, \quad (7)$$

$$\phi(z) = -\pi\theta(z + z_d) + \arctan \left(\frac{\sqrt{\frac{2v^2}{\tilde{\mu}}}\beta}{\exp[\sqrt{2\tilde{\mu}\beta}(z + z_0)] - 2\beta + 1} \right), \quad (8)$$

where $\beta = 1 - v^2/(2\tilde{\mu})$, z_0 is some parameter that determines the origin and z_d is the point where \arctan reaches $\pi/2$. It is worthwhile noting that the solution for $v < 0$ is Φ^* . The solution from Eqs. (7) and (8) is plotted in Fig. 1; for simplicity it is plotted in the interval $-L/2 < z < L/2$, the region $0 < z < L$ easily follows.

To describe an interacting impurity, we combine two moving solitons with $\pm z_0$, which creates a singularity at $z = 0$ [1, 4]. Therefore, a dressed impurity in our model is a topological defect with a dissipationless propagation. We write the corresponding ‘wave function’ as

$$\Phi = \sqrt{\frac{\tilde{\mu}}{\tilde{\lambda}(N-1)}} \left(1 - \beta \operatorname{sech}^2 \left[\sqrt{\frac{\tilde{\mu}\beta}{2}}(z \pm z_0) \right] \right)^{\frac{1}{2}} e^{i\phi(z)}, \quad (9)$$

with

$$\phi(z) = \delta\phi\theta(-z) + \arctan \left(\frac{\sqrt{\frac{2v^2}{\tilde{\mu}}}\beta}{\exp[\sqrt{2\tilde{\mu}\beta}(z \pm z_0)] - 2\beta + 1} \right), \quad (10)$$

where $z_0 > 0$ is discussed below, the parameter $\delta\phi$ is not important for the further derivations, it reassures that the phase is a continuous function; the plus sign in \pm corresponds to $z > 0$ and the minus sign to $z < 0$. This function is illustrated in Fig. 1. The density has a non-analytic derivative at $z = 0$. The phase is a continuous function at $z = 0$ (its derivative is also continuous). Note that the wave function is not periodic (see Eq. (10)). This non-periodicity is not important for our discussion, because we are interested in the behavior of the bosons close to the impurity. It suggests that a grey soliton must be formed upon a change of interaction parameters to take care of the phase slip.

The parameter $\tilde{\mu}$ is found from the normalization condition $\int \Phi^2 = 1$. For $N \rightarrow \infty$, we obtain

$$\tilde{\mu} = \gamma\rho^2 \frac{N-1}{N} \left(1 - 2\sqrt{2\beta_0} \frac{(\tanh(d) - 1)}{\sqrt{\gamma}N} \right), \quad (11)$$

where $\gamma = \tilde{\lambda}/\rho$, $\rho = N/L$, $\beta_0 = 1 - v^2/(2\gamma\rho^2)$, and $d = \sqrt{\frac{\gamma\beta_0}{2}}\rho z_0$. The equation to determine z_0 is found by using the boundary conditions at $z = \{0, L\}$

$$\frac{\tilde{g}}{\rho\sqrt{2\gamma}} = \frac{\beta_0^{\frac{3}{2}} \tanh(d)}{-\beta_0 + \cosh^2(d)}. \quad (12)$$

This equation is cubic (in $\tanh(d)$), hence, the solutions can be found in a closed form. There are three solutions. However, only two will lead to the acceptable values of z_0 . We will refer to these steady solutions as the ‘polaron’ and the ‘polaron-soliton’ pair, because in the limit $g \rightarrow 0$ the former corresponds to the ground state, and the latter to a gray soliton. The ‘polaron-soliton’ pair is expected to be unstable (small perturbations lead to a decay of this steady solution [1]), therefore, we do not consider it. The solutions merge for z_m

$$\tanh^2 \left(\sqrt{\frac{\gamma\beta_0}{2}} \rho z_m \right) = \frac{\sqrt{1 + \frac{4v^2}{\gamma\rho^2}} - (1 + \frac{v^2}{\gamma\rho^2})}{2\beta_0}, \quad (13)$$

which is derived by taking a derivative of Eq. (12) with respect to z_0 and equating the resulting expression to zero – this determines the maximum value of g for which (for a fixed β_0) there is a steady solution. Equations (12) and (13) give the equation for the critical value of v_c :

$$\frac{\tilde{g}}{\rho\sqrt{\gamma}} = \frac{3 - \sqrt{1 + \frac{4v^2}{\gamma\rho^2}}}{-1 + \sqrt{1 + \frac{4v_c^2}{\gamma\rho^2}}} \sqrt{\sqrt{1 + \frac{4v_c^2}{\gamma\rho^2}} - 1 - \frac{v_c^2}{\gamma\rho^2}}. \quad (14)$$

For $v > v_c$ (see Fig. 4 of the main text) there is no steady solutions.

Now we can calculate the energy of the dressed impurity in the thermodynamic limit

$$\mathcal{E} \equiv \lim_{N \rightarrow \infty, \frac{N}{L} \rightarrow \rho} [E(c, P) - E(c = 0, P = 0)], \quad (15)$$

where

$$E(c, P) = \frac{P^2}{2M} + \mu N - \frac{\hbar^2 A^2 N(N-1)}{2M} - \lambda N(N-1) \int_0^{L/2} |\Phi|^4 dz. \quad (16)$$

Using these expressions we derive

$$\mathcal{E} = \frac{P^2}{2M} + \frac{\hbar^2 \rho^2 \sqrt{2\gamma\beta}}{2\kappa} \frac{3}{3} [4b + (-4b + \beta \text{sech}^2(d)) \tanh(d)] + \frac{\hbar P}{M} \lim_{N \rightarrow \infty} AN, \quad (17)$$

where $b = 1 + \frac{v^2}{4\lambda\rho} = 1 + \frac{\kappa P^2}{2M^2\lambda\rho}$. This energy for $v \rightarrow 0$ can be written as

$$\mathcal{E} \simeq \epsilon + \frac{P^2}{2m_{\text{eff}}}, \quad (18)$$

where ϵ is the effective energy of the dressed impurity, and m_{eff} is the effective mass.

The parameters m_{eff} and ϵ calculated using Eq. (18) agree well with the results in the literature [5], supporting the use of the non-linear Schrödinger equation for solving the problem. However, further work is required to understand other properties of a dressed impurity in this formalism. First of all, it will be interesting to investigate the critical momentum, which is supersonic in the employed model for $g \rightarrow 0$ and for not heavy impurities. Indeed, the model we solve is equivalent to a heavy impurity moving in a gas of bosons with mass κ , which has a different speed of sound. Note that Fig. 4 of the main text reports on a heavy impurity ($M/m \gg 1$) for which this problem does not occur. It will be also interesting to investigate the residue – the overlap between the wave function that describes a state with $g = 0$ and the wave function that describes an interacting state. In the present model, the impurity changes the order parameter only locally, which means a non-zero residue (see [6] for $P = 0$), contradicting other studies on the topic [7, 8]. To understand this disagreement, one could calculate the overlap using an exactly solvable model, e.g., a heavy impenetrable impurity in a Bose gas (solvable by Bethe ansatz).

BOUNDARY-AUGMENTED COST FUNCTION

Equation (6) shows the boundary-augmented cost function which includes a term that increases the cost for link-potential solutions that extend beyond the support region $x \in [-x_0, x_0]$. This added terms is

$$J_{\text{boundary}} = \alpha \sum_i^N J_{\text{boundary}}^i, \quad (19)$$

where

$$J_{\text{boundary}}^i = \int_{|x| > x_0} dx |V_i(x; A_i, \mu_i, \sigma_i)|^2. \quad (20)$$

Assuming the Gaussian potential form as in Eq. (5), this evaluates to

$$J_{\text{boundary}}^i = \frac{\sqrt{\pi}}{2} A_i^2 \sigma_i \left[\text{erfc} \left(\frac{x_0 + \mu_i}{\sigma_i} \right) + \text{erfc} \left(\frac{x_0 - \mu_i}{\sigma_i} \right) \right], \quad (21)$$

where erfc is the complementary error function.

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