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

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

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: $N, L \to \infty$ 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 $e^{2\pi i\frac{n_1 x_1 + \ldots + n_N x_N + my}{L}}$, where $n_1, \ldots, n_N$ and m are arbitrary integers. For non-vanishing interactions we use these functions to write an eigenfunction of the Hamiltonian as $\Psi = \sum_{\{n_j\},m} a_{\{n_j\},m} e^{2\pi i\frac{\sum n_j x_j + my}{L}}$. 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 $\Psi = e^{i\frac{\mathcal{P}y}{\hbar}}\sum_{\{n_j\},m} a_{\{n_j\},m} e^{2\pi i\frac{\sum n_j z_j}{L}} \equiv e^{i\frac{\mathcal{P}y}{\hbar}}\psi(z_1, ..., z_N)$ 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 $\psi(0 < z_i < L)$

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

which must be supplemented with the boundary conditions:

$$\psi(z_i = 0) = \psi(z_i = L); \qquad \left.\frac{\partial\psi}{\partial z_i}\right|_{z_i=L^-}^{z_i=0^+} = \frac{2g\kappa}{\hbar^2}\psi(z_i = 0), \tag{3}$$

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

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

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

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

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 because A is determined by P, there is a unique value of $\mathcal{P}$ for a given P_I. The boundary conditions for Eq. (5) read

$$\Phi(z = 0) = \Phi(z = L); \qquad \left.\frac{\partial\Phi}{\partial z}\right|_{z=L^-}^{z=0^+} = \tilde{g}\Phi(0), \tag{6}$$

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

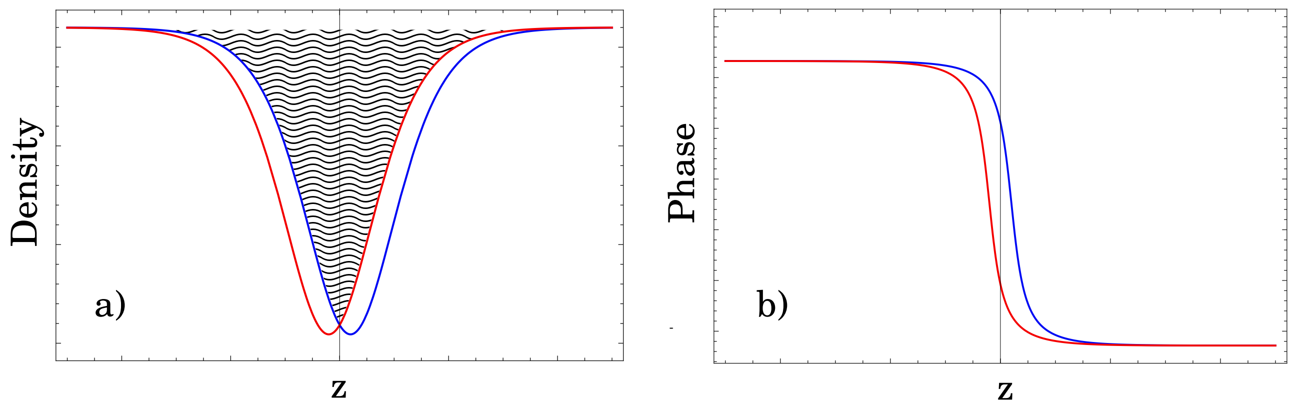

FIG. 1. Panel **a)**: The density, $|\Phi|^2 N$, of the Bose gas for $z_0 = a$ (red curve), $z_0 = -a$ (blue curve) ($a > 0$). Note that the minimum of the density is at $-a$. The shaded area is a combination of the two solutions with the singularity at $z = 0$. Panel **b)**: The phase, ϕ, of the Bose gas for the densities from **a)**.

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

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

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

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

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

with

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

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 $N \to \infty$, we obtain

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

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 $z=\{0,L\}$

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

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 $g\to 0$ 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 will lead to a decay of this steady solution [1]), therefore, we do not consider it. The solutions merge for z_m

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

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:

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

For $v>v_c$ (see Fig. 1 of the main text) there is no steady solutions.

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

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

where

$$E(c,P)=\frac{P^2}{2M}+\mu N-\frac{\hbar^2A^2N(N-1)}{2M}-gN(N-1)\int_0^{L/2}|\Phi|^4\mathrm{d}z. \tag{16}$$

Using these expressions we derive

$$\mathcal{E}=\frac{P_I^2}{2M}+\frac{\hbar^2\rho}{2\kappa}\frac{\sqrt{2\tilde{g}\rho\beta}}{3}\left[4b+(-4b+\beta\mathrm{sech}^2(d))\tanh(d)\right]+\frac{\hbar P_I}{M}\lim_{N\to\infty}AN, \tag{17}$$

where $b=1+\frac{v^2}{4\tilde{g}\rho}=1+\frac{\kappa P_I^2}{2M^2g\rho}$. This energy for $v\to 0$ can be written as

$$\mathcal{E}\simeq\epsilon+\frac{P_I^2}{2m_{\mathrm{eff}}}, \tag{18}$$

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 the non-linear Schrödinger equation agree well with the results in the literature [5]. This agreement supports methods for our discussion. Still, further work is required to understand properties of a dressed impurity in our formalism. First of all, it will be interesting to investigate the critical momentum, which is supersonic in the employed model for $g\to 0$ and for not heavy impurities. Indeed, the model we solve may have a different speed of sound, because it is equivalent to a heavy impurity in a gas of bosons with a mass κ. It will also be interesting to calculate the residue – the overlap between wave functions that describe a state with $g=0$ and an interacting state. In the present model, the impurity changes the order parameter only locally, which means a non-zero residue; see [6] for $P=0$. It will be interesting to calculate the overlap using an exactly solvable model, e.g., a heavy impenetrable impurity in a Bose gas (solvable by Bethe ansatz) to check this result.

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

$$J_{\text{boundary}} = \alpha \sum_{i}^{N} J^{i}_{\text{boundary}}, \tag{19}$$

where

$$J^{i}_{\text{boundary}} = \int\limits_{|x|>x_0} dx \, |V_i(x; A_i, \mu_i, \sigma_i)|^2. \tag{20}$$

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

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

where erfc is the complementary error function.

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