Streaming Instability with Multiple Dust Species: I. Favourable Conditions for the Linear Growth

Zhaohuan Zhu (朱照寰)1⋆ and Chao-Chin Yang (楊朝欽)1

1Department of Physics and Astronomy, University of Nevada, Las Vegas, 4505 S. Maryland Parkway, Box 45402, Las Vegas, NV 89154-4002, USA

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ABSTRACT
Recent study suggests that the streaming instability, one of the leading mechanisms for driving the formation of planetesimals, may not be as efficient as previously thought. Under some disc conditions, the linear growth rate of the instability decreases significantly when multiple dust species are considered, and the instability growth timescale can be longer than the disc lifetime. To further explore this finding, we use both linear analysis and direct numerical simulations with gas fluid and dust particles to mutually validate and study the unstable modes of the instability in more detail. We extend the previously studied parameter space by one order of magnitude in both the range of the dust-size distribution \([T_{s,\text{min}}, T_{s,\text{max}}]\) and the total solid-to-gas mass ratio \(\varepsilon\) and introduce a third dimension with the slope \(q\) of the size distribution. We find that the converged fast-growth regime and the non-converged slow-growth regime are distinctly separated by a sharp boundary in the \(\varepsilon – T_{s,\text{max}}\) space, while this boundary is not appreciably sensitive to \(q\) or \(T_{s,\text{min}}\). Moreover, it is not necessary that the largest dust species dominate the growth of the unstable modes, and the smaller dust species can either increase or decrease the growth rate significantly. In any case, we find that the converged fast-growth regime is bounded by \(\varepsilon \gtrsim 1\) or \(T_{s,\text{max}} \gtrsim 1\), which may represent the favourable conditions for planetesimal formation.

Key words: hydrodynamics – planets and satellites: formation – protoplanetary discs – instabilities

1 INTRODUCTION
One major obstacle for planet formation under the core accretion scenario is how solids can grow from cm/m-sized objects to km-sized planetesimals within a 1–10 Myr disc lifetime (Williams & Cieza 2011; Ansdell et al. 2016). Dust can grow from the ISM \(\mu m\) sizes to mm/cm sizes via electrostatic forces at collisions. Objects of km sizes and above can bind themselves and accrete materials via their own gravity (Benz & Asphaug 1999; Leinhardt & Stewart 2009; Bukhari Syed et al. 2017; Sebastián et al. 2020). However, it is difficult for solids to grow from pebble sizes to km sizes (Johansen et al. 2014). Collisions between dust at these sizes often lead to bouncing or fragmentation instead of growth (Blum & Wurm 2008; Zsom et al. 2010). Furthermore, mm/cm-sized pebbles in the outer disc or meter-sized boulders in the inner disc radially drift inward problematically fast in protoplanetary discs. In a smooth disc, these solids should drift to the central star within \(\sim 10^4\) years, which is known as the radial-drift barrier for planetesimal formation (Adachi et al. 1976; Weidenschilling 1977; Birnstiel et al. 2016).

Several mechanisms have been proposed to overcome these barriers to planetesimal formation, including dust traps at a local pressure maximum (Whipple 1972; Johansen et al. 2009; Bai & Stone 2014) or within vortices (Barge & Sommeria 1995; Lyra et al. 2009), growth of porous icy dust aggregates (Kataoka et al. 2013), secular gravitational instability (Youdin 2011; Michikoshi et al. 2012; Takahashi & Inutsuka 2014), and the streaming instability (Youdin & Goodman 2005; Youdin & Johansen 2007; Johansen & Youdin 2007; Lin & Youdin 2017). Among these, the streaming instability is one promising mechanism to concentrate dust particles of a wide range of sizes (Carrera et al. 2015; Yang et al. 2017; R. Li et al., in preparation). Unlike other mechanisms, which passively rely upon the underlying disc structures, dust particles actively participate in the dust-gas dynamics and spontaneously concentrate themselves via the reaction of the aerodynamic drag back onto the gas (Yang & Johansen 2014; Li et al. 2018).

However, Krapp et al. (2019) found that the linear growth of the streaming instability can be significantly dif-
different when considering a range of dust sizes instead of a single dust species as in previous studies. For some dust-size distributions and total solid-to-gas mass ratios, the growth rate of the instability decreases with increasing number of discrete species representing the distribution. It appears that for these cases, the growth timescale can be much longer than the typical disc lifetime for large number of dust species. This implies that taking the limit of a continuous dust-size distribution, the instability may not operate at all in protoplanetary discs. Interestingly, we note that when including the effects of vertical dust sedimentation, the streaming instability with multiple dust sizes appears to operate and can even drive strong concentration of dust particles according to previous numerical simulations (Bai & Stone 2010; Schaffer et al. 2018). Furthermore, the effects of background turbulence have not been considered in this scenario yet (Yang et al. 2018; Chen & Lin 2020; Unurman et al. 2020), and it appears that turbulence may play an important role in determining the efficiency and scale of planetesimal formation (Gerbig et al. 2020; Gole et al. 2020; Klahr & Schreiber 2020). Therefore, further studies of the multi-species streaming instability seem warranted.

In this work, we augment the study by Krapp et al. (2019) as follows. We validate the linearly unstable modes of the instability by using both linear analysis and direct numerical simulations (Sec. 2). We expand the parameter space by one order of magnitude in both the range of dust sizes and the total solid-to-gas ratio, and moreover, we explore the effects of the slope of the dust-size distributions (Sec. 3). Then we analyze in detail the properties of the most unstable mode (Sec. 4) and the contributions from different dust species (Sec. 5). Finally, we briefly summarize our results (Sec. 6).

2 METHODS

2.1 Linear analysis

We carry out the linear analysis for the multi-species streaming instability using the linearized perturbation equations presented in Appendix E of Benítez-Llambay et al. (2019), which assumes no vertical stratification and no background turbulence. The underlying dust-size distribution is assumed to follow a power law \( n(s) \propto s^q \) (Mathis et al. 1977) from \( s_{\text{min}} \) to \( s_{\text{max}} \), where \( s \) is the size of the dust particle. Since dust particles under the conditions of a typical protoplanetary disc are mostly in the Epstein regime, we assume that the dust’s dimensionless stopping time \( (T_s) \) is proportional to the particle size.

Under these assumptions, we consider dust with sizes from \( T_{s,\text{min}} \) to \( T_{s,\text{max}} \) (i.e., \( T_s \in [T_{s,\text{min}}, T_{s,\text{max}}] \)) and a total dust-to-gas mass ratio of \( \varepsilon \) in a disc. To discretize the continuous distribution into \( N_{sp} \) dust species, we divide the dust distribution into \( N_{sp} \) bins uniformly in the log \( T_s \) space. The dust particles in each bin have identical stopping time \( T_{s,i} \), being at the linear center of the bin. The dust-to-gas mass ratio for each bin is

\[
\varepsilon_i = \frac{T_{s,i+1} - T_{s,i}}{T_{s,\text{max}} - T_{s,\text{min}}},
\]

where \( T_{s,i+1} \) and \( T_{s,i} \) are the upper and lower dust size limit for each dust bin. In this case, \( \varepsilon = \sum \varepsilon_i \) (Schaffer et al. 2018). When we increase the number of species \( N_{sp} \) with the same distribution, the total mass of the dust remains constant.

Under the local-shearing-box approximation, Benítez-Llambay et al. (2019) derived the equations describing the gas and \( N_{sp} \) dust species in the radial-vertical \( (x,z) \) plane assuming axisymmetry. The linearized equations have been written in terms of the perturbed variables \( \delta f(k_x,k_z) = e^{i(k_xx + k_zz + \omega t)}c_{s,i} \) in the Fourier space. The wave number \( (k_x, k_z) \) and the complex eigenvalue \( \omega(k_x, k_z) \) can be expressed in the dimensionless form of \( K = k_x R_0 \) with \( i = x, z \) and \( \omega = \omega/\Omega(R_0) \), where \( \eta \) is related to the radial pressure gradient at the orbital radius \( R = R_0 \) by

\[
\eta \equiv \frac{\hbar^2}{2} \frac{d \log P}{d \log R},
\]

\( \hbar \equiv \frac{H_0}{R_0} \) with \( H_0 \) being the disc scale height at \( R_0 \), and \( \Omega(R) \) is the Keplerian angular frequency (Nakagawa et al. 1986). We choose \( \eta_{1/2} = 0.05 \) as our fiducial radial pressure gradient, where \( \eta_{1/2} = R\Omega_{K} \) and \( \Omega_{K} \) is the Keplerian velocity and the local speed of sound at \( R_0 \), respectively. We have also tried \( \eta_{1/2} = 0.1 \) for the outer disc, but the results are almost identical to those with the fiducial gradient. The eigenvalues \( \omega \) of the linearized equations are computed using Python NumPy function \texttt{linalg.eigvals}, and the growth rate of the multi-species streaming instability is hence \( \sigma = -\text{Re}(\omega) \). All growth rates \( \sigma \) in this paper is scaled to \( \Omega_K \).

We consider three different power-law indices \( q = -3.5, -2.5, \) and \( -1.5 \) for the dust-size distribution, motivated by protoplanetary disc observations and dust coagulation/fragmentation calculations (e.g., Pérez et al. 2015, Birnstiel et al. 2012). The smallest dust particles are fixed at \( T_{s,\text{min}} = 10^{-4} \) or \( 10^{-3} \). Given the maximum dust stopping time \( T_{s,\text{max}} \) and the total solid-to-gas mass ratio \( \varepsilon \), we calculate the maximum growth rate from all the eigenmodes for each \( K_x \) and \( K_z \). We then search for the maximum growth rate among the Fourier space \((K_x, K_z)\). This space is infinite, so we need to confine our search in practice. Youdin & Goodman (2005) have suggested that \( K_x \sim K_z \sim 1/T_s \) is roughly where the fastest growing mode is for the single-species streaming instability. Therefore, centred around \( K_x = K_z = 1/T_{s,\text{max}} \), we uniformly choose 54 values of \( \log_{10} K_x \) in \([A-1.5, A+2.5]\) and 54 values of \( \log_{10} K_z \) in \([A-3, A+3]\), where \( A = -\log_{10} T_{s,\text{max}} \). By inspection, we find that this domain size generally captures the absolute maximum of the growth rate. Thus, we define the maximum growth rate \( \sigma \) for any given \( T_{s,\text{max}} \) and \( \varepsilon \) as the maximum among the 54\times54 computed growth rates.

For each given dust distribution, we systematically increase the number of dust species \( N_{sp} \) from 2 to 1024 and use the aforementioned method to find the maximum growth rate \( \sigma \) for each \( N_{sp} \). However, the linear algebra becomes quite computationally intensive when \( N_{sp} \) is more than 1024. To estimate the maximum growth rate with more dust species (e.g., \( N_{sp} = 2048 \) and \( N_{sp} = 4096 \)), therefore, we simply use the \( K_x \) and \( K_z \) of the fastest growing mode found with 1024 dust species and only calculate the growth rate for this combination of \( K_x \) and \( K_z \) for 2048 and 4096 dust species, leading to our \( \sigma_{2048} \) and \( \sigma_{4096} \), respectively. Our experience with \( N_{sp} \leq 1024 \) is that, in most cases, increasing \( N_{sp} \) does not change the wave number of the fastest growing
mode, so our approach should give a good approximation of the maximum growth rate with 2048 and 4096 dust species. On the other hand, we caution that, under some circumstances (one example is given in Sec. 4), the fastest growing mode may occur at another $K_x$ and $K_z$ and may have a higher rate than $\sigma_{2048}$ and $\sigma_{4096}$ derived here.

2.2 Numerical validation

In addition to linear analysis, we use a simulation code to reproduce a linear mode for several cases, which serves for two purposes. First, the results from our linear analysis and the code are mutually validated, and in this process we demonstrate the resolution requirement for simulating the streaming instability with multiple dust species. Second and perhaps more importantly, by using a code equipped with Lagrangian dust particles, we can gauge the validity of the multi-fluid approximation for dust particles used in the linear analysis, especially for relatively large ones ($T_s \sim 1$, Garaud et al. 2004) which also happen to have the highest growth rates.

For these purposes, we use the Pencil Code$^1$ (Brandenburg & Dobler 2002). It employs sixth-order finite differences to approximate any spatial derivatives and integrates the system of (magneto-)hydro-dynamical equations in time using third-order Runge–Kutta method. To stabilize the scheme, we use sixth-order hyper-diffusion with fixed Reynolds number (Yang & Krumholz 2012). The dust component is modelled as Lagrangian super-particles, and their trajectories are integrated in tandem with the Runge–Kutta steps. The drag interaction between each dust particle and its surrounding gas is achieved via the standard particle-mesh method (Youdin & Johansen 2007).

For each dust distribution [$T_{s,\text{min}}, T_{s,\text{max}}$] and total solid-to-gas density ratio $\epsilon$, we explore a mode with a wave number $K_x = K_z$ that is close to the fastest growing mode. We normalize the eigenvector such that the amplitude of the perturbation in total particle density relative to the equilibrium density is about $10^{-6}$. We use a square computational domain that accommodates one wavelength per dimension. While it is straightforward to seed the mode in the gas component with Eulerian formulation, it is not trivial to do so in the dust component with Lagrangian super-particles. We describe in detail in Appendix A the algorithm of how to position the particles to focus the perturbations onto a desired mode. The velocities of the particles are then assigned according to their positions. For all cases, we allocate four particles per species per cell. With that, we conduct each simulation up to a time on the order of one $\epsilon$-folding time, and measure the growth rate of the mode in each field and compare it with the theoretical growth rate obtained from the linear analysis.

3 TWO REGIMES OF THE INSTABILITY

We explore the 3D parameter space spanned by the maximum dust stopping time $T_{s,\text{max}}$, the total solid-to-gas mass ratio $\epsilon$, and the power-law index $q$ for the dust-size distribution. While fixing the minimum dust size with $T_{s,\text{min}} = 10^{-4}$, we select 21 different $\log_{10} T_{s,\text{max}}$ values from $-3$ to 1 and 16 different $\log_{10} \epsilon$ values from $-2$ to 1. Therefore, both our $T_{s,\text{max}}$ and our $\epsilon$ are one order of magnitude larger than those investigated by Krapp et al. (2019). Furthermore, we expand their parameter study with a third dimension by considering three different $q = -3.5$, $-2.5$, and $-1.5$. We describe our findings in this section.

3.1 Characteristic conditions

The top-left panel in Fig. 1 shows the maximum growth rate $\sigma_{1024}$ for 1024 dust species following the dust-size distribution with the power-law index $q = -3.5$, restricting our attention to the parameter space of $T_{s,\text{max}} \leq 1$ and $\epsilon \leq 1$, we have reproduced the growth rate found by Krapp et al. (2019) (see their Fig. 5). The growth rate generally increases with increasing $\epsilon$. Two distinct regimes appear separated by roughly $\epsilon \sim 0.3$, above which the growth rate of the instability is high ($\sigma \gtrsim 0.01\Omega_{K,\text{crit}}^3$) and below which it is appreciably lower ($\sigma \lesssim 0.01\Omega_{K,\text{crit}}^{-1}$). As we expand the parameter space up to $\epsilon = 10$, we find that the trend continues, as $\sigma$ increases with increasing $\epsilon$. Moreover, we find that $\sigma$ also increases with decreasing $T_{s,\text{max}}$ above the transition. The maximum growth timescale is shorter than the orbital time near our smallest $T_{s,\text{max}} \simeq 10^{-3}$ and our largest $\epsilon \simeq 10$.

More interestingly, as we increase the maximum dust size up to $T_{s,\text{max}} = 10$, we find another transition zone where the maximum growth rate changes from low to high. As shown by the top-left panel in Fig. 1, this transition lies at roughly $T_{s,\text{max}} \sim 1$. Therefore, it appears that high growth rate occurs when either the maximum size $T_{s,\text{max}}$ or the total solid-to-gas mass ratio $\epsilon$ is high, while low growth rate occurs when both $T_{s,\text{max}}$ and $\epsilon$ are low.

We further investigate the effects of changing the slope of the dust-size distribution. The top panels in Fig. 1 compares the maximum growth rate $\sigma_{1024}$ for different power-law index $q$, with flatter size distribution (more top-heavy) towards the right (see Eq. 1). As shown by the panels, the general trend found above remains the same, while there are only slight changes of the transition zone separating fast and slow growth of the instability. With a more top-heavy dust distribution, the transition at $\epsilon \sim 1$ becomes less sensitive to $T_{s,\text{max}}$, and there is a larger parameter space which extends to $T_{s,\text{max}} \sim 0.1$ for high growth rates. On the other hand, the most unstable modes for cases at $0.1 \lesssim T_{s,\text{max}} \lesssim 1$ have small $K_x$ which may not fit into the disc thickness, which will be discussed in Sec. 4.

After studying the effects of $T_{s,\text{max}}$ and $q$ on the instability growth rate, we explore the effects of $T_{s,\text{min}}$ by increasing $T_{s,\text{min}}$ from $10^{-4}$ to $10^{-3}$. The resulting growth rates are shown in Fig. 2. By comparing Fig. 2 with Fig. 1, we can see that the growth rate is not appreciably changed by $T_{s,\text{min}}$ as long as $T_{s,\text{max}}$ is not close to $T_{s,\text{min}}$. For the convenience of time-step constraint by the small dust species in direct numerical simulations, we use $T_{s,\text{min}} = 10^{-3}$ to validate the unstable modes in several representative cases in Fig. 2.

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1 The Pencil Code and its documentation is publicly available at http://pencil-code.nordita.org/.

2 We find that with one particle per species per cell, grid noise of small amplitudes appear at high resolutions. Using four particles per cell effectively eliminates this noise.
3.2 Transition between the two regimes

As discovered by Krapp et al. (2019), the fast and slow growth regimes discussed in Sec. 3.1 also have distinct growth rate convergence with the number of discrete dust species $N_{sp}$ representing the distribution. The growth rate in the fast-growth regime converges to a finite value, while in the slow-growth regime, the growth rate appears to approach zero, i.e., the system seems to be virtually stable to the streaming instability. In this section, we attempt to identify the transition between these two regimes.

In the middle panels of Figs. 1 and 2, we plot the ratio between $\sigma_{1024}$ and $\sigma_{512}$ for the same parameters as in the top panels. This ratio decreases quickly from one (converged rates, which corresponds to the red colour) to $\sim 0.5$ (blue colour) as either $\varepsilon$ or $T_{s,max}$ decreases across some critical values. The transition zone separating the two regimes appears to be excessively sharp, and thus we overplot the contour of $\sigma_{1024}/\sigma_{512} = 0.99$ with dashed curves in the middle panels of Figs. 1 and 2.
the top panels to mark this transition. If $\sigma_{2N_{sp}}/\sigma_{N_{sp}} \approx 1$, the growth rate should approach to a finite value, while if $\sigma_{2N_{sp}}/\sigma_{N_{sp}} < 1$, the growth rate continues to approach to zero as $N_{sp}$ increases. Therefore, with more and more dust species, we can expect that the growth rate remains the same in the upper and right sides of the dashed curve, while the growth rate below the dashed curve continues to decrease so that the blue region in the top panels (σ panels) will become darker and darker, i.e., $\sigma_{N_{sp}} \ll 1$.

The bottom panels in Figs. 1 and 2 show the $K_x$ of the fastest growing mode. The $K_x$ value is normalized to $K_a$. $K_{a0}$ represents the $K_x$ of the fastest growth mode for a single dust species having $T_s = T_{s,\text{max}}$. Squire & Hopkins (2018) and Umurhan et al. (2020) use the wave-drift resonance to show that the fastest growing short-wavelength mode for a single dust species with dust-to-gas mass ratio $\varepsilon \lesssim 1$ and stopping time $T_s$ occurs at

$$K_x = K_a \equiv \frac{(1 + \varepsilon)^2 + T_s^2}{2(1 + \varepsilon)T_s}.$$  \hspace{1cm} (3)

When $\varepsilon \ll 1$, $K_a$ is insensitive to $\varepsilon$ so that we use $K_{a0}$, which is $K_a$ with $\varepsilon = 0$, to scale $K_x$. We can see that the converged and non-converged regimes have very different fastest growing modes, which will be discussed in more detail in Sec. 4.

To study how sharp this transition between the two regimes is, we conduct two additional sets of calculations. For one set, we fix $T_{s,\text{max}} = 0.01$ while varying $\varepsilon$ with 192 different values from $10^{-2}$ to 10. For the other set, we fix $\varepsilon = 1$ while varying $T_{s,\text{max}}$ with 192 different values from $10^{-3}$ to 10. For both sets, we consider only the dust-size distribution with power-law index $q = -3.5$. The trace of these two fine scans are schematically drawn with the two dotted lines in the top-left panel of Fig. 1, and the resulting maximum growth rates are shown in Figs. 3 and 4, respec-
Figure 3. The growth rate $\sigma_{N_{sp}}$ (in $\Omega_K^{-1}$) and the dimensionless radial wave number $K_x$ of the fastest growing mode (top panels) and the growth rate ratio $\sigma_{2N_{sp}}/\sigma_{N_{sp}}$ (bottom panels) as a function of the total dust-to-gas mass ratio $\varepsilon$ for discs with a dust distribution of $T_s \in [10^{-4}, 10^{-2}]$ and $q = -3.5$ (along the vertical dotted line in the top-left panel of Fig. 1). Number of dust species $N_{sp}$ representing the distribution increases from the left to the right panels.

Figure 4. The growth rate $\sigma_{N_{sp}}$ (in $\Omega_K^{-1}$) and the dimensionless radial wave number $K_x$ of the fastest growing mode (upper panels) and the growth rate ratio $\sigma_{2N_{sp}}/\sigma_{N_{sp}}$ (bottom panels) as a function of the the maximum size $T_{s,max}$ in a dust-size distribution with power-law index $q = -3.5$ (along the horizontal dotted line in the top-left panel of Fig. 1). The minimum size is $T_{s,min} = 10^{-4}$ and the total dust-to-gas mass ratio is fixed at $\varepsilon = 1$. Number of dust species $N_{sp}$ representing the distribution increases from the left to the right panels.
tively. The number of dust species \( N_{sp} \) increases from 256 in the left panels to 4096 in the right panels.

As shown by the bottom panels of Fig. 3, the growth rate converges with number of dust species to finite values (\( \sigma_{2N_{sp}}/\sigma_{N_{sp}} = 1 \)) for \( T_s \in [10^{-3}, 10^{-2}] \) and \( \varepsilon \geq 0.1 \). The transition from \( \sigma_{2N_{sp}}/\sigma_{N_{sp}} \sim 0.5 \) to \( \sigma_{2N_{sp}}/\sigma_{N_{sp}} = 1 \) becomes sharper and sharper with increasing \( N_{sp} \), which can also be seen in the upper panels. While the growth rate for \( \varepsilon \geq 0.1 \) remain the same from the left to the right top panels (increasing \( N_{sp} \)), the growth rate for \( \varepsilon \lesssim 0.1 \) becomes smaller and smaller. This leads to a discontinuity of the growth rate which can be identified as the boundary between the two regimes. With larger number of dust species, the fast-growth regime remains to have high growth rate while the slow-growth regime has decreasingly lower growth rate.

We now consider the simulations with a fixed \( \varepsilon = 1 \) and different \( T_{s,\text{max}} \), along the horizontal dotted line in the top-left panel of Fig. 1. The growth rate as a function of \( T_{s,\text{max}} \) is shown in the top panels of Fig. 4 with various \( N_{sp} \). For \( T_{s,\text{max}} \lesssim 0.02 \) and \( T_{s,\text{max}} \gtrsim 0.2 \), the profile of the growth rate remains the same with increasing \( N_{sp} \), as also evident in the bottom panels where \( \sigma_{N_{sp}}/\sigma_{N_{sp}} = 1 \). For \( 0.02 \lesssim T_{s,\text{max}} \lesssim 0.2 \), on the contrary, the rate becomes lower and lower with increasing \( N_{sp} \), leading to a growth rate orders of magnitude lower than in the fast-growth regime when \( N_{sp} = 4096 \). Similar to the case of fixed dust-size distribution but varying \( \varepsilon \), the transitions at \( T_{s,\text{max}} \approx 0.02 \) and \( T_{s,\text{max}} \approx 0.2 \) become sharper and sharper with increasing \( N_{sp} \). Therefore, the two regimes appear to be distinctly separated by a well defined boundary, as delineated by the dashed lines in Figs. 1 and 2.

### Table 1. Growth rate \( \sigma \) (in \( \Omega_i^{-1} \)) of fast-growing eigenmode in multi-species streaming instability

| \( N_{sp} \) | \( K_s = K_z = 60 \) | \( K_s = K_z = 10 \) | \( K_s = K_z = 1 \) |
|---|---|---|
| 1 | 0.009922 | 0.00748144 | 0.0885570 |
| 2 | 0.0616073 | 0.00787742 | 0.0857477 |
| 4 | 0.169425 | 0.0615058 | 0.0794737 |
| 8 | 0.127082 | 0.00334111 | 0.0519613 |
| 16 | 0.0976177 | 0.00283122 | 0.0573683 |
| 32 | 0.0980250 | 0.00169562 | 0.0450016 |
| 64 | 0.0386043 | 0.0097249 |

3.3 Numerical validation

As described in Sec. 2.2, we use the \textsc{Pencil Code} to mutually validate the eigenmodes derived from our linear analysis. We select three different dust distributions: (1) \( T_s \in [10^{-3}, 0.1] \) and \( \varepsilon = 2 \), (2) \( T_s \in [10^{-3}, 0.1] \) and \( \varepsilon = 0.2 \), and (3) \( T_s \in [10^{-3}, 2] \) and \( \varepsilon = 0.2 \), all of which have a power-law index of \( q = -3.5 \). For each distribution, we choose an eigenmode with a wave number \( K_x = K_z \) that is close to the fastest growing mode. The three cases are marked by the triangles in Fig. 2, and the growth rate of the mode as a function of number of dust species \( N_{sp} \) is listed in Table 1.

First, we consider the distribution \( T_s \in [10^{-3}, 0.1] \) and \( \varepsilon = 2 \). As shown in Fig. 2, this case belongs to the converged fast-growth regime. The growth rate approaches to a constant with increasing number of dust species and convergence occurs at \( N_{sp} \sim 16 \), as indicated by Table 1. Figure 5 shows the growth rate measured by the \textsc{Pencil Code} with various \( N_{sp} \) and resolutions \( \lambda/\Delta \), where \( \lambda = 2\pi/K_i \) is the wavelength per dimension with \( i = x, z \) and \( \Delta \) is the grid spacing. The simulation data demonstrate convergence with resolution to the theoretical rate at each given \( N_{sp} \). For \( N_{sp} > 2 \), convergence of gas velocity and dust density is seen at \( \lambda/\Delta \sim 32 \) while convergence of dust velocity and gas density is seen at \( \lambda/\Delta \sim 64 \). For the case of \( N_{sp} = 1 \), the convergence with resolution is similar while it is slightly worse for the case of \( N_{sp} = 2 \).

We next consider the dust distribution \( T_s \in [10^{-3}, 0.1] \) and \( \varepsilon = 0.2 \). It only differs from the previous case by the much decreased solid-to-gas mass ratio \( \varepsilon \), leading to longer critical wavelengths and into the non-converged slow-growth regime (Fig. 2). As shown by Table 1, the growth rate continues to decrease with increasing number of dust species \( N_{sp} \). Again we use the \textsc{Pencil Code} to measure the growth rate up to \( N_{sp} = 32 \) with varying resolutions, and the results are shown in Fig. 6. The code can still capture the instability accurately at such a low growth rate of \( \sigma \approx 0.0017\Omega_i^{-1} \) and convergence with resolution can be seen at \( \lambda/\Delta \sim 64 \). For comparison, the LinB mode for the single-species streaming instability (\( T_s = 0.1 \) and \( \varepsilon = 0.2 \)) has a growth rate of \( \sigma \approx 0.015\Omega_i^{-1} \), the lowest ever used for code validation in the previous literature (Youdin & Johansen 2007; Balsara et al. 2009; Bai & Stone 2010; Miniati 2010; Yang & Johansen 2016; Benitez-Llambay et al. 2019; Mignone et al. 2019; Krapp et al. 2019). The case we validate here has a growth rate one order of magnitude lower and hence is more challenging.

Finally, we change the maximum size of the dust distribution from the previous case to \( T_{s,\text{max}} = 2 \), the latter of which is in the converged fast-growth regime (Fig. 2). This case is valuable in the sense that the largest dust particles probe into the regime of \( T_s \sim 1 \), above which the fluid approximation used by the linear analysis may be broken because the trajectories of the particles may begin to cross (Garaud et al. 2004). The growth rate measured with the \textsc{Pencil Code} as a function of the number of dust species \( N_{sp} \) and the resolution \( \lambda/\Delta \) is shown in Fig. 7. Once again, convergence of the growth rate to the theoretical rate with resolution at any given \( N_{sp} \) is achieved. The growth in the velocity and density field of the gas converges at \( \lambda/\Delta \sim 16–32 \), while that of the dust particles converges at \( \lambda/\Delta \sim 32–64 \). This experiment indicates that the fluid approximation for the dust particles is still valid in the linear growth of the instability for the largest particles up to \( T_{s,\text{max}} \sim 2 \). However, it remains to be seen if the approximation holds valid in the nonlinear saturation of the instability.

### 4 ON THE CRITICAL WAVE NUMBER

To explore further the nature of the instability in these two distinct regimes, we turn our attention to the most unstable mode itself for any given system. Based on the linear analysis of the single-species streaming instability, Youdin & Goodman (2005) found that the most unstable mode occurs along
Figure 5. Numerical validation of linear modes of the streaming instability for different numbers of dust species using the Pencil Code. The dots are the growth rate $\sigma$ of a mode in units of $\Omega^{-1}$, measured from the simulation data at various resolution in terms of number of grid points per wavelength $\lambda/\Delta$. Different colors represent different numbers of dust species $N_{\text{sp}}$ in the system. The solid lines are the theoretical growth rates. The top panels show the components of the velocity field and the density of the gas, while the bottom panels show the components of the mass-weighted velocity field and the total density of the dust particles. In this case, the dimensionless stopping time is in the range of $T_s \in [10^{-3}, 0.1]$, and the total solid-to-gas mass ratio is $\epsilon = 2$. The selected mode has the wave number $K_x = K_z = 60$, which is close to the fastest growing mode. We note that the results are close to identical between the $N_{\text{sp}} = 16$ and the $N_{\text{sp}} = 32$ cases.

Figure 6. Same as Fig. 5, except that $\epsilon = 0.2$ and $K_x = K_z = 10$.

$K_z \sim T_s K_x^2$ on the long-wavelength side and $K_x \sim \text{constant}$ on the short-wavelength side, which are bridged roughly at $K_x \sim K_z \sim 1/T_s$. Usually, the maximum growth rate can be found near $K_x \sim K_z \sim 1/T_s$ or on the vertical $K_x \sim 1/T_s$. This property is closely related with the resonant drag instability, in which the relative drift velocity between the gas and the dust resonates with the projected wave speed of the gas (Squire & Hopkins 2018). With this new insight into the streaming instability, Squire & Hopkins (2018) gave a more accurate $K_x - K_z$ condition for the long-wavelength branch (their equation (33)) and $K_x = K_a$ (equation (3)) for the short-wavelength branch, assuming $\epsilon \lesssim 1$ (see also Umurhan et al. 2020). In the following, we use it as a reference to analyze what we find in the multi-species streaming instability.
The lowest panels in Figs. 1 and 2 show $K_x$ of the mode that has the highest growth rate. The dimensionless radial wave number $K_x$ is normalized by $K_{a0}$. Therefore, if the fastest growing mode is near the vertical branch $K_x = K_{a0}$, the color should be white in these panels, and it can be implied that the largest dust particles drives the instability in the white region. As shown by the panels, the non-convergent cases (which correspond to the blue region in the panels in the middle row) roughly have $K_x/K_{a0} \sim 1-3$. The convergent cases can be divided by $\varepsilon \sim 1$. For $\varepsilon \gtrsim 1$, $K_x \gtrsim 10K_{a0}$. For $\varepsilon \lesssim 1$, $K_x$ depends on the maximum stopping time $T_{s,\text{max}}$: When $T_{s,\text{max}}$ is small, the fast growing mode has $K_x \ll K_{a0}$ (the vertical wave number $K_x$ is similarly small such that the modes may not fit within the disc thickness, as discussed below), and when $T_{s,\text{max}} \gtrsim 1$, $K_x \sim K_{a0}$.

As in Sec. 3.2, we perform a vertical cut in the bottom-left panel of Fig. 1 as in the top-left panel and plot in Fig. 3 $K_x$ of the fastest growing mode (blue curves) as a function of $\varepsilon$ with a fixed dust distribution $T_s \in [10^{-5}, 10^{-1}]$ and $q = 3.5$. Similar to the convergence of the growth rate, we notice that $K_x$ also has a dramatic change at the $\varepsilon \sim 0.1$ convergence boundary, indicating that non-convergent and convergent cases may have different types of the fastest growing modes. When $\varepsilon \lesssim 0.1$, $K_x$ is close to $1-2K_{a0}$. At $\varepsilon \sim 0.1$, $K_x$ jumps to $20K_{a0}$ for 256 dust species; for 1024 and 4096 dust species, there is only a narrow $\varepsilon$ space for these high $K_x$ values. For convergent cases with $\varepsilon \gtrsim 0.1$, $K_x$ drops to $\sim K_{a0}$ and then increases with larger $\varepsilon$.

To study these modes in detail, we plot in Fig. 8 the growth rate with respect to $K_x$ and $K_{s}$ for three cases with the same $T_{s,\text{max}}$ but different $\varepsilon$ (located at the triangles in the top-left panel of Fig. 1). It can be seen that the fast growing modes (red coloured) may lie in two separate regions: the region that is close to the dust-gas drag resonance with single dust species $T_s = T_{s,\text{max}}$ (dashed curves; Youdin & Goodman 2005; Squire & Hopkins 2018; Umurhan et al. 2020), and another region whose $K_x$ is about one order of magnitude larger (which was also pointed out by Krapp et al. 2019). When $\varepsilon$ is as small as $\sim 0.01$ (not shown), the fastest growing mode lies in the region that is close to the dashed curves. With larger $\varepsilon \sim 0.1$ (the uppermost panels of Fig. 8), the most unstable mode lies in the larger $K_x$ region. As shown in the upper right panel, both red regions do not show convergent rates with increasing $N_{sp}$. Thus, the instability growth rate does not converge to finite values when $\varepsilon \lesssim 0.1$, consistent with Fig. 3. When $\varepsilon$ continues to rise (the middle row in Fig. 8), the narrow region with $K_x \sim T_{s,\text{max}}K_{a0}^2/10$ and small $K_x$ starts to show convergence and hence this region maintains its high growth rate with increasing $N_{sp}$ (left and middle panels). This converged region extends to higher $K_x$ and $K_{s}$ when $\varepsilon$ is even larger (the bottom panels). These changes of the convergent regions with $\varepsilon$ explain the trend of $K_x$ shown in Fig. 3.

We next consider the horizontal cut in the upper-left panel of Fig. 1, i.e., dust distributions with fixed $\varepsilon = 1$, $q = 3.5$, and $T_{s,\text{min}} = 10^{-4}$ but with varying $T_{s,\text{max}}$. The blue curves in the top panels of Fig. 4 show the radial wave number $K_x$ of the fastest growing mode, and Fig. 9 shows the map of the growth rate with respect to $K_x$ and $K_{s}$ for three selected cases (located at the crosses in Fig. 1). For cases shown in both the top and the bottom panels of Fig. 9, the growth rate converges, while the growth rate does not converge for the case in the middle panels. The top panels show that when $T_{s,\text{max}} \ll 1$, the fastest growing mode is at the large $K_x$ branch. When $T_{s,\text{max}}$ increases to $\sim 1$, the convergent region shrinks significantly (right panels), and the fastest growing mode occurs in the single-species resonant region $K_x \sim K_{a0}$, which does not show convergence with $N_{sp}$. When $T_{s,\text{max}}$ increases to even larger values (e.g., $T_{s,\text{max}} = 5$; the bottom panels), the fastest growing mode remains in this $K_x \sim K_{a0}$ region, but the region becomes converged with $N_{sp}$.

Figures 8 and 9 show that unstable modes have con-
Figure 8. Growth rate of the most unstable mode $\sigma$ (in $\Omega_K^{-1}$) as a function of the dimensionless wave number ($K_x, K_z$). The discs have the same dust distribution $T_s \in [10^{-4}, 10^{-2}]$ and $q = -3.5$, but the total solid-to-gas mass ratio $\epsilon$ increases from the top to the bottom panels. The three cases are represented by the triangles in the top-left panel of Fig. 1. The left panels show the growth rate for discs with 512 dust species, while the middle panels show the growth rate for discs with 1024 dust species. The right panels show the ratio between the left two panels. If the ratio at one point is one, the growth rate of that mode converges between $N_{sp} = 512$ and 1024. The dashed curves in the left two columns are calculated using equation (33) in Squire & Hopkins (2018) near which the system with a single dust species having $\epsilon$ and $T_s = T_{s,\text{max}}$ is the most unstable. The cross in each panel labels where the fastest growing mode is.

Figure 9. The maximum growth rate $T_{s,\text{max}}$ and the solid-to-gas mass ratio $\epsilon$ as a function of $\log_{10}K_z$, with $\log_{10}K_x = -3$. The left panel shows the growth rate for discs with 512 dust species, while the middle panels show the growth rate for discs with 1024 dust species. The right panels show the ratio between the left two panels. If the ratio at one point is one, the growth rate of that mode converges between $N_{sp} = 512$ and 1024. The dashed curves in the left two columns are calculated using equation (33) in Squire & Hopkins (2018) near which the system with a single dust species having $\epsilon$ and $T_s = T_{s,\text{max}}$ is the most unstable. The cross in each panel labels where the fastest growing mode is.

5 Interaction Between Dust Species

Krapp et al. (2019) showed that when the total solid-to-gas density ratio $\epsilon \ll 1$ for a given dust-size distribution, the instability is as if being driven by the largest dust species alone. Therefore, as more and more discrete species $N_{sp}$ are involved, the mass fraction of the leading species becomes smaller and smaller, resulting in increasingly small growth rate with increasing $N_{sp}$ and hence its non-convergence. Counter-intuitively, as $\epsilon$ becomes significant, the growth of the instability with multiple species is even slower than the leading species in isolation would have driven. In this section, we use a different approach to explore this property in a different angle and attempt to gain some more insight into the role of the leading dust species and the interaction between the species.

Our experiment is designed as follows. As in Sec. 2.1, we divide a given dust-size distribution $T_s \in [10^{-4}, T_{s,\text{max}}]$ into the role of the leading dust species and the interaction between species.
Figure 9. Similar to Fig. 8 but for discs with the same $\varepsilon = 1$ and $T_{s, \min} = 10^{-4}$ but varying $T_{s, \max}$. The value of $T_{s, \max}$ increases from the top to the bottom panels, and these cases are located at the three crosses in the top-left panel of Fig. 1.

Figure 10. Similar to Fig. 1 but only the unstable modes with $k_z \geq 1/H_0$ are considered.
with total solid-to-gas density ratio $\varepsilon$ into $N_{sp}$ regular logarithmic bins, with either $N_{sp} = 512$ or $N_{sp} = 1024$. Each bin then has a solid-to-gas density ratio $\varepsilon_j$ (equation (1)) and is represented by identical dust particles with dimensionless stopping time $T_{s,j}$, where $T_{s,1} < T_{s,2} < \cdots < T_{s,N_{sp}}$. We begin with the bin with the largest dust species $T_{s,N_{sp}}$ and find the fastest growing mode assuming that it is the only species present in the distribution. Then, we activate the bin with the second largest dust species $T_{s,N_{sp}-1}$ in the distribution and find the fastest growing mode again for this case. In this manner, we systematically add more and more smaller dust species until we recover the full distribution.

The results for various $T_{s,\text{max}}$, $\varepsilon$, and $q$ are shown in Fig. 11. Comparing the black dots ($N_{sp} = 512$) with the red dots ($N_{sp} = 1024$), it can be seen that the growth rate remains similar between the two cases when the lower cutoff of the distribution is high ($T_{s,\text{cut}} \gtrsim 10^{-3}$). When $T_{s,\text{cut}} \lesssim 10^{-3}$, the left panels show smaller growth rates with $N_{sp} = 1024$ than with $N_{sp} = 512$, indicating non-convergence, while the middle and the right panels continue to show consistent growth rates between $N_{sp} = 512$ and $N_{sp} = 1024$, indicating convergence. Therefore, the two distinct regimes of convergence and non-convergence shown by Fig. 1 are only manifested when sufficiently small dust species are included.

Moreover, it is not apparent that the largest particles alone can determine the maximum growth rate of multiple dust species in a distribution. The smaller particles contribute to the instability in a sophisticated way. As shown in Fig. 11, the growth rate first increases when the next largest particles are activated in the distribution in both convergent and non-convergent cases. This can be understood as particles near $T_{s,\text{max}}$ contribute constructively to the instability. This trend continues until $T_{s,\text{cut}} \approx 0.7T_{s,\text{max}}$ at which the growth rate reaches maximum except the case of $\varepsilon = 1$, $T_{s,\text{max}} = 0.01$, and $q = -1.5$ whose rate reaches maximum at $T_{s,\text{cut}} \approx 0.37T_{s,\text{max}}$. When even smaller particles are included, however, they can either constructively or destructively contribute to the instability. We note also that the radial wave number often begins near the resonant drag regime $K_\ast \sim K_{\text{drag}}$ and shifts to the region with larger $K_\ast$ when sufficiently small dust particles are included (see Sec. 4).

Overall, it is apparent that the small dust particles (e.g. $T_s \lesssim 10^{-3}$) in a given distribution can have a strong effect on the instability, either positively or negatively. The combined mass for dust with stopping times between $T_a$ and $T_b$ is

$$m(T_a < T < T_b) = \frac{T_b^{q+4} - T_a^{q+4}}{T_{s,\text{max}}^{q+4} - 10^{-4(q+4)}}.$$  

Therefore, dust with $T_s \lesssim 10^{-3}$ are 24% of the total dust mass for $T_{s,\text{max}} = 0.01$ and $q = -3.5$ (upper panels) or only 0.3% of the total dust mass for $T_{s,\text{max}} = 0.01$ and $q = -1.5$ (lower panels). We can see that, in the top middle panel, the growth rate jumps significantly at $T_{s,\text{cut}} \approx 10^{-3}$, which accompanies the sudden change of $K_\ast$. This indicates that the most unstable mode suddenly jumps from one $K_\ast$ region to another region, and the small particles affect the instability in a complicated way. In this regard, it is not necessary that the instability can be considered as if being driven by the largest dust particles, or that the smaller dust particles can only contribute to the instability negatively, as suggested by Krapp et al. (2019).

6 SUMMARY

We have conducted analytical calculations and direct numerical simulations to study the linear phase of the streaming instability with multiple dust species. We have explored various dust distributions with different maximum dust sizes $T_{s,\text{max}}$, total solid-to-gas mass ratios $\varepsilon$, and power-law indices $q$. In general, the instability has a high growth rate when either the maximum size $T_{s,\text{max}}$ or the total solid-to-gas mass ratio $\varepsilon$ is high ($T_{s,\text{max}} \gtrsim 1$ or $\varepsilon \gtrsim 1$). Under these conditions, the growth rate is converged with increasing number of dust species $N_{sp}$, representing the distribution. By contrast, the growth rate in the complimentary region of the parameter space, i.e., $T_{s,\text{max}} \lesssim 1$ and $\varepsilon \lesssim 1$, continues to decrease significantly with successively larger $N_{sp}$ and does not appear to converge to non-zero finite values. For more top-heavy dust distributions (e.g. $q = -1.5$), there is a larger parameter space for high growth rates extending down to $T_{s,\text{max}} \sim 0.1$ (but the fastest growing modes for $0.1 \lesssim T_{s,\text{max}} \lesssim 1$ cases may not fit in the thickness of a real protoplanetary disc). The instability growth rate is hardly affected by the minimum dust size $T_{s,\text{min}}$ of the distribution.

We find that the transition between the converged (fast-growth) and the non-converged (slow-growth) regimes is ex cessively sharp. The more dust species $N_{sp}$, the sharper the transition becomes. Therefore, the growth rate map with respect to $T_{s,\text{max}}$ and $\varepsilon$ is clearly separated into converged and non-converged regions by a discontinuity-like boundary (Figs. 1 and 2). Interestingly, for $\varepsilon \gtrsim 1$, the most unstable mode in the converged region has a dimensionless radial wave number $K_\ast \approx 10K_{\text{drag}}$ which is in a different branch from $K_\ast \sim K_{\text{drag}}$ identified as the resonant drag instability driven by the largest species (Squire & Hopkins 2018). For $\varepsilon \lesssim 1$ and $T_{s,\text{max}} \gtrsim 0.1$, on the other hand, the most unstable mode in the converged region has a variety of $K_\ast$ depending on $T_{s,\text{max}}$. When $T_{s,\text{max}} \gtrsim 1$, $K_{\ast}$ is close to $K_{\text{drag}}$. When $T_{s,\text{max}}$ is small ($0.1 \lesssim T_{s,\text{max}} \lesssim 1$), the fastest growing mode has $K_\ast \ll K_{\text{drag}}$, but these modes also have small $K_\ast$ such that they cannot fit into typical disc thickness and should not operate in protoplanetary discs.

We also notice that, for a disc with a given $\varepsilon$ and $T_{s,\text{max}}$, only unstable modes in a limited range of wave numbers have converged non-zero growth rates with increasing number of dust species $N_{sp}$. Thus, when the disc condition changes (either $\varepsilon$ or $T_{s,\text{max}}$), the most unstable mode can move from outside the converged $K_\ast$ region into the converged region. In this case, the growth rate of the instability changes from being non-convergent to convergent. This may help explain the sharp transition between the converged and the non-converged regions in the $\varepsilon$-$T_{s,\text{max}}$ growth rate maps.

Different dust species in a distribution appear to interact and contribute to the instability in non-trivial ways. We find that for a wide range of conditions, the dynamics may not be simplified to the one driven by the largest species in isolation, as may have been suggested by Bai & Stone (2010), Schaefer et al. (2018), and Krapp et al. (2019). Smaller dust species can either contribute positively or negatively to the instability. Moreover, they can change the relative importance of the unstable modes between different branches in the Fourier space to which the growth rate depends on sensitively (Figs. 8 and 9).

Finally, we have used hybrid numerical simulations to
reproduce the unstable modes for several representative cases. Numerical convergence has been achieved in all cases, and the corresponding analytical growth rates down to unprecedentedly low $\sigma \sim 10^{-3} \Omega$ as well as for large leading species ($T_{s, \text{max}} \sim 2$) are recovered. In the process, we have demonstrated the resolution requirement for simulating the instability with the code, which generally lies within 16–64 grid points per wavelength of the unstable modes. This experiment will serve us for future investigations of the streaming instability with multiple dust species using direct numerical simulations.

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DATA AVAILABILITY

The data underlying this article are available in the article and in its online supplementary material.

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APPENDIX A: SEEDING DENSITY PERTURBATIONS BY LAGRANGIAN PARTICLES

Youdin & Johansen (2007) in their Appendix C described how to seed a sinusoidal perturbation in density with Lagrangian particles. When there exist multiple perturbations with an arbitrary phase, cross correction terms are needed to maintain high order of accuracy. In this appendix, we illustrate how this can be achieved.

Following Youdin & Johansen (2007), we consider the superposition of two waves with wave numbers \( k_x \equiv k_x 0 \hat{e}_x \pm k_z 0 \hat{e}_z \), resulting in one horizontally propagating but vertically standing wave. In this case, the initial density field of the particles in the \( xz \)-plane reads (see their Equation (10a))

\[
\rho_p(r) = \rho_0 [1 + (A_R \cos k_z 0 x - A_I \sin k_z 0 x) \cos k_z 0]
\]

\[
= \rho_0 \left[ 1 + \frac{1}{2} A_R (\cos k_+ \cdot r + \cos k_- \cdot r) - \frac{1}{2} A_I (\sin k_+ \cdot r + \sin k_- \cdot r) \right],
\]

where \( r \equiv x \hat{e}_x + z \hat{e}_z \) is the position, \( \rho_0 \) is the mean density, \( A \equiv A_R + i A_I \) is the complex amplitude of the waves relative to \( \rho_0 \).

To approximate the continuous density field (Equation (A1)) using discrete particles, we begin with a periodic domain accommodating integral numbers of wavelengths \( \lambda_{x, 0} \equiv 2 \pi / k_{x, 0} \) and \( \lambda_{z, 0} \equiv 2 \pi / k_{z, 0} \) in both directions. We uniformly distribute \( N_p \) identical particles with positions \( r_j \) and shift the position of each particle by \( \xi_i \). The density field of the particles is then

\[
\rho_p(r) = m_p \sum_j \delta (r - r_j - \xi_j),
\]

where \( m_p \) is the mass of each particle and \( \delta(r) \) is the Dirac \( \delta \) function.\(^3\) Fourier transforming Equation (A3) over the domain gives

\[
\tilde{\rho}_p(k) = m_p \sum_j \exp (i k \cdot r_j) \left[ 1 + i k \cdot \xi_j - \frac{1}{2} (k \cdot \xi_j)^2 + O ([k \cdot \xi_j]^3) \right].
\]

Equation (A2) suggests that to first order in \( |A| \), the position shifts should be

\[
\xi_i^{(1)} = - \frac{A_R}{2 k_0^2} (k_+ \sin k_+ \cdot r_j + k_- \sin k_- \cdot r_j) - \frac{A_I}{2 k_0^2} (k_+ \cos k_+ \cdot r_j + k_- \cos k_- \cdot r_j),
\]

where \( k_0 \equiv \sqrt{k_{x, 0}^2 + k_{y, 0}^2} \). Substituting \( \xi_i = \xi_i^{(1)} \) into Equation (A4) results in

\[
\tilde{\rho}_p(k) = N_p m_p \left[ 1 + \frac{1}{4} A_R (\delta_{k_0,k_0} + \delta_{k_0,-k_0} + \delta_{k_0,k_0} + \delta_{k_0,-k_0}) - \frac{i}{4} A_I (\delta_{k_0,k_0} - \delta_{k_0,-k_0} + \delta_{k_0,k_0} - \delta_{k_0,-k_0}) 
\right.

\[
\left.+ \frac{1}{8} (A_R^2 - A_I^2) (\delta_{k_0,2k_0} + \delta_{k_0,-2k_0} + \delta_{k_0,2k_0} + \delta_{k_0,-2k_0}) - \frac{i}{4} A_R A_I (\delta_{k_0,2k_0} - \delta_{k_0,-2k_0} + \delta_{k_0,2k_0} - \delta_{k_0,-2k_0}) 
\right.

\[
\left.+ \frac{1}{4} (A_R^2 + A_I^2) \left( \frac{k_x 0}{k_0} \right)^4 (\delta_{k_0,2k_0,0} \hat{e}_x + \delta_{k_0,-2k_0,0} \hat{e}_x) + \frac{1}{4} (A_R^2 - A_I^2) \left( \frac{k_x 0}{k_0} \right)^4 (\delta_{k_0,2k_0,0} \hat{e}_x + \delta_{k_0,-2k_0,0} \hat{e}_x) 
\right.

\[
\left. - \frac{i}{2} A_R A_I \left( \frac{k_x 0}{k_0} \right)^4 (\delta_{k_0,2k_0,0} \hat{e}_x - \delta_{k_0,-2k_0,0} \hat{e}_x) + O (|A|^3) \right].
\]

where \( \delta_{u,v} \equiv \delta(u - v) \) for any \( u \) and \( v \). In other words, perturbations of amplitude on the order of \( |A|^2 \) appear in the second harmonics. These overtones can be cancelled by introducing the second-order correction shifts

\[
\xi_i^{(2)} = \frac{A_R^2 - A_I^2}{8 k_0^4} (k_+ \sin 2k_0 \cdot r_j + k_- \sin 2k_0 \cdot r_j) + \frac{A_R A_I}{4 k_0^2} (k_+ \cos 2k_0 \cdot r_j + k_- \cos 2k_0 \cdot r_j)
\]

\[
+ \frac{1}{4} (A_R^2 + A_I^2) \left( \frac{k_x 0}{k_0} \right)^4 \hat{e}_x \sin 2k_x 0 z_j + \frac{1}{4} (A_R^2 - A_I^2) \left( \frac{k_x 0}{k_0} \right)^4 \hat{e}_x \sin 2k_x 0 z_j + \frac{A_R A_I k_x 0^4}{2 k_0^2} \hat{e}_x \cos 2k_x 0 z_j.
\]

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\(^3\) We note that any of the weighting schemes of the particle-mesh method has the properties of a \( \delta \) function.