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# Bragg spectroscopy of a superfluid Bose–Hubbard gas

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**Abstract.** Bragg spectroscopy is used to measure the excitations of a trapped, quantum-degenerate gas of $^{87}$Rb atoms in a three-dimensional (3D) optical lattice. The measurements are carried out over a range of optical lattice depths in the superfluid phase of the Bose–Hubbard model. For a fixed wavevector, the resonant frequency of the excitation is found to decrease with increasing lattice depth. A numerical calculation of the resonant frequencies based on Bogoliubov theory shows a less steep rate of decrease than the measurements.

Quantum degenerate atoms in optical lattices form a strongly interacting many-body system whose parameters can be readily controlled. In particular, Jaksch *et al* [1] have pointed out that bosonic atoms in an optical lattice constitute a nearly ideal realization of the Bose–Hubbard model [2]. This model predicts a quantum phase transition from superfluid to the Mott insulator that has been confirmed by experimental observations [3]. Quantum degenerate gases trapped in optical lattices have since opened up new perspectives into the field of quantum computation and quantum simulation of strongly correlated many-body systems [4].

A key property of a quantum gas is its excitation spectrum. Previous observations of excitations of a Bose–Hubbard gas have been made using either a gradient of magnetic

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field [3] or a modulated optical lattice depth [5, 6]. Neither of the two techniques, however, directly probes the linear excitation spectrum of the gas, since a tilted lattice perturbs the gas only at zero frequency, whereas a modulated optical lattice affects only at zero quasi-momentum. The latter case, in particular, results in a nonlinear excitation spectrum that has been analyzed only very recently [6, 7].

On the other hand, Bragg spectroscopy [8] has gradually emerged as a fundamental and precise tool to investigate the excitation spectrum of Bose–Einstein condensates (BECs) in unprecedented detail. Important progress has been made in Bragg spectroscopy, especially in investigating BECs with lattice-free geometries, first to probe the higher-energy particle-like excitations [9, 10] and later to measure low-energy phonons [11]. The measurements using Bragg spectroscopy in these experiments [9]–[11], however, were restricted to isolated points on the excitation spectrum. The first measurement of the full momentum dependence of the excitation spectrum was reported in [12]. More recently, Bragg spectroscopy has also been applied to explore strongly interacting bosonic [13] and fermionic gases [14].

In this paper, we report the first application of Bragg spectroscopy to a quantum-degenerate Bose gas in a three-dimensional (3D) optical lattice. We observe resonant excitations of the gas in the superfluid regime of the Bose–Hubbard model. Furthermore, we carry out a numerical calculation of the resonant frequencies based on Bogoliubov theory, and find that the calculated frequencies decrease with increasing lattice depth at a lower rate than the measured ones. It is necessary to mention that, after we posted our work online [15], several other Bragg spectroscopic studies of ultracold atomic gases in optical lattices were reported. Clement *et al* [16] reported the Bragg spectroscopy of interacting 1D Bose gases loaded in an optical lattice across the phase transition from superfluid to the Mott insulator. A comprehensive study of superfluids in optical lattices by Bragg spectroscopy was reported in [17], which presented full momentum-resolved measurements of the band structure and the associated interaction effects at several lattice depths. These two papers together complete the observation of the excitations of a BEC by Bragg spectroscopy, covering both the superfluid and insulating phases as well as their transition regime. More elaborate theoretical treatments for Bragg spectroscopy have been presented in [18]–[24].

In our experiment, a BEC of about $N = 5 \times 10^5$ $^{87}$Rb atoms in the hyperfine state $|F = 1,$ $m_F = -1\rangle$ is prepared in a 'cloverleaf' magnetic trap [25] with an axial trapping frequency of 11.6 Hz and a radial trapping frequency of 20.7 Hz. The condensate has an ellipsoidal shape and an inverted parabolic density profile $n(\mathbf{r})$ [26] with Thomas–Fermi axial and radial radii being $z_0 = 26 \,\mu$m and $r_0 = 15 \,\mu$m, respectively. The initial condensate fraction is greater than 90%, and its peak density is $n_0 = (5.2 \pm 1) \times 10^{13} \,\text{cm}^{-3}$.

A 3D optical lattice is created with three mutually orthogonal optical standing waves, formed by three retro-reflected, linearly polarized laser beams from a single-frequency Ti:sapphire laser with a wavelength $\lambda_L = 830$ nm. The 'axial' lattice laser beams propagate parallel to the symmetry axis of the BEC and have a spot size ($1/e^2$ intensity radius) at the BEC of 130 $\mu$m. The two sets of 'radial' lattice beams have a spot size at the BEC of 260 $\mu$m. Frequency shifts of several tens of MHz between these three beam pairs suppress the effects of interference between them. The resulting optical dipole potential has the form $V(x, y, z) = V_0[\sin^2(k_L x) + \sin^2(k_L y) + \sin^2(k_L z)]$ and lattice constant $a = \lambda_L/2 = 0.415 \,\mu$m. The lattice height $V_0$ is calibrated to an accuracy of about 10% with measurements of the diffraction pattern of the atoms from a short pulse of each beam pair. Such a gas provides a realization of the Bose–Hubbard model [1], and for our parameters the gas is entirely superfluid
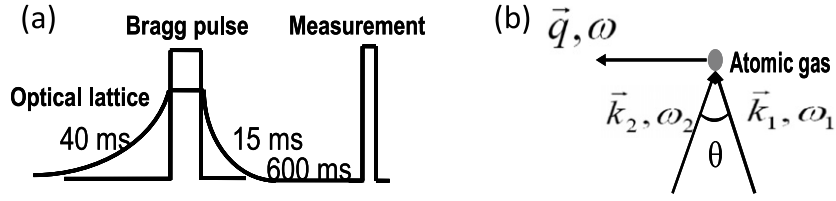
**Figure 1.** (a) Time sequence of the experiment. (b) Schematic diagram of Bragg spectroscopy.

below the critical lattice height $V_{0c} \approx 13 E_R$, where $E_R = \hbar^2 k_L^2/2m = h \times 3.33\,\text{kHz}$ is the lattice recoil energy with $m$ being the atomic mass.

The experimental sequence is illustrated in figure 1(a). The BEC is loaded into the optical lattice by ramping up the lattice laser intensity with a quadratic function in a time period of 40 ms. After the lattice is turned on, we induce Bragg excitation with two laser beams of wavevector $\mathbf{k}_1$ and $\mathbf{k}_2$ and frequencies $\omega_1$ and $\omega_2$, respectively, as illustrated in figure 1(b). These two beams perturb the gas with a traveling wave optical dipole potential $V_B \cos(\mathbf{q} \cdot \mathbf{r} - \omega t)$ with wavevector $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$ and frequency $\omega = \omega_1 - \omega_2$. The Bragg beams have a wavelength of 781.05 nm and are 400 GHz red-detuned from the atomic transition $5s_{1/2} \to 5p_{3/2}$, their intensities ranging between 70 and 320 mW cm$^{-2}$, which corresponds to $V_B$ in the range from 0.45 to 1.3 $E_R$. In our experiment, the Bragg wavevector $\mathbf{q}$ is held fixed and directed perpendicular to the symmetry axis of the gas and at an angle of $\pm 45°$ with respect to the radial lattice beams. Bragg pulse durations are 20 ms for zero and 1.1 $E_R$ lattice depth and 5 ms for 2.2 $E_R$ lattice depth, and they vary from 2 to 5 ms for higher lattice depths. The angle between the two Bragg beams is $30.6° \pm 0.6°$, corresponding to $q = 4.25 \pm 0.08\,\mu\text{m}^{-1}$. Thus, the Bragg wavelength is $\lambda_B = 2\pi/q = 1.48\,\mu\text{m}$, which corresponds to 3.56 lattice constants.

The Bragg pulse produces excitations in the gas with the wavevector $\mathbf{q}$. In order to measure the degree of excitation of the gas, we ramp the lattice beams back down to zero depth in 15 ms, wait for 600 ms for the gas to re-thermalize and finally measure the condensate fraction with time-of-flight absorption imaging. Excitation of the gas leads to an increased final temperature of the gas after thermalization or equivalently to a reduced condensate fraction. We used this procedure rather than measuring outcoupled atoms [10]–[12], [18] because at the higher lattice strengths, the gas acquires a large momentum spread due to quantum depletion [3, 27], and this makes it difficult to clearly observe the Bragg-diffracted atoms in a time-of-flight image.

Figure 2 shows experimental Bragg spectra recorded at five different lattice depths ranging from 0 to 9.9 $E_R$. In each case, resonant heating of the gas is observed. The results differ substantially from previous zero quasi-momentum excitation studies [5, 6], where almost no excitations were observed for lower optical lattice depths and a broad resonance appeared for higher optical lattice depths. We have searched for but found no dependence of the resonance frequencies on the Bragg beam intensities and pulse durations that is significant relative to the experimental error. In other words, our measurements are performed in the linear response regime. The heating that appears off-resonance for lattice strengths greater than about 7 $E_R$ is due to non-adiabatic effects rather than Bragg excitation.

The results of the experiment are summarized in figure 3. Approximately 40 spectra in total were taken for ten different lattice depths, and from each spectrum we obtained a resonance frequency $\omega_0$ and an rms width $\Delta\omega$ from a Gaussian fit to the data. Figure 3 shows the measured
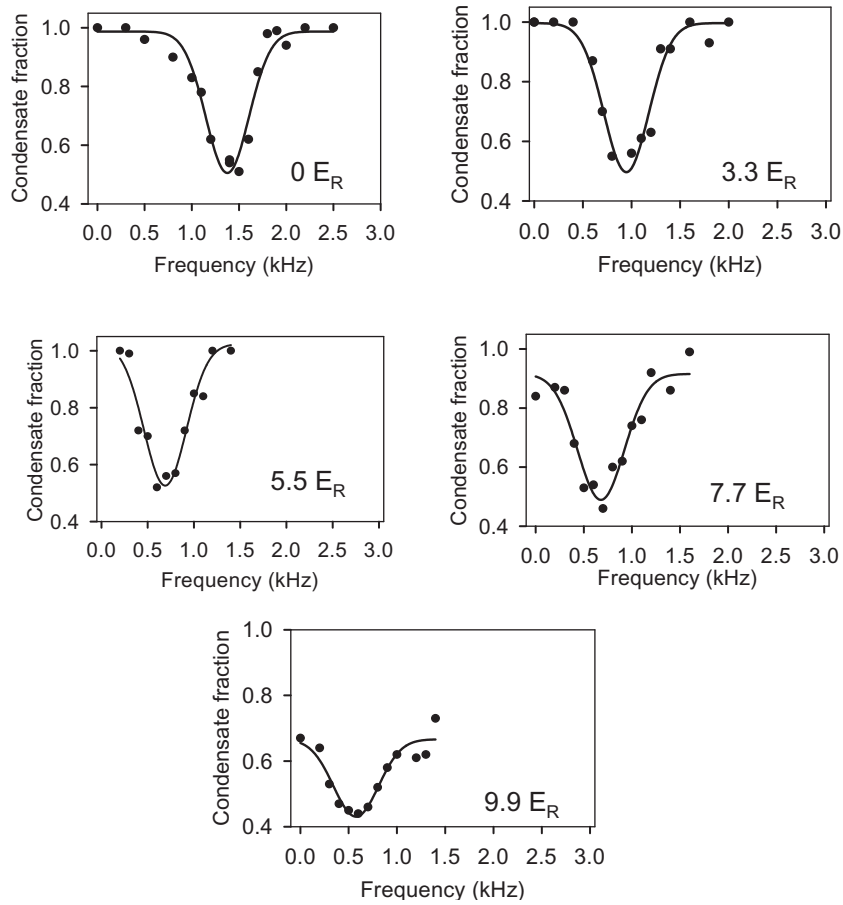
**Figure 2.** Bragg spectra at the optical lattice depths $V_0 = 0$, 3.3, 5.5, 7.7 and 9.9 $E_R$, respectively. Each peak is fitted with a Gaussian.
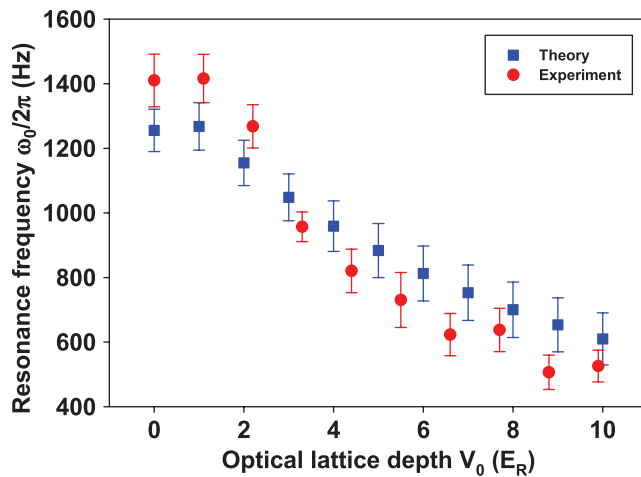


**Figure 3.** Comparison between the experimental (circles) and theoretical values (squares) of the resonant excitation frequency versus optical lattice depth. The theory shows the calculated frequency for the density $n = 0.57 n_0(V_0)$.

resonance frequency as a function of lattice depth. Each data point is an average over several measurements, whereas the error bars indicate the statistical variation between measurements.

At zero lattice strength, the results correspond to previous measurements of Bragg excitation in condensates. In our experiment, the Bragg wavelength is small relative to the condensate radius $r_0$, and the Doppler spread $\hbar q/mr_0$ of the Bragg resonance is much less than $\mu/\hbar$. Here, $\mu = gn_0 = h \times 404\,\text{Hz}$ is the chemical potential of the gas, where $g = 4\pi\hbar^2 a/m$ with $a = 5.31\,\text{nm}$ [28] being the scattering length. Therefore a local density approximation applies [10]–[12], [18], and the gas is resonantly excited only at points with density $n(\mathbf{r})$ such that the condensate dispersion relation $\omega_{\text{res}}(q) = \sqrt{\omega_q^0(\omega_q^0 + 2gn/\hbar)}$ is satisfied, where $\omega_q^0 = \hbar q^2/2m = 2\pi \times 1050\,\text{Hz}$. The excitation is phonon-like if $q\xi \ll 1$, and particle-like if $q\xi \gg 1$, where $\xi = \sqrt{1/8\pi na}$ is the local healing length of gas [10]–[12], [18]. In our case, $\xi(n_0)^{-1} = 2.64\,\mu\text{m}^{-1}$, so that $q\xi(n_0) = 1.60$; hence the Bragg excitation is intermediate between the phonon and particle-like regimes. Our lineshape function is expected to be $\omega \times I(\omega)$, where $I(\omega) = (15/8)(\omega^2 - \omega_q^{02})/(\omega_q^0(\mu/\hbar)^2)\sqrt{1 - (\omega^2 - \omega_q^{02})/(2\omega_q^0\mu/\hbar)}$ [18], and the extra factor of $\omega$ arises from the fact that we measure energy input to the gas, rather than outcoupled atoms. Accounting for our 20% uncertainty in the density as well as the uncertainty in $q$, our calculated first moment of this lineshape function is $\omega_0/2\pi = 1260 \pm 50\,\text{Hz}$, in reasonable agreement with our measured value of $1410 \pm 80\,\text{Hz}$. This frequency corresponds to resonant excitation at the density $n = 0.57n_0$.

The results for nonzero lattice strength show a strong decrease in the resonant frequency with increasing lattice strength. This can be understood qualitatively with Bogoliubov theory [29]–[32]. The excitations in our experiment can be roughly understood as Bogoliubov sound waves with a resonant frequency $\omega_{\text{res}} = c_s q$, where $c_s = \sqrt{1/\kappa m^*}$ is the sound speed. Here, $\kappa = [n(\partial\mu/\partial n)]^{-1}$ is the compressibility of the gas, while the effective mass $m^* = (\partial^2\varepsilon/\partial q^2)$ can be obtained from the energy dispersion $\varepsilon(q)$ of the Bloch states. When the lattice depth increases, the band becomes flatter, leading to an increased $m^*$, which tends to decrease the sound speed, whereas an increasing lattice depth also results in enhanced interatomic interaction and the compressibility, thereby causing the sound speed to increase. However, the relative rate of change in the effective mass is much greater than that of the compressibility, so the overall effect of increased lattice depth leads to decreased sound speed.

In our experiment, there are two effects that cause the peak value of the (unit-cell averaged) density $n_0$ to change with lattice depth $V_0$. One effect is the increasing repulsion between the atoms due to their localization within the lattice sites. The other is an additional contribution to the harmonic trapping force from the optical dipole force of the lattice laser beams, which have a Gaussian intensity profile. These effects can be modeled by a modified Thomas–Fermi approach [33]. The resulting peak density as a function of lattice depth is shown in figure 4(a). For $V_0 = 10\,E_R$, we calculate that the axial and radial trapping frequencies increase to 24.2 and 39.54 Hz, respectively. Going from $V_0 = 0$ to $10\,E_R$, we calculate that the peak density $n_0(V_0)$ decreases from $5.2 \times 10^{13}$ to $3.2 \times 10^{13}\,\text{cm}^{-3}$, corresponding to a decrease in the mean site occupancy from 3.7 to 2.3.

We have carried out a numerical calculation of excitation frequencies based on Bogoliubov theory [29]–[32]. The details of our numerical method can be found in [32]. In the calculation, the trapped Bose gas in an optical lattice is treated as a uniform system. In figure 3, we show the result for the density $n = 0.57n_0(V_0)$. Here, the prefactor 0.57 for the measurement of the energy transfer equals the calculated value 4/7 in [18] for the dynamic structure factor. According
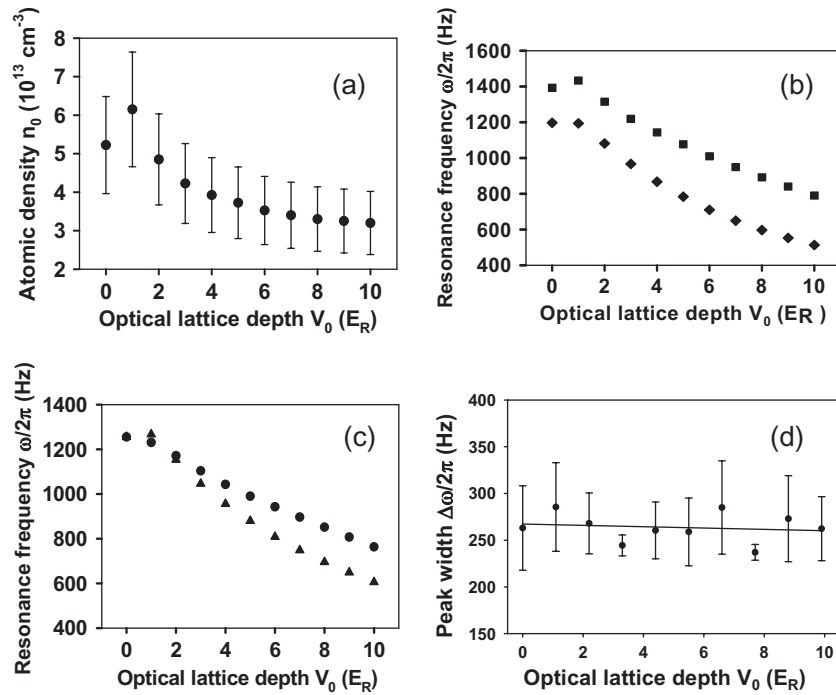
**Figure 4.** (a) Peak atomic density $n_0(V_0)$. (b) Calculated resonance frequencies for peak density $n_0(V_0)$ (squares) and for average density $0.40n_0(V_0)$ (diamonds). (c) Calculated resonance frequencies for density $n = 0.57n_0(V_0)$ (triangles) and fixed density $n = 0.57n_0(0) = 3.0 \times 10^{13}$ (circles). (d) Measured rms peak width versus optical lattice depth. A linear fit to the data is shown.

to previous discussions, the frequency for this density agrees with the first moment of the theoretical lineshape at zero lattice strength. For nonzero lattice strength, the density $0.57n_0(V_0)$ should still provide a reasonable definition of the 'average' density. In figure 3, the error bars on the experimental points account for the statistical error of repeated measurements, whereas the error bars on the theoretical points account for the uncertainty in density and the uncertainty in **q**. We have confirmed that the calculated frequencies do not depend on the direction of **q** relative to the principal lattice vectors.

Figure 3 has shown general agreement between the mean-field calculations and experimental values regarding the change in resonant frequencies as a function of the lattice depth, except for a much larger slope of decrease observed in the experiment than that expected from Bogoliubov theory. We now explore whether such a discrepancy arises from the density $n = 0.57n_0(V_0)$ used in the calculation as a function of the lattice parameter in figure 3. As a first point, we note that the prefactor (0.57) in the density $n = 0.57n_0(V_0)$ is closely related to the value of the first moment of the lineshape function in the particle-like regime. However, an increase in lattice strength leads to decreased healing length $\xi$, or $q\xi$ for fixed **q**, consequently shifting the optically trapped gas toward the phonon-like regime where the first moment of the lineshape function takes a comparatively smaller value [12, 18]. To observe the consequence of this changing lineshape at different lattice depths, a mean density $0.40n_0(V_0)$ appropriate to the phonon-like regime is adopted instead, whereas the rate of decrease in the resulting resonance frequencies shown in figure 4(b) still deviates from the experiment (see figure 3). As a second comparison, we keep the prefactor (0.57); instead, we calculate excitation frequencies

at a fixed density $n = 0.57n_0(0) = 3.0 \times 10^{13}$ cm$^{-3}$ and compare them with those obtained for $n = 0.57n_0(V_0)$ that is a function of the lattice depths. As shown in figure 4(c), when the lattice depth increases from 0 to 10 $E_R$, the frequency drops by approximately 500 Hz for a fixed $n$, even smaller than the corresponding drop of 650 Hz obtained for $n = 0.57n_0(V_0)$. We thereby conclude from the above analysis that the change in the density function $n = 0.57n_0(V_0)$ constitutes a minor contribution in causing the deviation of Bogliubov's theoretical prediction for the frequency-decreasing rate from experimental observations.

Therefore, in this paper, we suggest that the modest discrepancy between the theory and experiment may reflect the inaccuracy of our Bogoliubov approximation calculation, which neglects the effects of quantum depletion [27]. Depletion starts to become important when $U > J$, where $U$ and $J$ are characteristic parameters of the Bose–Hubbard Hamiltonian [1, 2],

$$H = \sum_i \varepsilon_i n_i - J \sum a_i^\dagger a_j + \frac{U}{2} \sum n_i(n_i - 1). \tag{1}$$

In equation (1), the index $i$ labels the lattice sites, $n_i = a_i^\dagger a_i$ is the atomic number operator for site $i$ with $a_i^\dagger$ and $a_i$, respectively, being the raising and lowering operators, and $\varepsilon_i$ is the single particle energy for site $i$. The second sum is over all pairs of nearest neighbor sites, $J$ is the amplitude for particles to hop between nearest neighbor sites, and $U$ is the contact energy of two particles in the same lattice site. For our parameters, we estimate that $U = J$ at a lattice height of about $V_0 = 3.5 E_R$. On the other hand, it happens that the slopes of the two curves in figure 3 also differ most strongly at $V_0 = 3.5 E_R$. This coincidence suggests an intimate relation between the quantum depletion and the modest deviation of mean-field predictions from the observed decreasing rate of frequencies. For a lattice height $V_0 > 13E_R$, Bogoliubov theory must fail since the Bose–Hubbard gas becomes an insulator and cannot support long-wavelength sound waves. For further investigations taking the effects of quantum depletion into account, we would like to mention [34, 35] going in this direction.

The rms width resonance versus optical lattice depth is given in figure 4(d). The width is relatively constant as the lattice strength increases. Note that this may be partly explained by the density dependence of the resonance frequency illustrated in figure 4(b), which shows that the spread in resonance frequencies from the peak to the mean density is roughly constant versus lattice strength.

In conclusion, we have applied Bragg spectroscopy to measure the linear excitation spectrum of a quantum degenerate gas of bosons in the superfluid regime. The results show that the resonant frequency decreases with increasing lattice strength at a rate that is modestly higher than predicted by a Bogoliubov theory. In the future, Bragg spectroscopy may be useful to determine the excitation spectrum in the insulating phase of the Bose–Hubbard model[6] and other quantum gases.

**Acknowledgments**

[6] After posting our manuscript online, we noticed that Clement *et al* [16] have reported the Bragg spectroscopy of interacting Bose gases loaded in an optical lattice across the superfluid-to-Mott insulator phase transition.

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