Generalizing Similarity Laws for Radio-Frequency Discharge Plasmas across Nonlinear Transition Regimes

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We generalize similarity theory based on the scaling and solution invariance of the Boltzmann equation, coupled with the Poisson equation, and demonstrate similarity laws for radio-frequency (rf) discharge plasmas across three nonlinear transitional regimes, namely, the alpha-gamma mode transition, the stochastic-Ohmic-heating mode transition, and the bounce-resonance-heating mode transition. Fundamental plasma parameters, e.g., the electron power absorption, under similar discharge conditions are examined via fully kinetic particle-in-cell simulations, and electron-kinetic invariance is exemplified in similar rf discharge plasmas. The results unambiguously confirm the applicability of similarity laws for rf plasmas in extended operating regimes, and strengthen the foundations and framework of similarity physics with universality.

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I. INTRODUCTION

Similarity laws map out how discharge conditions change in such a way that they retain the same characteristics [1–4]. They have been explored and demonstrated in discharge phenomena ranging from the laboratory to nature, such as glow discharges [5,6], streamers [7], pulsed electrical breakdown [8,9], fusion plasmas [10], and mesosphere red-sprite discharges [11,12]. The studies of similarities in gas discharges date back to those of Paschen [13] and Townsend [14], which initiated the usage of combined parameters, such as the reduced gap length $pd$ (gas pressure times gap distance) and the reduced electric field $E/p$ (electric field divided by gas pressure) for characterizing discharge behaviors, e.g., the use of the Townsend coefficient with a local-field approximation to describe the ionization process under a direct-current (dc) voltage. Historically, most of the initial investigations of similarity were done for dc discharges, but in 1948 Margenau [15] showed theoretically a similarity principle for high-frequency discharges. He proposed an additional combined parameter, the reduced frequency $f/p$ (driving frequency divided by gas pressure), and this principle was later experimentally verified by Jones and Morgan [16]. In 2008, Lisovskiy et al. [17] experimentally validated the similarity laws for breakdown, e.g., Paschen’s law [13], for radio-frequency (rf) discharges in both atomic and molecular gases, including argon, nitrogen, and hydrogen. Nowadays, due to the widespread application of rf discharge plasmas [18,19], it is of fundamental importance to elucidate the applicability of similarity laws to more comprehensive discharge regimes, and this is essential for correlating discharge parameters between rf plasma systems with different dimensional scales.

In more recent years, Puač et al. [20] and Lee et al. [21] have demonstrated breakdown similarity laws for rf discharges at macroscopic and microscopic scales, respectively. Loveless and Garner [22] conducted a nondimensionalized equation analysis of gas breakdown under rf and microwave-driven electric fields and inferred the universality of scaling laws for alternating-current gas breakdown. Very recently, rather than using a fluidic method with the local-field approximation, Fu et al. [23] confirmed the similarity of alpha-mode capacitive rf plasmas in nonlocal kinetic regimes through particle simulations.
However, the understanding of discharge similarity laws is still far from complete; for example, to date, the effects of nonlinear physical mechanisms on discharge similarities have rarely been investigated, and the applicability of similarity laws in the discharge-mode transition regimes of rf plasmas, e.g., the alpha-gamma (AG) mode transition [24], the stochastic-Ohmic (SO)-heating mode transition [25,26], and the bounce-resonant-heating (BRH) mode transition [27–29], has not yet been confirmed, which severely limits the application of similarity theory.

In this paper, we generalize the similarity laws for rf discharge plasmas across the three aforementioned nonlinear transition regimes, i.e., the AG, SO, and BRH mode transitions. Based on fully kinetic particle-in-cell (PIC) and Monte Carlo collision simulations, the AG, SO, and BRH mode transitions are observed in rf plasmas by tuning the applied rf voltage, the gas pressure, and the gap distance, respectively, showing distinctive nonlinear parameter-scaling relations. By simultaneously manipulating the external discharge-condition parameters \([p, d, f]\), we find that the nonlinear characteristics can be exactly replicated under similar discharge conditions, which unambiguously confirms the validity of the similarity laws across the nonlinear transition regimes considered. The results of the present work provide additional knobs and more flexibility for characterizing rf discharges across a wider range of parameter regimes, which is essential for the optimization and fabrication of plasma devices.

II. THEORY AND MODEL

Similarity laws are usually utilized for the correlation of discharges in geometrically similar gaps, the linear dimensions of which are proportional in every direction, i.e., \(d_{tj} = kd_{kj}\), where \(j = [x, y, z]\) represents the coordinate direction, \(d_t\) is the dimension in the base (or prototype) case, and \(d_k\) is the dimension in a scaled case that, compared with the base case, has a geometrical scaling factor of \(k\). According to similarity theory [30], a physical parameter \(G(x, t)\) at the corresponding spatiotemporal points \((x, t)\) in similar discharge systems can be transformed through

\[
G(x_1, t_1) = k^{\alpha[G]} G(x_2, t_2),
\]

where the subscripts 1 and 2 indicate the prototype gap and the scaled gap, which has a scaling factor of \(k\), respectively; \((x_1, t_1)\) and \((x_2, t_2)\) are the corresponding spatiotemporal points in the gaps being compared, which are defined by the scaling factor \(k = x_1/x_2 = t_1/t_2\); and \(\alpha[G]\) is the similarity factor for the parameter \(G\). Note that the scaling factor \(k\) need not be an integer and can be less than one. The most common similarity factors include \(\alpha[n_e] = \alpha[J_e] = -2\) for the electron density \(n_e\) and electron current density \(J_e\), \(\alpha[E] = \alpha[p] = -1\) for the electric field \(E\) and gas pressure \(p\), \(\alpha[\varepsilon_e] = \alpha[v_e] = 0\) for the electron energy \(\varepsilon_e\) and electron velocity \(v_e\), and \(\alpha[d] = \alpha[x] = \alpha[t] = 1\) for the gap dimension \(d\), position \(x\), and time \(t\) [31]. In particular, from the transformation in Eq. (1), the parameters having \(\alpha[G] = 0\) are similarity invariants, such as the combined parameters \(E/p\) and \(n_e/p^2\) [32].

Previously, similarity theory has mostly been developed within the framework of local-field or local-energy approximations [15,33]. However, in low-pressure rf discharges, the electron kinetics can be highly nonlocal, and the local reduced electric field may not be proportional to the mean electron energy, which is a prerequisite for the conventional explanations. Here, in the following, we interpret the similarity laws using a more generalized approach, which is based on the scaling and solution invariance of the Boltzmann equation, coupled with the Poisson equation. Considering rf plasmas in weakly ionized regimes, the collisions are dominated by electron-neutral collisions, and the Boltzmann equation for the electrons can be expressed as

\[
\frac{\partial f_e}{\partial t} + v \cdot \nabla f_e - \frac{eE}{m_e} \cdot \nabla f_e = \sum_j C_{en}(f_{en}, v_{en}, \sigma_{en}(v_{en}))
\]

where \(f_e\) is the electron distribution function, \(v\) is the velocity, \(e\) is the elementary charge, and \(C_{en}(f_{en}, v_{en}, \sigma_{en}(v_{en}))\) is an integral term for the \(j\)th collision between electrons and neutrals, which depends on the relative velocity \(v_{en}\), the collision cross section \(\sigma_{en}(v_{en})\), and the distributions of electrons and neutrals \(f_e\) and \(f_{en}\) [34]. By dividing Eq. (2) by \(k^3\), we have

\[
\frac{\partial(f_e/k^2)}{\partial(kt)} + v \cdot \nabla(k^2 f_e/k^2) - \frac{e(E/k)}{m_e} \cdot \nabla f_e = \sum_j C^j_{en}(f_{en}/k^2)(f_{en}/k), v_{en}, \sigma_{en}(v_{en}))
\]

Note that once the systems to be compared are given, \(k\) is a constant and can be put inside the integration of the collision term. By substituting the scaled parameters, i.e., \(kt, kx, E/k, f_{en}/k, \) and \(f_e/k^2\), Eqs. (2) and (3) can be used to demonstrate solution invariance. Considering Eq. (2) for the base case and Eq. (3) for the scaled system, one can rewrite the parameter relation using Eq. (1) and then obtain \(\alpha[t] = \alpha[x] = 1\), \(\alpha[E] = -1\), \(\alpha[f_{en}] = -1\), and \(\alpha[f_e] = -2\), which consistently explains the scaling factors for different parameters.

Note that for more detailed descriptions of the collision term, one needs to refer to the Boltzmann collision integral or the Fokker-Planck collision term [35]. Since the main collisional processes in a weakly ionized plasma are between charged and neutral particles, the simultaneous Coulomb interactions between charged particles are not taken into account here and are beyond the scope of the
present work. Therefore, we employ a Krook-like relaxation model [35] that can be derived from the simplified Boltzmann collision integral, assuming that the neutral density \( n_0 \) is stationary and not perturbed by collisions. The relaxation model for the collision term is expressed as \( \delta f_e/\delta t_{\text{coll}} = -v_{\text{rc}}(f_e - f_{\text{eq}}) \), where \( v_{\text{rc}} = \sigma_m v_{\text{en}} N_0 \propto p \) is the velocity-dependent relaxation-collision frequency, with \( \sigma_m \) being the momentum-transfer cross section and \( N_0 \) the number density of neutral particles in the gas, and \( f_{\text{eq}} \) is the equilibrium distribution function of the electrons. In Eq. (3), when the collision term is divided by \( k^3 \), since \( \alpha[v_{\text{rc}}] = \alpha[p] = -1 \), \( \alpha[f_e] = \alpha[f_{\text{eq}}] = -2 \) can be directly concluded from the solution invariance of the equation. Although the collision term for the interparticle interactions is simplified, the general idea of the similarity scalings can be straightforwardly demonstrated in a kinetic manner.

From \( \alpha[f_e] = -2 \) and \( n_e = \int f_e(v) \, dv \), we can directly obtain the similarity factor for the electron density, \( \alpha[n_e] = -2 \). Further, we can also identify the similarity scaling for the Poisson equation, which is expressed as \(-\partial (\varepsilon E)/\partial x = e \int [f_e(v) - f_{\text{eq}}(v)] \, dv \), with \( \varepsilon \) being the permittivity constant. Here, \( \alpha[\partial E/\partial x] = \alpha[E] = \alpha[x] = -2 \) is equal to \( \alpha[f] = \alpha[f_e] = -2 \), which indicates that the Poisson equation also follows the similarity scaling. Similarly, for the electron current density, the scaling factor is \( \alpha[J_e] = \alpha[n_e] + \alpha[v_e] = -2 \), where \( \alpha[n_e] = -2 \) and \( \alpha[v_e] = 0 \); this is also the case for the ion and total current densities, i.e., \( \alpha[J_i] = \alpha[J_{\text{tot}}] = -2 \). Further, for rf discharge plasmas, since \( \alpha[f] = \alpha[1/t] = -1 \), the external driving frequency \( f \) needs to be tuned to keep the solution invariance, which indicates that the reduced frequency \( f/p \) needs to be constant, or is a similarity invariant in the systems being compared, i.e., \( \alpha[f/p] = 0 \). Here, mathematically, the similarity theory is self-consistently interpreted on the basis of the Boltzmann and Poisson equations with universality, which can be applied to rf discharge plasmas.

A schematic illustration of two similar discharge systems \((S, S')\) having different dimensional scales is shown in Fig. 1(a), where \( G(x, t) \) is a physical parameter at the corresponding spatiotemporal points. We hereby make a statement to distinguish between similarity and scaling laws. The former hold with multiple control parameters scaled simultaneously, e.g., if the similarity invariants \( pd \) and \( f/p \) are maintained to achieve similar rf discharges. The later usually determine the dependence of the discharge parameters on only one of the controlled parameters, e.g., the scaling of the discharge characteristics with the gas pressure [36,37], gap dimension [38,39], and driving frequency [40]. As illustrated in Fig. 1(b), the scaling laws establish the dependence of plasma parameters from \( S_1 \) to \( S_e \) [or from \( S'_1 \) to \( S'_e \)], whereas the similarity laws correlate plasmas between \((S_1, S_e)\) and \((S'_1, S'_e)\). Strategically, if the similarity laws are valid, discharge properties for \( S \) can be directly applied to \( S' \) and vice versa; thus the conventional scaling laws can be exactly extrapolated from one system to another, enabling extended parameter regimes for prediction in various rf plasma systems.

In the following, PIC simulations are employed to demonstrate the applicability of the similarity laws for rf discharge plasmas across the AG, SO, and BRH nonlinear transition regimes. The simulations of the rf plasmas are performed for argon at 300 K, accounting for three types of electron-neutral collisions (elastic, excitation, and ionization scattering) and two types of ion-neutral collisions (isotropic and backward scattering) [41]. A custom-developed electrostatic PIC code, ASTRA, is used for all the simulations (see [42] for the code benchmark with the results from Turner et al. [43] and other details). Argon ions and electrons are tracked as particles. The rf plasmas are geometrically symmetric between two parallel-plate electrodes for simplicity. The rf voltage waveform \( V_{\text{rf}}(t) = V_{\text{rf}} \sin(2\pi ft) \) (in units of volts), where \( f = 1/T \) is the driving frequency, with \( T \) being the rf period, is connected to the powered electrode (\( x = 0 \)), while the other electrode (\( x = d \)) is grounded. To satisfy the requirement for similar discharge conditions, the gas pressure \( p \), gap distance \( d \), and driving frequency \( f \) are simultaneously tuned with respect to the scaling factor \( k \), i.e., \( k = p_0/p_1 = d_1/d_e = f_1/f_e \), keeping \( f/p \) and \( pd \) constant in the systems being compared. The emission coefficient of the ion-induced secondary electron is \( \gamma_{\text{sc}} = 0.1 \) when it is considered, and the electron reflection probability is \( \gamma_{\text{re}} = 0.2 \) in all cases [44]. In the simulations, an implicit algorithm and an energy-conservation scheme are adopted; the grid number and time step are case dependent, while most of the cases have 300 grid points and 2000 time steps per rf period.

III. RESULTS AND DISCUSSION

We demonstrate similarity in rf discharges during the AG mode transition in Fig. 2. In the simulations, we set \([p, d, f] = [0.3 \text{Torr}, 6.7 \text{cm}, 13.56 \text{MHz}]\) in \( S \) and...
respectively; (d) time-averaged scaled rates across the gap.

Taking $V_{rf}$ as an example to demonstrate the decomposed electron heating rates corresponding to their maxima in $S$ and $S'$, respectively; (d) time-averaged scaled rates across the gap.

$[p, d, f] = [0.6 \text{ Torr, } 3.35 \text{ cm, } 27.12 \text{ MHz}]$ in $S'$, with a scaling factor $k = 2$, and have $\gamma_{se} = 0.1$ in all cases. The AG mode transitions are obtained by varying $V_{rf}$ from 100 to 1000 V, i.e., we have ten cases AG1–AG10 in $S$ and $S'$ [see Fig. 2(a)]. The transition occurs around a critical voltage $V_{rf} = 500$ V (case AG5) as an example to demonstrate the dynamical similarities, (b), (c) spatiotemporal distributions of the elastic-collision rates normalized with the time domain scaled correspondingly. The correlation of the electron-neutral elastic-collision rate, $R_{el} = K_{el}n_eN_n$, where $K_{el}$ is the reaction-rate coefficient, normalized to their maxima in $S$ and $S'$ for $V_{rf} = 500$ V (case AG5), are found to be the same [see Figs. 2(b) and 2(c)]. It is confirmed that the similarities hold in a dynamical manner with the time domain scaled correspondingly. The corresponding time-averaged scaled reaction rates normalized to the gas number density, i.e., $R_{el}^{\text{avg}} = k^{-2}R_{el}N_n^{-1}$, are also exactly the same in $S$ and $S'$ [see Fig. 2(d)], which explicitly confirms that $\alpha[R_{el}^{\text{avg}}] = \alpha[n_e] = -2$ and quantitatively validates the similarity laws for the rf plasma systems being compared.

Figure 2 illustrates the electron density versus $V_{rf}$ under similar discharge conditions during the AG mode transition. In the simulations, we set $[p, d, f] = [0.3 \text{ Torr, } 6.7 \text{ cm, } 13.56 \text{ MHz}]$ for $S$ and $[p, d, f] = [0.6 \text{ Torr, } 3.35 \text{ cm, } 27.12 \text{ MHz}]$ for $S'$ with $\gamma_{se} = 0.1$. Taking $V_{rf} = 500$ V (case AG5) as an example to demonstrate the dynamical similarities, (b), (c) spatiotemporal distributions of the elastic-collision rates normalized with their maxima in $S$ and $S'$, respectively; (d) time-averaged scaled rates across the gap.

In Fig. 3(c), the scaled electron power absorption, $k^{-3}P_e$, at 0.01 Torr in $S$ and 0.02 Torr in $S'$ are the same, with the dominant electron heating rate being stochastic within the averaged sheath and the bulk Ohmic heating being negligible. Figure 3(d) shows the same scaled total electron power absorption in SO7, i.e., at 1 Torr in $S$ and 2 Torr in $S'$, with the Ohmic heating being dominant. In comparison with Fig. 3(c), the magnitudes of the electron heating rate are greatly increased, and there is significant positive electron heating in the bulk region. Figure 3(e) presents the decomposed electron heating rates corresponding to Fig. 3(d), with, correspondingly, the same scaled stochastic...
we have \( V \) are discharge conditions. The discharge-condition parameters \( S \) in Figs. 4(a)–4(c), which demonstrate a gradual transition and Ohmic heating components in similar discharge systems with \( p/k \) from 0.01 to 1 Torr. Time-averaged spatial distributions of the electron heating rate at (c) \( p/k = 0.01 \) Torr (SO1, stochastic-heating-dominated) and (d) \( p/k = 1 \) Torr (SO7, Ohmic-heating-dominated). (e) Decomposition of the electron heating rate in \( S \) and \( S' \) at \( p/k = 1 \) (SO7). In the simulations, we have \( V_{rf} = 300 \) V and \( \gamma_{ne} = 0.1 \) in all cases, and set \( [d,f] = [6.7 \text{ cm, 13.56 MHz}] \) in \( S \) and \( [d,f] = [3.35 \text{ cm, 27.12 MHz}] \) in \( S' \).

and Ohmic heating components in \( S \) and \( S' \). Note also that \( P_{e,\text{Ohm}} \geq P_{e,\text{st}} \) holds across the gap. Thus the similarity laws apply to rf plasmas dominated by either stochastic or Ohmic heating, as well as in the transition regime.

Under certain conditions, electrons can be bounced back and forth many times between rf sheath fields and continuously accelerated without experiencing collisions; the discharge is then operating in the BRH mode, which is considered as a typical nonlinear mechanism in rf plasmas [27–29]. Here we examine the BRH nonlinear transition with \( V_{rf} = 40 \) V and \( \gamma_{ne} = 0 \) under similar discharge conditions. The discharge-condition parameters are \( [p,f] = [0.025 \text{ Torr, 13.56 MHz}] \) in \( S \) and \( [p,f] = [0.05 \text{ Torr, 27.12 MHz}] \) in \( S' \). The BRH mode transitions are identified by tuning the gap distance, i.e., \( d' = (2.5, 1.25), (4.5, 2.25), \) and \( (5 \text{ cm, 2.5 cm}) \) for \( (S, S') \). The temporal evolution of the electron kinetic energy \( \varepsilon_e(t) \) obtained from test-particle simulations is shown in Figs. 4(a)–4(c), which demonstrate a gradual transition across the BRH mode. The test-particle simulations are conducted using spatiotemporal electric fields obtained from PIC simulations of the rf discharges in the steady state. Under the BRH condition [see Fig. 4(b)], the electron energy is highly enhanced, up to 9 eV, whereas \( \varepsilon_e(t) \) is generally less than 3 eV when BRH is less significant [see Figs. 4(a) and 4(c)]. Note that the efficiency of the BRH mode demonstrated here is even higher than that obtained by Park et al. [27], since the discharge-condition parameters in the BRH mode are further optimized. Although the BRH mode and its transition are considered to be nonlinear, this phenomenon can actually be reproduced in similar discharge systems. The corresponding normalized trajectories of the test particles, \( \langle x(t)/d \rangle \), where \( x(t) \) is the temporal position of the test particle, also overlap in \( S \) and \( S' \) [see Figs. 4(d)–4(f)], which ensures the applicability of similarity laws in the rf plasmas during the BRH mode transition.

Further, we examine the behavior of the electron kinetics in rf plasmas under similar discharge conditions. As mentioned before, we have \( \alpha[f_e/n_e] = \alpha[f_e] - \alpha[n_e] = 0 \) in similar discharges, and thus the normalized electron distribution function \( f_e/n_e \) should be an invariant. Converting \( f_e \) to the normalized electron energy probability function (EEPF) \( f_{\varepsilon} \), using \( \sqrt{\varepsilon} f_{\varepsilon}(\varepsilon) \, d\varepsilon = 4\pi V^2 f_e(\varepsilon) \, d\varepsilon/n_e \), we have \( \alpha[f_{\varepsilon}] = \alpha[f_e/n_e] = 0 \) from Eq. (1), from which we conclude that the EEPF is also invariant. The temporal and time-averaged EEPFs in the full space under various similar discharge conditions are shown in Fig. 5. In Figs. 5(a)–5(c), we show the temporal EEPFs in (a) the alpha mode with \( V_{rf} = 100 \) V (AG1), (b) the stochastic-heating-dominated mode with \( p/k = 0.01 \) Torr (SO1), and (c) the BRH mode with a gap length of 4.5 cm in \( S \). Figures 5(d)–5(f) show the corresponding EEPFs in \( S' \) under similar discharge conditions. Although the EEPFs in different discharge modes are quite different,
the independent, and any two of them can be chosen and considered \[17,52]\). The three combined parameters are not pressures, where the pressure effect is not typically considered, which usually occur in vacuum or at rather low discharge conditions, whereas the \[\pi\] theorem is also typically utilized for dimensional analysis.

In the present paper, similarity laws are demonstrated for a scaling factor \(k = 2\) and a one-dimensional geometry. Similarity properties are also expected for larger scaling factors and for higher-dimensional geometrically similar systems when the fundamental physical processes are maintained. For example, similar rf discharges can still be obtained in systems being compared for \(k = 10\) [31]. However, for larger values of \(k\), the scaled rf discharge parameters may enter high-pressure and high-ionization-degree regimes, in which other collision processes (e.g., stepwise ionization and Coulomb collisions [54]) could be important, and their effects need further investigation. Also, currently the results are for atomic gases only, and the scaling laws could be more complicated for electronegative or molecular gases, since negative ions and ion-ion recombination should be additionally considered.

IV. CONCLUSION

We generalize and demonstrate similarity laws for rf plasmas across various nonlinear transition regimes, based on theoretical interpretations and fully kinetic particle simulations. From the perspective of similarity theory, the nonlinear transition behaviors, such as the AG, SO, and BRH mode transitions, can be exactly replicated in similar discharge systems, and thus the scaling laws during the transitions can be extrapolated from one system to another. The fundamental mechanisms, such as the invariance of the electron kinetics, that maintain the similarity laws are elucidated based on the scaling and solution invariance of the Boltzmann equations and the coupled Poisson equation. The results of the present work bring comprehensive insights and additional flexibility to plasma characterization in extended parameter regimes, and provide valuable guidance for developing upscaled plasma devices, e.g., next-generation plasma-processing facilities for etching applications. Moreover, the generalization of the similarity laws also suggests a strategy for scale
reduction in large-scale simulations when the model equations can be treated as absolute invariants. The effects of stepwise ionization at high pressures, Coulomb collisions in highly ionized regimes, and possible electromagnetic mechanisms [55,56] at high frequencies, as well as the applicability of the similarity laws to discharge plasmas in electronegative gases [57–59], will be explored in future work.

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