This is the accepted manuscript made available via CHORUS. The article has been published as:

Quasiparticle Energy in a Strongly Interacting Homogeneous Bose-Einstein Condensate
Raphael Lopes, Christoph Eigen, Adam Barker, Konrad G. H. Viebahn, Martin Robert-de-Saint-Vincent, Nir Navon, Zoran Hadzibabic, and Robert P. Smith
DOI: [10.1103/PhysRevLett.118.210401](http://dx.doi.org/10.1103/PhysRevLett.118.210401)
Quasiparticle energy in a strongly interacting homogeneous Bose-Einstein condensate

Raphael Lopes,* Christoph Eigen, Adam Barker,† Konrad G. H. Viebahn,
Martin Robert-de-Saint-Vincent,‡ Nir Navon, Zoran Hadzibabic, and Robert P. Smith
Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Using two-photon Bragg spectroscopy, we study the energy of particle-like excitations in a strongly interacting homogeneous Bose-Einstein condensate, and observe dramatic deviations from Bogoliubov theory. In particular, at large scattering length $a$ the sign of the excitation resonance changes from positive to negative. For an excitation with wavenumber $q$, this sign change occurs at $a \approx 4/(\pi q^2)$, in agreement with the Wilson operator product expansion and the static structure factor expressed in terms of the two-body contact. For $a \gtrsim 3/q$ we also see a breakdown of this theory, and better agreement with calculations based on the Wilson operator product expansion. Neither theory explains our observations across all interaction regimes, inviting further theoretical efforts.

PACS numbers: 03.75.Hh, 67.85.De, 67.85.-d, 67.85.Hj

Spectroscopy of elementary excitations in a many-body system is one of the primary methods for probing the effects of interactions and correlations in the ground state of the system, which are at the heart of macroscopic phenomena such as superfluidity [1, 2]. In ultracold atomic gases, two-photon Bragg spectroscopy provides a measurement of the excitation energy $\hbar \omega$ at a well defined wavenumber $q$ [3–9]. For a weakly interacting homogeneous Bose-Einstein condensate (BEC), the excitation spectrum is given by the Bogoliubov dispersion relation [10], with low-$q$ phonon excitations and high-$q$ particle-like excitations. Predictions of the Bogoliubov theory have been experimentally verified both in harmonically trapped gases, invoking the local density approximation [4, 5], and in homogeneous atomic BECs [9].

Much richer physics, including phenomena traditionally associated with superfluid liquid helium, such as the roton minimum in the excitation spectrum [11], is expected in strongly interacting atomic BECs (for a recent review see [12]). The strength of two-body interactions, characterised by the $s$-wave scattering length $a$, can be enhanced by exploiting magnetic Feshbach resonances [13]. However, this also enhances three-body inelastic collisions, making the experiments on strongly interacting bulk BECs [6, 14–16] challenging and still scarce [17]. A deviation from the Bogoliubov spectrum was observed in Bragg spectroscopy of large-$q$ excitations in a harmonically trapped $^{85}$Rb BEC [6], and has inspired various theoretical interpretations [6, 12, 18–22], with no consensus or complete quantitative agreement with the experiments being reached so far.

In this Letter, we use Bragg spectroscopy to study the large-$q$, particle-like excitations in a strongly interacting homogeneous $^{39}$K BEC, produced in an optical box trap [24]. Our homogeneous system allows more direct comparisons with theory, and we also explore stronger interactions than in previous experiments. We show that at large $a$ the excitation-energy shift from the free-particle dispersion relation strongly deviates from the Bogoliubov theory and even changes sign from positive to negative. For $a \gtrsim 3/q$ our measurements are in excellent agreement with the calculation based on the Feynman energy relation, with a static structure factor that accounts for short-range two-particle correlations. However, for even stronger interactions we also observe a breakdown of this approximation, and find better agreement with a recent prediction [22] based on the Wilson operator product expansion.

In Bogoliubov theory, the excitation energy $\hbar \omega$ is given by

$$\omega = \omega_0 \sqrt{1 + \frac{2}{q^2 \xi^2}},$$

(1)

where $\omega_0 = \hbar q^2/(2m)$ is the free-particle dispersion relation, $m$ the atom mass, $\xi = 1/\sqrt{8\pi n a}$ the healing length, and $n$ the BEC density. For particle-like excitations, with $q \gg 1/\xi$, the Bogoliubov prediction for the interaction shift $\Delta \omega = \omega - \omega_0$ is $\Delta \omega_B = 4\pi n a \hbar /m$ [see Fig. 1(a)]. This theory assumes $\sqrt{n a^3} \ll 1$. Moreover, it is valid only for $q \ll 1/a$, because it does not consider the short-range two-particle correlations, at distances $r \lesssim a$.

For $\sqrt{n a^3} \ll 1$, the Feynman energy relation gives the excitation resonance at $\omega = \omega_0 / S(q)$, where $S(q)$ is the static structure factor. Considering short-range correlations, for $q \xi \gg 1$:

$$S(q) = 1 + \frac{C}{8n} \left( \frac{1}{q} - \frac{4}{\pi a q^2} \right),$$

(2)

where $C(n, a)$ is the two-body contact density, and the expression in the brackets reflects the two-body correlations at short...
distances [22, 25]; this ‘factorisation’ of the effects of many-body correlations (captured by $C$) and the short-distance two-body physics was highlighted by Tan [26]. For $\sqrt{n a^3} \ll 1$, the contact density is $C \approx (4\pi n a^2)^2$, and for our experimental parameters $|S(q) − 1| < 0.03$, so $1/S(q) − 1 \approx 1 − S(q)$. This ‘Feynman-Tan’ (FT) approach thus gives the interaction shift of the excitation resonance

$$\Delta\omega_{\text{FT}} = \frac{4\pi\hbar a}{m} \left( 1 - \frac{\pi q a}{4} \right).$$

For $q a \to 0$, $\Delta\omega_{\text{FT}}$ reduces to $\Delta\omega_B$, but for increasing $a$ (at fixed $q$) it back-bends and changes sign at $a = 4/(\pi q)$ [see Fig. 1(a)]. In Ref. [6] the largest value of $a$ reached was $0.8/q$ and back-bending was observed, but $\Delta\omega$ remained positive.

Let us also consider the dispersion relation, $\omega(q)$ at fixed $a$. The energy of the low-$q$ phonons is above the free-particle dispersion ($\Delta\omega > 0$) [22, 27], while according to Eq. (3) the energy of particle-like excitations with $q > 4/(\pi a)$ is below it ($\Delta\omega < 0$); finally, for $q \to \infty$ the quasiparticle energy is expected to approach the free-particle dispersion from below ($\Delta\omega \to 0^−$) [22, 23]. As illustrated in Fig. 1(b), for a large enough $a$ the dispersion relation has an inflection point, which is a precursor of the roton minimum that fully develops only for extremely strong interactions [22, 23]. In Eq. (2) the maximum in $S(q)$ for fixed $n$ and $a$, which is conceptually associated with the roton [22, 28], occurs at $q = 8/(\pi a)$, independently of $n$, and only for $\sqrt{n a^3} \sim 1$ this coincides with the familiar result for liquid helium, $q_{\text{roton}} \sim n^{1/3}$.

In our experiments the regime $\sqrt{n a^3} \sim 1$ is not reachable due to significant losses on the timescale necessary to perform high-resolution Bragg spectroscopy. Nevertheless, we reach the regime where interactions are strong enough to observe a dramatic departure from Bogoliubov theory and the precursors of roton physics.

Our setup is described in Ref. [29]. We produce quasi-pure homogeneous $^{39}$K BECs of $N = (50−160) \times 10^3$ atoms in a cylindrical optical box trap of variable radius, $R = (15−30) \mu$m, and length, $L = (30−50) \mu$m. The BEC is produced in the lowest hyperfine state, which features a Feshbach resonance centred at 402.70(3) G [30]. The condensed fraction in our clouds is $>90\%$ and we hold them in a trap of depth $\approx k_B \times 20$ nK. By varying $N$, $L$, and $R$, we vary $n$ in the range $(0.2−2.0) \times 10^{12}$ cm$^{-3}$. The three-body loss rate is $\propto n^2 a^4$, so working at such low $n$ is favourable for increasing both $q a$ and $\sqrt{n a^3}$. We prepare the BEC at $a = 200 a_0$, where $a_0$ is the Bohr radius, and then ramp $a$ in 50 ms to the value at which we perform the Bragg spectroscopy. For each $n$ we limit $a$ to values for which the particle loss during the whole experiment is $<10\%$; note that in our trap the three-body recombination does not lead to any observable heating. By varying the angle between the Bragg laser beams we also explore three different $q$ values: 1.1, 1.7 and 2.0 $k_{\text{rec}}$, where $k_{\text{rec}} = 2\pi/\lambda$ and $\lambda = 767$ nm. For all our parameters we stay in the regime of particle-like excitations, with $q \xi$ values between 5 and 40.

In Fig. 2(a) we show an example of an absorption image taken after Bragg diffraction, and in Fig. 2(b) an example of a Bragg spectrum used to determine the resonance shift $\Delta\omega$. The diffracted fraction of atoms is determined from the centre of mass of the atomic distribution [6, 8]. In all our measurements we keep the maximal diffracted fraction to $\lesssim 10\%$; this should result in $\lesssim 10\%$ systematic errors in our interaction frequency shifts [5, 31].

In Fig. 3(a) we plot $\Delta\omega$ versus $a$ for two different combinations of the BEC density $n$ and excitation wavenumber $q$. In both cases we observe good agreement with the prediction of Eq. (3), without any adjustable parameters; for the lower $n$ we reach higher $a$ and clearly observe that $\Delta\omega$ changes sign.

Defining a dimensionless interaction frequency shift

$$\alpha \equiv \frac{mq}{4\pi\hbar n} \Delta\omega,$$

the FT prediction of Eq. (3) is recast as:

$$\alpha_{\text{FT}} = q a \left( 1 - \frac{\pi q a}{4} \right),$$

which is a universal function of $qa$ only; with the same normalisation the Bogoliubov theory gives $\alpha_B = qa$. Note that the normalisation in Eq. (4) also allows us to correct for the small ($\pm 10\%$) density variations between measurements taken with different values of $a$ and the same nominal $n$. In Fig. 3(b) we show measurements of $\alpha$ with three different combinations of $n$ and $q$, which all fall onto the same universal curve, in good agreement with the FT theory.

In Fig. 3(b), for our most strongly interacting samples $qa \approx 2.5$ and $\sqrt{n a^3} \approx 0.05$. In the final part of the paper we explore even stronger interactions and observe that the FT theory also breaks down. In Fig. 4(a) we show measurements of $\Delta\omega$ with $n \approx 0.2 \times 10^{12}$ cm$^{-3}$ and $q = 2k_{\text{rec}}$, for which we explore scattering lengths up to $\approx 8 \times 10^3 a_0$, corresponding to $qa \approx 7$.  

![Graph](image_url)
and $\sqrt{\alpha a^3} \approx 0.1$. Here we observe a clear deviation from the FT prediction.

Tuning $a$ at fixed $n$ and $q$ simultaneously changes $qa$ and $\sqrt{\alpha a^3}$, making it non-obvious which of the two dimensionless interaction parameters is (primarily) responsible for the breakdown of the FT theory. In an attempt to disentangle the two effects, we collect data with many \{n, q, a\} combinations, and group them into sets with (approximately) equal $\sqrt{\alpha a^3}$, but varying $qa$ values. In Fig. 4(b) we plot $\alpha - \alpha_{\text{FT}}$ versus $qa$, with different symbols corresponding to different $\sqrt{\alpha a^3}$. These measurements suggest that, at least for our range of parameters, the breakdown of the FT theory occurs for $qa \gtrsim 3$, independently of the value of $\sqrt{\alpha a^3}$.

At $qa \gtrsim 3$, the deviation of our data from the FT theory is captured well by a recent calculation based on the Wilson operator product expansion (OPE) [22]. Assuming $C = (4\pi n a)^2$, and with the same normalisation as in Eq. (4), $\alpha_{\text{OPE}} = qa[2/(1 + (qa/2)^2) - 1]$ (see also [27]); in Fig. 4(b) the dashed black line shows $\alpha_{\text{OPE}} - \alpha_{\text{FT}}$.

This theory also allows for self-consistent inclusion of beyond-mean-field corrections to $C$. Including the Lee-Huang-Yang (LHY) correction [32–34], $\alpha_{\text{OPE}}$ depends on both $qa$ and $\sqrt{na^3}$; we show the LHY-corrected $\alpha_{\text{OPE}}$ (dotted-dashed black line) only for our largest $\sqrt{na^3}$, where it appears to provide a slightly better agreement with the experiments, but this observation is not conclusive (see also [15]). Note that at this point the LHY correction to $C$ is about a factor of two, but beyond-LHY corrections, which additionally depend on the van der Waals length, could also be significant and the two effects could partially cancel [35, 36].

Finally, we note that while the OPE theory successfully describes our large-$qa$ measurements, it does not agree with our low-$qa$ data, in particular because it predicts the zero-crossing of $\Delta \omega$ at $qa = 2$ instead of $qa = 4/\pi$; this is highlighted in the inset of Fig. 4(b).

In conclusion, we have probed the quasiparticle excitations in a strongly interacting homogeneous BEC, pushing the experiments far beyond the regime of validity of the Bogoliubov theory. For a range of interaction strengths, $qa \lesssim 3$, our data can still be quantitatively explained in the framework of the FT theory. The solid line shows the FT prediction. (b) Deviation of the dimensionless frequency shift $\alpha$ versus $qa$ for three different combinations of $n$ and $q$. Solid lines in (a) and (b) show the FT predictions from Eqs. (3) and (5), respectively, with no adjustable parameters. The dashed lines show the corresponding Bogoliubov predictions. Vertical error bars show statistical fitting errors and horizontal error bars reflect the uncertainty in the position of the Feshbach resonance.

**FIG. 3.** (color online) Breakdown of the Bogoliubov approximation and observation of negative frequency shifts. (a) $\Delta \omega$ as a function of $a$ for $n \approx 2.0 \times 10^{12}$ cm$^{-3}$ and $q = 1.1 k_{\text{rec}}$ (blue circles), and for $n \approx 0.8 \times 10^{12}$ cm$^{-3}$ and $q = 2 k_{\text{rec}}$ (orange diamonds). (b) Dimensionless frequency shift $\alpha$ versus $qa$ for three different combinations of $n$ and $q$. Solid lines in (a) and (b) show the FT predictions from Eqs. (3) and (5), respectively, with no adjustable parameters. The dashed lines show the corresponding Bogoliubov predictions. Vertical error bars show statistical fitting errors and horizontal error bars reflect the uncertainty in the position of the Feshbach resonance.

**FIG. 4.** (color online) Deviation from the Feynman-Tan prediction. (a) Frequency shift versus $a$ for $n \approx 0.2 \times 10^{12}$ cm$^{-3}$ and $q = 2 k_{\text{rec}}$. The solid line shows the FT prediction. (b) Deviation of the dimensionless frequency shift $\alpha$ from the FT theory as a function of $qa$, for various values of $\sqrt{na^3}$ (see the legend). The dashed line is the OPE prediction with $C = (4\pi n a)^2$ and no adjustable parameters. The dot-dashed line is the OPE prediction that also includes the LHY correction with $\sqrt{na^3} = 0.093$, corresponding to the open-circles data. Inset: comparison of the FT (solid) and OPE (dashed) calculations with the data at low $qa$. 

\[ \alpha = \frac{\Delta \omega}{2\pi} \]
of the Feynman energy relation, by taking into account the short-range two-particle correlations in the spirit introduced by Tan. For \( qa \gtrsim 3 \) this theory also fails, pointing to the need for more sophisticated theoretical approaches. One such approach, based on the Wilson operator product expansion, indeed accounts well for our observations at \( qa \gtrsim 3 \), but not at \( qa \lesssim 3 \). Providing a unified description of quasiparticle resonances in all interaction regimes thus remains a theoretical challenge.

We thank Richard Fletcher, Sandro Stringari, Wilhelm Zwerger, Johannes Hofmann, Eric Cornell, Nir Davidson and Stefano Giorgini for inspiring discussions. This work was supported by the Royal Society, EPSRC [Grant No. EP/N011759/1], ERC (QBox), AFOSR, and ARO. R.L. acknowledges support from the E.U. Marie-Curie program [Grant No. MSCA-IF-2015 704832] and Churchill College, Cambridge. N.N. acknowledges support from Trinity College, Cambridge.

---

† Present Address: Laboratoire de physique des lasers, CNRS UMR 7538, Université Paris 13, Sorbonne Paris Cité, F-93430, Villetaneuse, France.
‡ Present Address: Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

[17] This is in contrast to Fermi gases near Feshbach resonances, and Bose and Fermi gases in optical lattices, where the regime of strong correlations is readily reached experimentally.