Semiclassical dynamics of atomic Bose-Einstein condensates
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An atomic Bose-Einstein condensate (BEC) is often described as a macroscopic object which can be approximated by a coherent state. This, on the surface, would appear to indicate that its behavior should be close to being classical. In this paper, we clarify the extent of how “classical” a BEC is by exploring the semiclassical equations for BECs under the mean field Gaussian approximation. Such equations describe the dynamics of a condensate in the classical limit in terms of the variables \( \langle x \rangle \) and \( \langle p \rangle \) as well as their respective variances. We compare the semiclassical solution with the full quantum solution based on the Gross-Pitaevskii Equation (GPE) and find that the interatomic interactions which generate nonlinearity make the system less “classical.” On the other hand, many qualitative features are captured by the semiclassical equations, and the equations to be solved are far less computationally intensive than solving the GPE which make them ideal for providing quick diagnostics, and for obtaining new intuitive insight.

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We note that the “Gaussian dynamics” in this context includes a “squeezed coherent state” i.e. Gaussian of variable width, and the state is assumed to remain a Gaussian throughout the evolution.

Despite the coherent state/Gaussian ansatz, the solution to the GPE does not necessarily give classical dynamics. This apparent “contradiction” arises simply because the coherent state assumption used to derive the GPE is made at the level of second quantization – the ansatz turns the many-body quantum field operator into a classical field of condensate wave function. The resulting wave function in real space can, in principle, take any form depending on the boundary and external conditions. In order for the classical dynamics to emerge from the condensate wave function, a further “coherent state” assumption within the mean-field level of theory – that the condensate wave function takes on a Gaussian profile – is needed. The fact that a BEC is not strictly a “coherent state” within the mean-field regime is evident from examining the Q-function for the condensate at the level of GPE: a Gaussian wave packet gives a circular Q-function expected of a coherent state while the Thomas-Fermi approximation for which most experiments are valid, gives an elliptical Q-function indicative of its nonclassical nature.

The Gaussian profile approximation can, in fact, be a good approximation for the stationary condensates with a small number of atoms or with an attractive interatomic interaction. However, the inherent nonlinearity of the system can destroy any Gaussian profile approximation very quickly during the dynamical evolution. We note that a Gaussian description was used previously in the context of studying surface collective mode of a BEC with attractive interactions, where the results based on variational methods were used. In the early works based on variational principle, it was shown that many of the features of a BEC can be captured using the Gaussian ansatz. However, the semiclassical aspect and the validity of the Gaussian dynamics compared to the full quantum dynamics was not fully explored. Also
the results were restricted to the harmonic trapping potential, which doesn’t demonstrate a more general picture of deviation from the GPE.

In this paper, we ask the question “Just how classical is a BEC and under what conditions?” We explore the dynamics of the atomic BECs in the semiclassical limit and compare with the full quantum solution described by the GPE. The semiclassical limit is obtained by assuming that a BEC maintains a Gaussian profile (of variable mean and variance) throughout the evolution and deriving the corresponding effective Gaussian semiclassical equations. Strictly speaking, only the ground state for a harmonic trap with \( U_0 = 0 \) in the GPE of Eq. (1) is precisely Gaussian; for \( U_0 \neq 0 \), a Gaussian profile provides an idealized classical limit that acts as a “baseline” for comparison with the full quantum result. The motivation for this study comes not just from addressing fundamental questions on the quantum-classical nature of a BEC but also in the context of advancing quantum engineering and control methods [13] via simpler equations that relate relevant observables. The semiclassical equations can provide us a means to understand complex quantum behavior in terms of the more familiar and intuitive classical picture, providing a new insight into how to manipulate atomic BECs.

The usual derivation of Dirac’s time-dependent variational principle states that an action of the form \( \Gamma = \int dt \langle \Psi | i \hbar \partial / \partial t - H | \Psi \rangle \) \( \delta \Gamma = 0 \) results in the Schrödinger Equation. The solution is obtained by restricting \( | \Psi, t \rangle \) to a subspace of the full Hilbert space. For deriving the semiclassical Gaussian dynamics, the subspace is assumed to be that of a “squeezed state” wave function of the form [7]:

\[
\psi(x,t) = \frac{1}{(2\pi \rho^2)^{1/4}} \exp \left\{ -\alpha \frac{\rho^2}{4\rho^2}(x - \langle x \rangle)^2 + ip(x - \langle x \rangle) \right\}
\]

where, with the definition \( \Delta A \equiv A - \langle A \rangle \), \( \alpha = 1 - \frac{i}{2} \Delta x \Delta p + \Delta p \Delta x \) and \( \rho \) is defined such that

\[
\langle \Delta x^{2m} \rangle = \frac{\rho^{2m}(2m!)}{2^m m!}
\]

with \( m = 1 \) corresponding to the position variance, \( \langle \Delta x^2 \rangle = \rho^2 \). The use of a squeezed state ansatz is reminiscent of the time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory [14]. The major difference is that with TDHFB the squeezed state ansatz is applied for both the condensate and non-condensate atoms, as it is a finite temperature theory. Further, the mean field solution used is the precise ground state for the system, not a Gaussian approximation i.e. it has nothing to do with the classical dynamics. TDHFB is also a very difficult problem to solve. Here, we are interested in the semiclassical dynamics at the mean field level, i.e. where all the atoms are assumed to be in the condensate.

With such an ansatz, the dynamics of the system characterized by a Hamiltonian \( H = p^2/2 + V(x) \) (here we set the mass to unity) can be represented as an extended classical gradient system for the average and fluctuation variables. The dynamical equations for the coordinate variable \( \langle x \rangle \) and its standard deviation, \( \rho \) are:

\[
\frac{d^2 \langle x \rangle}{dt^2} = -\sum_{m=0}^{\infty} \frac{\rho^{2m}}{m!^2} \times V(2m+1)(\langle x \rangle)
\]

\[
\frac{d^2 \rho}{dt^2} = \frac{\hbar^2}{4\rho^3} - \sum_{m=1}^{\infty} \frac{\rho^{2m-1}}{(m-1)!^2} \times V(2m)(\langle x \rangle)
\]

where \( V^{(n)}(\langle x \rangle) = \frac{\partial^n V(x)}{\partial x^n} \big|_{x=\langle x \rangle} \).

By integrating the above equations once with respect to time, the dynamics of the respective conjugate variables \( \langle p \rangle \) and \( \Pi \) are obtained:

\[
\langle p \rangle = \frac{d\langle x \rangle}{dt} \quad \text{and} \quad \Pi = \frac{d\rho}{dt},
\]

where

\[
\Pi \equiv \frac{\langle \Delta x \Delta p + \Delta p \Delta x \rangle}{2\rho}.
\]

From the uncertainty relation

\[
\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} + \frac{\langle \Delta x \Delta p + \Delta p \Delta x \rangle^2}{4}.
\]

the momentum variance can be written in terms of \( \rho \) and \( \Pi \) as

\[
\langle \Delta p^2 \rangle = \frac{\hbar^2}{4\rho^2} + \Pi^2,
\]

implying that whenever \( \Pi = 0 \), we have the minimum uncertainty state. We note that Eqs. (4-7) are the most general equations of motion for \( \langle x \rangle \), \( \langle p \rangle \), \( \rho \) and \( \Pi \) for a squeezed coherent state in an arbitrary potential \( V(x) \).

We use this set of self-contained equations to model our case. It is noted that these equations may also be derived alternatively using an operator expansion method [13]. A point of interest is how to include the interatomic interaction in the equations of motion.

As shown in Eq. (1), the GPE for the condensate wave function is a nonlinear Schrödinger equation with an additional mean field potential term \( U_0|\psi(x,t)\rangle^2 \). We therefore model nonlinearity by extending our potential to introduce the “internal” mean field potential experienced by an atom in the condensate i.e., \( V(x,t) = V_{\text{ext}}(x,t) + V_{\text{int}}(x,t) \) where \( V_{\text{ext}}(x,t) \) is the usual externally imposed potential (such as the harmonic trap) and \( V_{\text{int}}(x,t) \) is the internal “mean field” potential due to the interatomic interactions experienced by the condensate atoms:

\[
V_{\text{int}}(x,t) \equiv U_0|\psi(x,t)\rangle^2 = \frac{U_0 e^{-(x-\langle x \rangle)^2}}{\sqrt{2\pi \rho^2}},
\]

where we have assumed that the condensate wave function is given by the squeezed state Eq. (2). Since the
semiclassical equations are essentially equations governing \( \langle x \rangle \) and \( \rho \) and \( V_{\text{int}}(x, t) \) is itself a function of the time-dependent variables \( \langle x \rangle \) and \( \rho \), it should provides the necessary nonlinear effect consistent within this framework. We shall check this by comparing with the equations derived independently in Ref. [12] where the Lagrangian itself contained the nonlinear interaction term from the outset.

For the purposes of deriving the semiclassical equations for atomic BECs, we shall consider a most general (practical) form for the external potential:

\[
V_{\text{ext}}(x, t) = \frac{1}{2} \omega^2 x^2 - \alpha \cos(kx - \Omega t) - 1 + \beta x \tag{11}
\]

where \( \omega \) provides the frequency of the harmonic trap, \( \alpha \) is the amplitude of an optical lattice, \( \beta \) is the gradient of the tilt of the optical lattice, and \( \Omega \) allows the possibility of a travelling lattice at speed \( \Omega/k \). By setting \( \alpha = \beta = \Omega = 0 \) and \( \omega \neq 0 \) one is considering the case of a harmonically trapped condensate, while setting \( \alpha \neq 0 \) and \( \omega = 0 \) would imply the presence of an optical lattice only. It is noted that all of these parameters \( \alpha, \beta, k, \Omega \) and \( \omega \) can, in general, be time-dependent quantities. The form of the optical lattice potential was chosen so that at time \( t = 0 \) it approximates the standard harmonic potential for a condensate initially at mean position \( \langle x \rangle = 0 \).

It was found that the infinite series of Eqs. (4) and (5) involving the \( V_{\text{ext}}(x, t) \) part can be obtained relatively straightforwardly, while that involving \( V_{\text{int}}(x, t) \) was less straightforward, and required the use of the definition of the Hermite polynomials \( H_n(x) \),

\[
H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{12}
\]

the identity

\[
H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{(1/2)}(x^2), \tag{13}
\]

where \( L_n^{(\alpha)}(x) \) are the generalized Laguerre polynomials, and the generating function for the Laguerre polynomials

\[
e^{-xt/(1-t)} \frac{1}{(1-t)^{\alpha+1}} = \sum_{n=0}^{\infty} L_n^{(\alpha)}(x) t^n. \tag{14}
\]

After some work, the semiclassical equations that describe a BEC in the general external potential and in the presence of a mean field is finally obtained as:

\[
\frac{d^2 \langle x \rangle}{dt^2} = -\alpha k \sin(k \langle x \rangle - \Omega t) e^{-\beta^2 k^2/2 - \omega^2 \langle x \rangle} - \beta \langle x \rangle \tag{15}
\]

\[
\frac{d^2 \rho}{dt^2} = -\left[ \alpha k^2 \cos(k \langle x \rangle - \Omega t) e^{-\beta^2 k^2/2 + \omega^2 \langle x \rangle} \right] \rho + \frac{\hbar^2}{4 \rho^3} + \frac{U_0}{4 \sqrt{\pi} \rho^3}. \tag{16}
\]

These equations in \( \langle x \rangle \) and \( \rho \) can be very easily solved numerically compared to the GPE which requires a dense grid in both position and time for accuracy. In particular, the equations are essentially identical to those obtained in Ref. [12]. This proves the validity of the assumption that at least for the Gaussian ansatz, the effect of non-linearity can be modeled exactly by assuming that the interatomic interaction effectively results in a modified potential. This insight can help in analyzing equations in other contexts.

The variables in the semiclassical equations yield an extended potential system where the fluctuation and average variables are treated on equal footing. The extended Hamiltonian \( H_{\text{ext}} \equiv \langle H \rangle \) in our case is given by

\[
H_{\text{ext}} = H_x + H_\rho + H_{x\rho} \tag{17}
\]

\[
H_x = \langle p \rangle^2 \over 2 + \beta \langle x \rangle + \frac{1}{2} \omega^2 \langle x \rangle^2 \tag{18}
\]

\[
H_{x\rho} = -\alpha \cos(k \langle x \rangle - \Omega t) e^{-\beta^2 k^2/2} \tag{19}
\]

The form of the extended Hamiltonian indicates effectively an infinite barrier potential \( H_{\text{ext}} \to \infty \) as \( \rho \to 0 \) i.e. the “quantum fluctuations” can never go to zero except in the limit \( \hbar \to 0 \) and \( U_0 \to 0 \). The last two terms of Eqs. (19) and (19) indicate that the effect of having a mean field interatomic interaction can be thought of as effectively modifying the Plank constant \( \hbar \to h_{\text{eff}} \) such that:

\[
h_{\text{eff}} = \sqrt{\hbar^2 + \frac{U_0}{\sqrt{\pi}}}. \tag{20}
\]

This formally supports the observation that nonlinear interatomic interactions (having \( U_0 > 0 \)) push the system deeper into the “quantum” regime.

Several interesting observations can be made simply by examining Eqs. (15) and (16) a bit more closely. For instance, it is clear how to directly set the accelerations, \( d^2 \langle x \rangle / dt^2 \) and \( d^2 \rho / dt^2 \) by choosing various initial parameters \( \alpha, k, \Omega, \omega, \beta \) and \( U_0 \). This can be useful in designing quantum control strategies to manipulate a wave packet’s acceleration. Such direct and intuitive information is not readily available from the GPE. In particular, the entire right hand side of Eq. (16) can be made to vanish i.e. one can figure out how to stop the variance of a wave packet from accelerating.

This is significant since, if one starts off with a stationary state i.e. with a zero initial rate of change \( dp/dt = 0 \), the width of the wave packet throughout the evolution is “frozen” at the initial value under such conditions. For a Gaussian this is tantamount to having its overall shape unaltered throughout its evolution. Although such a behavior is reminiscent of a soliton solution [17], they are better classified as solitary waves [18] as it has less to do with the nonlinearity of the system and more to do with being a stationary state of the extended Hamiltonian. Another way to look at this is to consider the gradient of the extended potential with respect to the position.
corresponding to various values of state wave packet represented by the position variance for variance. When one has

$$\frac{dH_{x\rho}}{d\rho} + \frac{dH_{\rho}}{d\rho} = 0, \quad (21)$$

$\rho$ continues on with its initial value without acceleration.

For the case of a harmonically trapped condensate ($\alpha = \beta = 0$, $\omega > 0$) the right hand side of Eq. (16) vanishes when the initial width of the wave packet is such that

$$\rho = \sqrt{\frac{\hbar}{2\omega}} \quad (22)$$

i.e. it gives the expected width of the stationary state solution for a given value of $U_0$. In Fig. 1 the prediction of the semiclassical equation for the stationary state solution is compared with those obtained using the full quantum ground state solution of the GPE. Figure 1(a) compares the shape of the Gaussian solitary wave solution for $U_0 = 5$ with the ground state of GPE for the same value of nonlinearity, while Fig. 1(b) compares the width of the stationary state wave function as a function of $U_0$. We have checked using the numerical ground state solution to GPE with a harmonic trap that for $U_0$ up to around 9, the profile of the condensate can be well-approximated by a Gaussian before going over to the inverted parabolic form of the Thomas-Fermi regime.

A common experimentally relevant situation is when the harmonic trap is turned off in the absence of an optical lattice, ($\alpha = \beta = 0$, $\omega = 0$, $U_0 > 0$). It is easy to see from the right hand side of Eq. (16) being positive that the position variance $\rho$ will start to increase without bound when the trap is suddenly turned off. In addition, as $\rho \to \infty$, $d^2\rho/dt^2 \equiv d\Pi/dt \to 0$ due to the last two terms of Eq. (16) i.e. $\Pi$ becomes a constant

$$\langle \Delta p^2 \rangle \equiv \frac{\hbar^2}{4\rho^2} + \Pi^2 \to \Pi^2 \quad (23)$$

i.e. it is expected that the momentum variance reaches a constant value after a while. Although this fact about the momentum variance is not at all obvious from the GPE or even from the theory of Fourier transforms – one would suspect the momentum variance tends towards zero as the position variance increases without bound – Fig. 1(c) and (d) indicate that the quantum simulation using GPE shows a good qualitative agreement with the semiclassical prediction.

What is also notable is that, if one wants to hold the wave packet together in the absence of any confining potential ($\alpha = \beta = 0$, $\omega = 0$), one needs $U_0 = -\hbar^2/\sqrt{\pi} < 0$ to get the right hand side of Eq. (16) to vanish i.e. an attractive interaction, as expected. This also presents the limit as to how far negative $U_0$ can be for a harmonically trapped BEC with an attractive interaction. This is because, with a harmonic potential present ($\alpha = \beta = 0$, $\omega > 0$), $U_0 = -\hbar^2/\sqrt{\pi}$ in Eq. (16) eliminates the infinite barrier potential so that $\rho$ can take on zero value after some time. This then makes $\langle \Delta p^2 \rangle \equiv \frac{\hbar^2}{4\rho^2} + \Pi^2$ to diverge, making the system unstable – this limit on $U_0$ shows that, according to a semiclassical argument, a given harmonically trapped BEC with a negative scattering length can support up to

$$N = \frac{1}{4\sqrt{\pi}|a|} \approx 0.141 \frac{|a|}{2\hbar/a} \quad (24)$$

atoms where the interatomic scattering length $a$ is in harmonic oscillator lengths $\sqrt{\hbar/m\omega}$. Ignoring additional considerations such as the dimensionality of the condensate this is of comparable order of magnitude to the prediction made using the full quantum theory for the upper limit in atom number, $N = 0.573/|a|$. Again the semiclassical equations can be a useful tool in finding order-of-magnitude predictions based on intuitive argument.

In a previous work, the case where the interaction strength $U_0$ of a harmonically trapped atomic BEC is suddenly tuned to zero was studied using the full quantum theory. In that work it was noted that a BEC starts to undergo oscillatory motion which correspond to the rotation of the error contour. We investigate here a similar effect using the semiclassical equations: starting with the stationary state with nonlinearity $U_0 > 0$, the nonlinearity is suddenly switched to $U_{\text{new}}$ at time $t = 0$ and the subsequent evolution of the position and momentum variances is observed. We consider four possible cases: (a) $U_{\text{new}} = 0$, (b) $0 < U_{\text{new}} < U_0$, (c) $U_{\text{new}} > U_0$ and
with the initial nonlinearity of $U_0 = 5$ is tuned to new nonlinearity $U_{\text{new}}$ at time $t = 0$. (a) $U_{\text{new}} = 0$, (b) $U_{\text{new}} = 2$, (c) $U_{\text{new}} = 7$, and (d) $U_{\text{new}} = -0.5$

(d) $-\hbar^2 \sqrt{\rho} < U_{\text{new}} < 0$ and compare the quantum calculations with the semiclassical prediction. We show in Fig. 2 the evolution of the correlations $\langle \Delta x^2 \rangle$ and $\langle \Delta p^2 \rangle$ of a trapped BEC with initial $U_0 = 5$ when the nonlinearity is tuned at time $t = 0$ to $U_{\text{new}} = 0$, 2, 7, and $-0.5$. It is noted that for $U_{\text{new}} = 0$ shown in Fig. 2(a), the evolution of both position and momentum variances vary sinusoidally with equal amplitudes, consistent with the previous observation on the rotation of the error contour, while for $U_{\text{new}} \neq 0$, the oscillation amplitudes are uneven, showing the effect of squeezing.

This result clearly indicates that the amount of quantum squeezing can be controlled by controlling the magnitude of $U_{\text{new}}$ relative to $U_0$. From further simulations with different values of $U_{\text{new}}$, it was found that in general, with a decreasing $U_{\text{new}} < U_0$ such as Fig. 2(b) the minimum value that the position variance takes during the oscillatory dynamics decreases, indicating position squeezing while, with an increasing $U_{\text{new}} > U_0$ such as Fig. 2(c), the maximum value that the position variance takes increases indicating momentum squeezing. This shows that the general effect of positive nonlinearity is to induce momentum squeezing. The case with a negative $U_0$ such as Fig. 2(d) showed that the momentum variance quickly diverges as $U_0$ becomes more negative.

All these behaviors may be understood from the structure of the extended Hamiltonian $H_{\text{ext}}$ and the changes in the infinite barrier potential term in Eq. (10). It should be noted that the semiclassical predictions differ only in the amplitude for the $U_{\text{new}} = 0$ case while for $U_{\text{new}} \neq 0$, there is also a phase difference so that over a long time, the semiclassical prediction gets worse. This feature due to the nonlinear effect agrees with the result observed in a different context of driven nonlinear systems[15], and indicates that the semiclassical dynamics are better for predicting short time evolutions.

Finally we consider the evolution of variances in an optical lattice instead of a harmonic trap. A salient aspect from the semiclassical equations is that, $\langle x \rangle$ and $\rho$ are coupled in the presence of an optical lattice, unlike the case of a simple harmonic trap ($\alpha = \beta = 0$) for which $\langle x \rangle$ and $\rho$ are completely decoupled. Also, due to the $e^{-x^2k^2/\rho}$ factor, the effect of the optical lattice is significantly diminished when the wave packet is extended over the lattice, i.e. when $t^2k^2 \gg 1$ or $\rho \gg \lambda_{OL}$ where $\lambda_{OL}$ is the wavelength of the optical lattice. Likewise, when $\rho$ is small, the effect of the optical lattice becomes more pronounced.

Figure 3 shows what happens when one places a condensate corresponding to $U_0 = 5$ and position variance $\rho^2$ in an optical potential of varying wavelengths. It was found that for wavelengths $\lambda_{OL} < \rho$ it is as if the optical lattice is not present, and shows ballistic expansion-like behavior. In such cases, the GPE simulation agreed very well with the semiclassical prediction. However, as Fig. 4(a) shows, although the semiclassical equation captures the mean and variance it does not capture the detailed structure formed in the wave packet. For $\lambda_{OL} = 2\rho$, we see in Fig. 4(b) that the semiclassical prediction starts to deviate from the calculation of the full GPE solution; this is understandable from Fig. 4(b) where it shows the breakup of the wave function such that the Gaussian approximation cannot be valid (In fact, the Gauss-
FIG. 4: (Color online) Spatio-temporal plot of the probability density $|\psi(x, t)|^2$ obtained from the GPE when a BEC with the initial nonlinearity $U_0 = 5$ and position variance $\rho^2$ is placed in an optical lattice with wavelength (a) $\lambda_{OL} = \rho$, (b) $\lambda_{OL} = 2\rho$, (c) $\lambda_{OL} = 10\rho$, and (d) $\lambda_{OL} = 20\rho$. This shows that especially for $\lambda_{OL} = \rho$ and $2\rho$ the Gaussian approximation is not valid.

The example with the optical lattice shows that there is rich physics to be explored, and that one needs to exercise caution in applying the semiclassical analysis to make detailed experimental predictions. The results show clearly that the quantitative differences between the semiclassical and the quantum result originate from the fact that the semiclassical limit is more or less a “coarse grained” representation of the full quantum dynamics. This is unavoidable since, fundamentally, classical mechanics deal with point particles in phase space whereas quantum mechanics deal with wave functions. Indeed, the semiclassical approach such as the one discussed in this paper has been originally developed as one of the many attempts to bridge the gap between the classical and quantum physics.

In summary, we have derived a set of equations for atomic BECs which describe the condensate dynamics in the semiclassical limit. The semiclassical equations have been derived by applying the Gaussian squeezed coherent state ansatz for the condensate wave function. From the comparison of the semiclassical dynamics with the expected full quantum dynamics, it was found that the interatomic interactions tend to push the condensate deeper into the quantum regime. The advantage of these equations was that it was easy to get a more intuitive picture of the behavior of the system under consideration. Intuitive understanding could be obtained either from the classical Hamiltonian energy landscape argument or from simply examining the equations carefully and considering the variables in various limits. Such an analysis is not possible with the GPE. Despite the additional advantages such as the very high numerical efficiency, if one wants to use the semiclassical equations as a predictive guide to the full quantum dynamics, one has to make sure that the Gaussian approximation is likely to be valid throughout the evolution. With this caveat, the semiclassical equations provide a quick diagnostics and a verifiable “baseline” with which one can gauge the classical or quantum nature of a condensate dynamics under different situations.

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