Supplemental material: Beyond-mean-field effects in Rabi-coupled two-component Bose-Einstein condensate

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BOGOLIUBOV SPECTRUM AND BMF ENERGY IN COUPLED BINARY MIXTURES

The expansion of the Hamiltonian (1) (hereafter, equation numbers without prefix S refer to the main text) up to quadratic terms in the fields $\hat{\phi}_{\sigma,\mathbf{p}}$ (we switch to momentum space) can be written as $E_{\rm MF}+E_0+\hat{H}_2$, where $E_{\rm MF}$ is given by Eq. (2),

$$E_0=\frac{1}{2}\sum_{\mathbf{p}}\left(-p^2-\frac{n_\uparrow+n_\downarrow}{\sqrt{n_\uparrow n_\downarrow}}\frac{\Omega}{2}-g_{\uparrow\uparrow}n_\uparrow-g_{\downarrow\downarrow}n_\downarrow+\frac{1}{p^2}\sum_{\sigma\sigma'}g^2_{\sigma\sigma'}n_\sigma n_{\sigma'}\right), \tag{S1}$$

and

$$\hat{H}_2=\frac{1}{2}(\hat{\phi}^\dagger_\uparrow\hat{\phi}^\dagger_\downarrow\hat{\phi}_\uparrow\hat{\phi}_\downarrow)\begin{pmatrix}\frac{p^2}{2}+g_{\uparrow\uparrow}n_\uparrow+\frac{\Omega}{2}\sqrt{\frac{n_\downarrow}{n_\uparrow}} & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2} & g_{\uparrow\uparrow}n_\uparrow & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}\\ g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2} & \frac{p^2}{2}+g_{\downarrow\downarrow}n_\downarrow+\frac{\Omega}{2}\sqrt{\frac{n_\uparrow}{n_\downarrow}} & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow} & g_{\downarrow\downarrow}n_\downarrow\\ g_{\uparrow\uparrow}n_\uparrow & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow} & \frac{p^2}{2}+g_{\uparrow\uparrow}n_\uparrow+\frac{\Omega}{2}\sqrt{\frac{n_\downarrow}{n_\uparrow}} & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2}\\ g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow} & g_{\downarrow\downarrow}n_\downarrow & g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2} & \frac{p^2}{2}+g_{\downarrow\downarrow}n_\downarrow+\frac{\Omega}{2}\sqrt{\frac{n_\uparrow}{n_\downarrow}}\end{pmatrix}\begin{pmatrix}\hat{\phi}_\uparrow\\ \hat{\phi}_\downarrow\\ \hat{\phi}^\dagger_\uparrow\\ \hat{\phi}^\dagger_\downarrow\end{pmatrix}. \tag{S2}$$

The first four terms in the brackets on the right-hand side of Eq. (S1) arise as a compensation for the "incorrectly" ordered terms added to the quadratic form (S2) in order to make it symmetric with respect the ordering of creation and annihilation operators. This symmetrized form is convenient since it stays symmetrized under the usual Bogoliubov transformation and diagonalizes into

$$\hat{H}_2=\frac{1}{2}\sum_{\mathbf{p},\pm}E_{p,\pm}(\hat{b}^\dagger_{\mathbf{p},\pm}\hat{b}_{\mathbf{p},\pm}+\hat{b}_{\mathbf{p},\pm}\hat{b}^\dagger_{\mathbf{p},\pm})=\sum_{\mathbf{p},\pm}E_{p,\pm}\hat{b}^\dagger_{\mathbf{p},\pm}\hat{b}_{\mathbf{p},\pm}+\frac{1}{2}\sum_{\mathbf{p},\pm}E_{p,\pm}. \tag{S3}$$

The last term in Eq. (S1) is due to the standard renormalisation of the coupling constant $g_{\sigma\sigma'}\to g_{\sigma\sigma'}(1+g_{\sigma\sigma'}\sum_p 1/p^2)$ in the MF term.

The dispersion relations $E_{p,\pm}$ of the Bogoliubov modes (created by operators $\hat{b}^\dagger_{\mathbf{p},\pm}$) can be written as

$$E_{p,\pm}=\sqrt{D_p\pm\sqrt{D_p^2-\frac{p^2}{2}\left(\frac{p^2}{2}+\frac{\Omega}{2}\frac{n_\uparrow+n_\downarrow}{\sqrt{n_\uparrow n_\downarrow}}\right)\left[\prod_\sigma\left(\frac{p^2}{2}+2g_{\sigma\sigma}n_\sigma+\frac{\Omega}{2}\sqrt{\frac{n_{\bar\sigma}}{n_\sigma}}\right)-\left(2g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2}\right)^2\right]}}, \tag{S4}$$

where

$$D_p=\frac{1}{2}\sum_\sigma\left(\frac{p^2}{2}+\frac{\Omega}{2}\sqrt{\frac{n_{\bar\sigma}}{n_\sigma}}\right)\left(\frac{p^2}{2}+2g_{\sigma\sigma}n_\sigma+\frac{\Omega}{2}\sqrt{\frac{n_{\bar\sigma}}{n_\sigma}}\right)-\frac{\Omega}{2}\left(2g_{\uparrow\downarrow}\sqrt{n_\uparrow n_\downarrow}-\frac{\Omega}{2}\right). \tag{S5}$$

From Eq. (S5) one sees that the mode $E_{p,-}$ is gapless, while $E_{p,+}$ has a gap $\sqrt{2D_0}\neq 0$. The former is just the Goldstone mode due to the breaking of the $U(1)$ symmetry in the condensed state, while the latter is related to the gap introduced by Ω in having a different phase for the two spinor components. The gap vanishes for $\Omega=0$, since in this case there exist two Goldstone modes of the broken $U(1)\times U(1)$ symmetry.

The BMF energy is obtained by adding the vacuum part of Eq. (S3) to the constant energy E_0. The BMF energy thus explicitly reads

$$E_{\rm BMF}=\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\left(E_{p,+}+E_{p,-}-p^2-\frac{n_\uparrow+n_\downarrow}{\sqrt{n_\uparrow n_\downarrow}}\frac{\Omega}{2}-g_{\uparrow\uparrow}n_\uparrow-g_{\downarrow\downarrow}n_\downarrow+\frac{1}{p^2}\sum_{\sigma\sigma'}g^2_{\sigma\sigma'}n_\sigma n_{\sigma'}\right), \tag{S6}$$

where we have replaced the sum over momenta by the integral. Equation (4) is obtained from Eq. (S6) under the conditions (3) as follows. We switch to the integration variable $z = p^2$ and express the integral in Eq. (S6) as a contour integral around the branch cut of $\sqrt{z}$ along the positive real semiaxis. We then deform this contour towards the negative semiaxis such that it now goes around the branch cut of $E_{p,+}$. This is a finite interval which we map onto $x \in [0, 1]$.

EXACT SOLUTION OF THE TWO-BODY PROBLEM IN THE ZERO-RANGE APPROXIMATION

In order to characterize the two-body scattering let us introduce the single-particle states (normalization will not be important) $|+\rangle = |\uparrow\rangle - \alpha_0 |\downarrow\rangle$ and $|-\rangle = |\uparrow\rangle + |\downarrow\rangle/\alpha_0$, which are eigenstates of the operator ξ corresponding to eigenvalues $\pm\sqrt{\Omega^2+\delta^2}/2$. For two bosons we thus have three possible "total spin" states, which correspond to three scattering channels equally separated in energy by $\sqrt{\Omega^2+\delta^2}$. We define these spin states by

$$
\begin{aligned}
|--\rangle &= |\uparrow\uparrow\rangle + (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\alpha_0 + |\downarrow\downarrow\rangle/\alpha_0^2, && \text{(S7)}\\
|+-\rangle &= |\uparrow\uparrow\rangle - (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\delta/\Omega - |\downarrow\downarrow\rangle, && \text{(S8)}\\
|++\rangle &= |\uparrow\uparrow\rangle - \alpha_0(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + \alpha_0^2 |\downarrow\downarrow\rangle. && \text{(S9)}
\end{aligned}
$$

Consider the scattering of two ground-state $|-\rangle$ bosons at the collision energy q^2 below the gap $\sqrt{\Omega^2+\delta^2}$. Since the atoms interact only at zero separation, the orbital wave functions in the three channels correspond to free motion, respectively, at energies $q^2 > 0$ (open channel), $q^2 - \sqrt{\Omega^2+\delta^2} < 0$, and $q^2 - 2\sqrt{\Omega^2+\delta^2} < 0$ (these channels are therefore closed). In addition, only s waves are important. Accordingly, introducing $\kappa_1 = \sqrt{\sqrt{\Omega^2+\delta^2} - q^2}$ and $\kappa_2 = \sqrt{2\sqrt{\Omega^2+\delta^2} - q^2}$ we write the two-body scattering state as

$$
\left[\frac{\sin(qr)}{qr} - a\frac{\cos(qr)}{r}\right]|--\rangle + C_1\frac{e^{-\kappa_1 r}}{r}|+-\rangle + C_2\frac{e^{-\kappa_2 r}}{r}|++\rangle, \tag{S10}
$$

where the parameters a, C_1, and C_2 are fixed by three zero-range Bethe-Peierls boundary conditions ensuring that for $r \to 0$ the projections of Eq. (S10) on the spin states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$ are proportional, respectively, to $1 - a_{\uparrow\uparrow}/r$, $1 - a_{\uparrow\downarrow}/r$, and $1 - a_{\downarrow\downarrow}/r$. Note that C_1, C_2, and the overall prefactor in Eq. (S10) absorb the normalization coefficients omitted in Eqs. (S7-S9). Performing the projection leads to the matrix equation

$$
\begin{bmatrix}
1/a_{\downarrow\downarrow} & -\alpha_0^2(\kappa_1 - 1/a_{\downarrow\downarrow}) & \alpha_0^4(\kappa_2 - 1/a_{\downarrow\downarrow})\\
1/a_{\uparrow\downarrow} & -\alpha_0(\delta/\Omega)(\kappa_1 - 1/a_{\uparrow\downarrow}) & -\alpha_0^2(\kappa_2 - 1/a_{\uparrow\downarrow})\\
1/a_{\uparrow\uparrow} & \kappa_1 - 1/a_{\uparrow\uparrow} & \kappa_2 - 1/a_{\uparrow\uparrow}
\end{bmatrix}
\begin{pmatrix} a \\ C_1 \\ C2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{S11}
$$

The energy-dependent scattering length $a(q)$ is related to the s-wave scattering amplitude by the equation

$$
f(q) = -\frac{1}{1/a(q) + iq} \tag{S12}
$$

and can be obtained from Eq. (S11) by eliminating C_1 and C_2. The corresponding explicit expression is analytic but bulky. However, in the limit of small $a_{\sigma\sigma'}$ one can recover the MF result $a(0) = a_{--}$, where a_{--} is defined in the main text. If one assumes $a_{\uparrow\downarrow} \sim a_{\downarrow\downarrow} \sim |a_{\uparrow\downarrow}|$ and $|\delta| \sim \Omega$, one can see from Eq. (S11) that $a(0)$ can be expanded in powers of the small parameter $|a_{\uparrow\downarrow}|\sqrt{\Omega} \ll 1$. The leading BMF correction to a is thus expected to be of order $a_{\uparrow\downarrow}^2\sqrt{\Omega}$. By solving Eq. (S11) exactly under the conditions Eq. (3) we obtain

$$
a(0) = \sqrt{2}a_{\uparrow\downarrow}^2\sqrt{\tilde{\Omega}}\frac{1 + a_{\uparrow\downarrow}\sqrt{\tilde{\Omega}}}{1 + [1 - 2\sqrt{2} + \sqrt{2}(\alpha_0^2 + 1/\alpha_0^2)]a_{\uparrow\downarrow}\sqrt{\tilde{\Omega}} - \sqrt{2}(\alpha_0 - 1/\alpha_0)^2 a_{\uparrow\downarrow}^2\tilde{\Omega}}, \tag{S13}
$$

the leading-order asymptote of which is indeed proportional to $a_{\uparrow\downarrow}^2\sqrt{\Omega}$ (since $a_{--} = 0$) and corresponds to the two-body coupling constant in Eq. (5).

The term $\propto a_{\uparrow\downarrow}^2\sqrt{\Omega}$ can be understood as the second-order Born correction to the scattering amplitude for small $a_{\sigma\sigma'}\sqrt{\Omega}$. This term accounts for virtual interaction-induced transitions of two atoms in the unperturbed ground $|--\rangle$ state with zero momenta to various spin states ($|--\rangle$, $|+-\rangle$, $|++\rangle$) and momenta $\mathbf{q}$ and $-\mathbf{q}$. In spite of the fact that the channels $|+-\rangle$ and $|++\rangle$ are strongly gapped at large Ω the second-order integral actually grows as $\sqrt{\Omega}$. This can be understood by looking at the structure of this integral, which behaves (qualitatively) as $\int g^2 d^3q/(q^2+\Omega)$. Its diverging part $\int g^2 d^3q/q^2$ is regularized in the standard manner by replacing the bare coupling constants $g_{\sigma\sigma'}$ by $4\pi a_{\sigma\sigma'}$ and the remaining part indeed scales as $\sqrt{\Omega}$ as the number of momentum states essentially contributing to the integral grows faster than the gap.

Finally, we note that the Bogoliubov quadratic Hamiltonian, which leads to the BMF energy Eq. (4), does take into account the virtual two-body processes which we have just described. Equation (5) therefore exactly reproduces the second-order Born term. On the other hand, the third-order two-body correction $\propto a_{\uparrow\downarrow}^3\Omega$ [present in Eq. (S13)] is not captured on the level of the Bogoliubov Hamiltonian [and we therefore do not see it in Eq. (5)] since it requires taking into account interactions between atoms excited from the condensate.