Modified parameterization of the Li-Petrasso Charged-Particle Stopping Power Theory

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Charged-particle energy loss, or 'stopping power' in plasmas has been studied theoretically and experimentally, with important applications to modeling fusion experiments. Dense plasmas relevant to inertial fusion are theoretically challenging but several models have been developed. Here we report several physically-motivated modifications to the parameterization of the Li-Petrasso stopping-power model. The modified parameterization has a larger difference compared with other models near the Bragg peak while agreeing better in the high-velocity limit. These results corroborate recent experimental conclusions that the LP theory overestimates the stopping power near the Bragg peak in some regimes.

I. INTRODUCTION

The basic principle of laboratory fusion is to use the energy produced from the nuclear reactions to self-heat the plasma, counteracting loss mechanisms and resulting in a sustained controlled burn or a rapidly increasing temperature and energy production. Magnetic fusion schemes operate with low density plasmas that have a large Coulomb logarithm and can be treated like classical plasmas. Inertial confinement fusion (ICF) systems, in contrast, operate with very high-density plasmas that have small Coulomb logarithms, and that are potentially cool enough to be strongly-coupled and electron degenerate, such as in the dense fuel of a typical hot-spot design[1].

Modeling the fusion self-heating in these systems requires a theory of the rate at which an energetic charged particle loses energy to the plasma, as the dominant fusion self-heating mechanism is by the DT fusion's α product, initially at 3.5 MeV. In this regime, large-angle Coulomb scattering can play a critical role, especially towards the end of the α range, resulting in a difference between the linear versus path-length energy transfer. α transport in an ICF hot spot is important for calculating the hot-spot energy balance and dynamical evolution[2], the thresholds for burning plasma and ignition regimes are sensitive to the choices of theoretical models used[3]. Stopping powers are also relevant to ICF diagnostics that employ charged particles including radiography[4,5] and spectroscopy[6–11]. In these applications the linear and path-length energy transfer are similar since scattering effects are insignificant. As an example, in Ref. 10 uncertainty in the stopping-power model is a significant source of systematic uncertainty in the inferred areal density (ρR). Experiments studying fusion-product spectra from nuclear reactions occurring in implosions[12], with applications to basic nuclear physics and nuclear astrophysics, may need to correct for energy loss[13,14].

Many theories of charged-particle energy loss applicable to ICF have been developed in the last three decades, notably the Maynard-Deutsch (MD)[15,16], Li-Petrasso (LP)[17,18], and Brown-Preston-Singleton (BPS)[19] theories, which are widely used in ICF modeling. The LP model was the first to treat a generalized Fokker-Planck equation for moderately-coupled plasmas[20], which results in a stopping-power evaluation including terms proportional to $1/\ln\Lambda$ (where $\ln\Lambda$ is the Coulomb logarithm), an important development since many ICF-relevant plasmas have $\ln\Lambda < 10$. In this model, contributions from large-angle Coulomb scattering are thus treated, which enhances the linear stopping power since the effective path length per linear distance increases, an effect which is also related to energy straggling and blooming. We note that the Fokker-Planck equation includes a number of approximations and is not as exact as other approaches to kinetic theory including Boltzmann and Lenard-Balescu approaches[21]. The lack of collective excitations in the Fokker-Planck equation leads to Li and Petrasso introducing a second term to account for plasmons, and modifying the result to account for quantum effects.

In contrast, theories based on the Lenard-Balescu kinetic equation include weak collisions and plasmon excitations, an example being MD. Theories based on convergent kinetic theory, such as BPS, combine both Lenard-Balescu and Boltzmann physics, including both collective excitations and strong collisions, but we note that the BPS theory does not include a treatment of quantum degeneracy effects.

In addition to theory new experimental measurements are being reported, including in warm-dense matter and ICF-relevant plasmas for the first time. Recent reports have been published of fast particles stopping in warm-dense matter plasmas (moderately coupled and degenerate)[22,23], in ICF hot-spot relevant plasmas generated by implosions[24,25], and in novel laser-generated plasmas probed by accelerator beams[26,27]. These experiments span a wide range of plasma

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conditions but the probing particles lose a relatively small fraction of their initial energy. A proper and well-documented treatment of the theory is necessary for comparisons to the data and other theories.

In this work, we discuss several modifications and generalizations to the original LP theory, specifically the parameterizations of physical quantities, and compare to the MD and BPS theories. Some of these modifications are already being used by the community and this paper serves, in part, to document the various choices that we recommend using in evaluating the LP model. The theoretical discussion of LP is given in Section II. Our modified LP results are compared to the originally-published LP theory and MD plus BPS in Section III, and the paper is concluded in Section IV.

II. MODIFIED LI-PETRASSO FORMALISM

The published LP stopping power is expressed as

$$\frac{dE}{dx} = -\left(\frac{Z_t e}{v_t}\right)^2 \omega_{pf}^2 \left\{ G(x^{t/f}) \ln\Lambda_b + \Theta(x^{t/f}) \ln\left(1.123\sqrt{x^{t/f}}\right) \right\}, \quad (1)$$

see Eq. 3 in Ref. 17. Here, Z_t is the test particle charge in atomic units, e is the fundamental charge, v_t is the velocity, and ω_{pf} is the plasma frequency for field particle species f (defined $\omega_{pf} = \sqrt{4\pi n_f e_f^2/m_f}$ where e_f is the field particle charge, m_f is the mass, and n_f is the particle number density. The parameter $x^{t/f}$ is a dimensionless ratio of the test-to-field particle velocity, which will be discussed later. In plasmas with multiple species (e.g. electrons and ions), the total stopping power is

$$\frac{dE}{dx} = \sum_f \frac{dE}{dx}_f. \quad (2)$$

The pre-factor in Eq. 1 gives the overall normalization. Inside the brackets, $G(x^{t/f})\ln\Lambda_b$ represents the stopping power from binary Coulomb collisions, and $\Theta(x^{t/f})\ln\left(1.123\sqrt{x^{t/f}}\right)$ represents slowing due to collective plasma effects (i.e. dielectric response).

A. Velocity ratio $x^{t/f}$

As clarified in the recent Erratum (Ref. 17), the original LP paper gave only one expression for the parameter $x^{t/f}$, inadvertantly implying that it was equivalent in the binary and collective terms. In the dielectric term, the parameter $\sqrt{x^{t/f}}$ is in fact $v_t/\omega_{pf}\lambda_{Df}$ (see Ref. 28), where λ_{Df} is the Debye length $\left(=\sqrt{k_B T_f/4\pi n_f e_f^2}\right)$. Thus, in the collective effects term, $x^{t/f} = v_t^2 m_f/k_B T_f$, while in the binary collision term, $x^{t/f} \equiv v_t^2/v_f^2$ with $v_f^2 = 2k_B T_f/m_f$, so $x^{t/f} = v_t^2 m_f/2k_B T_f$. Relative to the original publication, the LP erratum change the collective effects term by $\sqrt{2}$ inside the logarithm, which can be significant when the collective stopping is an appreciable fraction of the total. From here on we use $x^{t/f}$ only in the binary collision term, i.e. with $x^{t/f} \equiv v_t^2/v_f^2$ with $v_f^2 = 2k_B T_f/m_f$, and write the collective effects stopping in terms of $v_t/\omega_{pf}\lambda_{Df}$ for clarify.

Further, the form of the collective effects term published in Ref. 17 was derived under the assumption that $x^{t/f} \gg 1$ (see Ref. 28), but the regime $x^{t/f} \sim 1$ is important for hot-spot self-heating in ICF, where the α stopping often occurs near the 'Bragg peak'. A more general form of Eq. 1 can be written as

$$\frac{dE}{dx} = -\left(\frac{Z_t e}{v_t}\right)^2 \omega_{pf}^2 \left\{ G(x^{t/f}) \ln\Lambda_b + \left(\frac{\omega_{pf}\lambda_D}{v_t}\right) K_0\left(\frac{\omega_{pf}\lambda_D}{v_t}\right) K_1\left(\frac{\omega_{pf}\lambda_D}{v_t}\right) \right\}, \quad (3)$$

where K_0 and K_1 are the irregular modified cylindrical Bessel function of zeroth and first order, respectively. This expression places no limits on values of $x^{t/f}$.

The factor G in the binary collision term is sometimes referred to as the Chandrasekhar function, which as modified in Ref. 17 to include $1/\ln\Lambda$ terms is given by

$$G\left(x^{t/f}\right) = \mu\left(x^{t/f}\right) - \frac{m_f}{m_t}\left\{ \frac{d\mu\left(x^{t/f}\right)}{dx^{t/f}} - \frac{1}{\ln\Lambda_b}\left[\mu\left(x^{t/f}\right) + \frac{d\mu\left(x^{t/f}\right)}{dx^{t/f}}, \right] \right\}, \quad (4)$$

where

$$\mu\left(x^{t/f}\right) = \frac{2}{\sqrt{\pi}} \int_0^{x^{t/f}} e^{-\xi}\sqrt{\xi} d\xi, \quad (5)$$

$$= \frac{\sqrt{\pi}}{2}\mathrm{erf}\left(\sqrt{x^{t/f}}\right) - \sqrt{x^{t/f}} e^{-x^{t/f}}, \quad (6)$$

$$\frac{d\mu\left(x^{t/f}\right)}{dx^{t/f}} = \sqrt{x^{t/f}} e^{-x^{t/f}}. \quad (7)$$

As noted previously, G is evaluated where $x^{t/f} = v_t^2/v_f^2$ and $v_f^2 = 2k_B T_f/m_f$. Here, erf is the error function.

B. Coulomb logarithm

The Coulomb logarithm, $\ln\Lambda_b$, in the Li-Petrasso paper given by

$$\ln\Lambda_b = \ln\left(\frac{\lambda_D}{p_{min}}\right), \quad (8)$$

which is an approximation by Trubnikov[29] in the limit $\lambda_D \gg p_{min}$. A more general form is given by

$$\ln\Lambda_b = \frac{1}{2}\ln\left[1 + \left(\frac{\lambda_D}{p_{min}}\right)^2\right]. \quad (9)$$

While Eq. 9 will reduce to Eq. 8 in the appropriate limit, the approximation by Trubnikov is not valid for all ICF-revelant scenarios. For example if $\lambda_D \sim 3p_{min}$ then Eq. 9 and 8 differ by about 5%.

For the Coulomb logarithm, Li and Petrasso use the electron Debye length (λ_{De}). For stopping on electrons we also use $\lambda_D = \lambda_{De}$. However, for ion stopping the Debye length is taken as a total Debye length for all species in the plasma, as it represents the absolute screening length:

$$\lambda_D = \frac{1}{\sqrt{\sum_f 4\pi n_f e_f^2/k_B T_f}}. \tag{10}$$

This is particularly motivated by plasmas with a minority ion species. In that scenario, if the Debye length were evaluated for only the minority it would be significantly longer than physical. Potential applications include fusion product transport in mixed plasmas[30]. We note that plasma ion stopping is typically dominated by strong scattering and care must be taken applying theories in this regime.

C. Relative velocity u

The term p_{min} in Eqs. 8 and 9 corresponds to a minimum impact parameter (maximum momentum transfer), and is given by Li-Petrasso as

$$p_{min} = \sqrt{p_\perp^2 + \left(\frac{\hbar}{2m_r u}\right)^2}, \tag{11}$$

where $p_\perp = e_t e_f/m_r u^2$ is the classical impact parameter, and the second term represents maximum momentum transfer in the regime where the quantum de Broglie wavelength may be greater than the classical minimum impact parameter. In this equation, m_r is the reduced mass of test and field particles, and u is a relative velocity between test and field particles defined as $\vec{u} = |\vec{v}_t - \vec{v}_f|$. We suspect that the approximation $u = \sqrt{v_t^2 + v_f^2}$ is used in many evaluations of the LP dE/dx in the literature, which would be accurate only when $v_t \gg v_f$ or $v_f \gg v_t$, i.e. not when $v_t \sim v_f$, near the Bragg peak.

u can be rigorously derived by integrating the complete Maxwellian field particle distribution in three dimensions:

$$u \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \sqrt{(v_t - v_x)^2 + v_y^2 + v_z^2}\, A e^{-m_f v^2/2k_B T_f} dv_x dv_y dv_z, \tag{12}$$

where A is the normalization of the distribution function and v_t is the test particle velocity, which is taken as $\vec{v}_t \parallel \hat{x}$ without loss of generality. In the exponent, $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$. it is relatively straightforward to directly evaluate the integral of the distribution function, which results in the expression

$$u = \sqrt{\frac{2k_B T_f}{\pi m_f}} \exp\left[-\frac{m_f v_t^2}{2k_B T_f}\right] + v_t\left(1 + \frac{k_B T_f}{m_f v_t^2}\right) \mathrm{erf}\left[\sqrt{\frac{m_f v_t^2}{2k_B T_f}}\right]. \tag{13}$$

Since Eq. 13 is simple to evaluate numerically we recommend its use in all but the most demanding applications.

When the test particle is slow ($v_t \ll v_{th}$),

$$\sqrt{(v_t - v_x)^2 + v_y^2 + v_z^2} \to \sqrt{v_x^2 + v_y^2 + v_z^2} = v, \tag{14}$$

which means that the relative velocity reduces to

$$u = \int_0^\infty v A e^{-mv^2/2k_B T_f} dv = \sqrt{\frac{8k_B T_f}{\pi m_f}}. \tag{15}$$

In the high-velocity limit ($v_t \gg v_{th}$),

$$\sqrt{(v_t - v_x)^2 + v_y^2 + v_z^2} \to v_t, \tag{16}$$

and the relative velocity reduces to

$$u = v_t. \tag{17}$$

For intermediate values one can construct a 'simple relative velocity' from these two results, rather than evaluating the integral over the distribution function. This velocity is given by:

$$u_s = \sqrt{v_t^2 + \left(\frac{8k_B T_f}{\pi m_f}\right)^2}. \tag{18}$$

When $v_t \sim v_{th}$, this expression has an error of about 2.5% compared to the exact expression (Eq. 13). Generally, this is acceptable since u only appears in the Coulomb logarithm.

D. Electron degeneracy

In degenerate regimes where the Fermi energy can be comparable to the thermal temperature it is common to modify the plasma temperature to account for quantum degeneracy, which was noted in Ref. 17 but without an explicit prescription for an effective temperature. Ref. 31 gives an expression for an 'effective temperature' (T_{eff}) in terms of the Fermi temperature (T_F)

$$T_{eff} = \frac{3}{5}T_f\left[1 + \frac{5\pi^2}{12}\left(\frac{T_e}{T_F}\right)^2 - \frac{\pi^4}{16}\left(\frac{T_e}{T_F}\right)^4 + ...\right], \tag{19}$$

which is only valid in the strong-degeneracy regime $T_e \ll T_F$. Separately, given in Ref. 28, in the weak degeneracy regime the effective energy per electron is given as

$$E_{eff} = \frac{3}{2}k_B T_e\left[1 + \frac{1}{2^{5/2}}\frac{4}{3\sqrt{\pi}}\left(\frac{E_F}{k_B T_e}\right)^{3/2} - \frac{1}{3^{5/2}}\left(\frac{4}{3\sqrt{\pi}}\right)^2\left(\frac{E_F}{k_B T_e}\right)^3 ...\right] \tag{20}$$

with $T_{eff} = 2E_{eff}/3k_B$. To combine the two regimes, strong and weak degeneracy, Ref. 28 uses

$$\frac{1}{E_{eff}} = \sqrt{\frac{1}{E_{eff,weak}^2} + \frac{1}{E_{eff,strong}^2}} \tag{21}$$

Here, we use an effective field particle temperature correction following Drake[32]. The total pressure (p_e) of quasi-degenerate electron fluid may be written as (Ref. 32 Eq. 3.22)

$$p_e = \frac{2}{3} n_e k_B T_e \frac{F_{3/2}\left(\frac{\mu_e}{k_B T_e}\right)}{F_{1/2}\left(\frac{\mu_e}{k_B T_e}\right)}, \tag{22}$$

which leads to an expression for T_{eff}:

$$T_{eff} = T_e \frac{F_{3/2}\left(\frac{\mu_e}{k_B T_e}\right)}{F_{1/2}\left(\frac{\mu_e}{k_B T_e}\right)}. \tag{23}$$

In this expression, $F_{1/2}$ and $F_{3/2}$ are the Fermi integrals

$$F_j(x) = \frac{1}{\Gamma(j+1)} \int_0^\infty dt \frac{t^j}{\exp(t-x)+1}, \tag{24}$$

and μ_e is the chemical potential, which can be derived from the fit by Drake (Ref. 32 Eq. 3.20)

$$\frac{\mu_e}{k_B T_e} = -\frac{3}{2}\ln\Theta + \ln\left(\frac{4}{3\sqrt{\pi}}\right) + \frac{0.25054\Theta^{-1.858} + 0.072\Theta^{-1.858/2}}{1 + 0.25054\Theta^{-0.868}}, \tag{25}$$

where Θ is the ratio of temperature to Fermi temperature, given by:

$$\Theta = \frac{T_e}{T_F} = T_e \left[\left(\frac{8\pi}{3n_e}\right)^{2/3} \frac{2m_e k_B}{h^2}\right]. \tag{26}$$

In the non-degenerate limit of large Θ Eq. 23 gives $T_{eff} \to T_e$ and smoothly transitions to the degenerate regime. We note that this simple approximation is likely accurate only in the weakly degenerate regime and care must be taken in the strongly degenerate regime, as T_{eff} becomes less representative and other parts of the problem, such as the relative velocity u are affected.

E. Summary

To express the modified Li-Petrasso formalism, we use Eq. 3 with the modified Chandrasekhar function defined by Eq. 4, and the Coulomb logarithm calculated from Eqs. 9, 10, 11, and 13 with a quantum correction given by Eqs. 22 to 26.

III. COMPARISON

A comparison to the published version of the theory is shown in Fig. 1. In most regimes the significant changes are to the collective effects stopping term, specifically the factor of 2 error as noted in Ref. 18 and Section II A. We thus evaluate the LP stopping model in three ways:

- **LP # 1**: LP as published in 1993, i.e. Eq. 1 with $x^{t/f} = v_t^2 m_f / 2k_B T_f$ in all terms.
- **LP # 2**: LP Erratum (Ref. 18), i.e. Eq. 1 but with $x^{t/f}$ properly treated in the binary and collective terms, i.e. with the latter replaced by $v_t/\omega_{pf}\lambda_D$.
- **LP # 3**: This model, i.e. Eq. 3.

While the evaluation # 1 is superceded by Ref. 18, we include it to demonstrate the magnitude of the correction. LP # 1 and # 2 use the collective effects term with a step function (i.e. Eq. 1). All evaluations use the modified Coulomb logarithm (Eq. 9) and Debye length as prescribed in Section II B, plus the relative velocity and effective temperature from Sections II C and II D respectively. In Fig. 1 these models are evaluated for

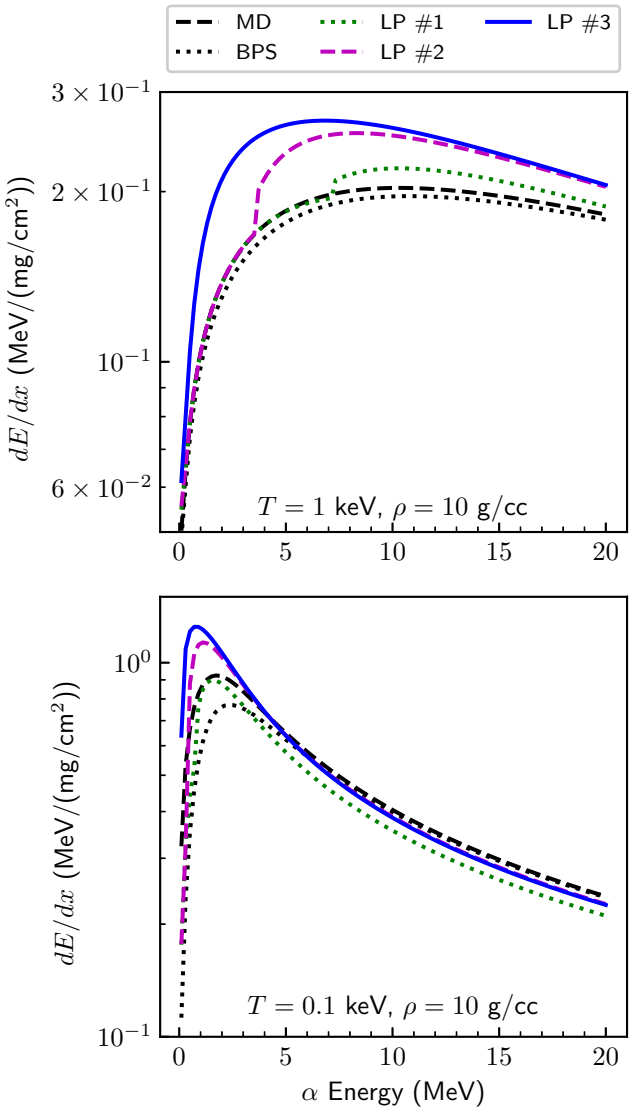

FIG. 1. Three evaluations of the LP stopping power (see text) compared to MD and BPS for αs stopping in a DT plasma at 10 g/cc and 1 (top) or 0.1 (bottom) keV.

α particles stopping in a DT plasma at temperatures of 1 keV (top) and 0.1 keV (bottom) and a density of 10 g/cc. The major effect is that the changes to the collective stopping treatment increases dE/dx, especially noticeable near the Bragg peak and in the high-velocity limit. The LP model as published in 1993, including the incorrect treatment of $x^{t/f}$, surprisingly is closest to the MD and BPS models around the Bragg peak, while the modified LP stopping power is closer to MD and BPS in the high-velocity limit.

Fig. 2 compares the modified LP stopping in this paper to a number of models over a range of relevant parameters for proton stopping. In addition to BPS and MD, we include Grabowski's classical molecular dynamics results[33], and cold-matter tabular stopping power from the SRIM code[34] in the first (and lowest temperature) case. These models are evaluated for protons in:

(a) Solid-density warm-dense-matter beryllium (relevant to Ref. 22)

(b) A D^3He plasma at modest density and temperature roughly relevant to Ref. 24

(c) In a CH plasma at high density and low temperature, relevant to stopping in imploding shells (Ref. 10 and 11)

(d) In an ignition-relevant hot spot

In the lower-density examples (a and b), the modified LP model agrees well with MD and BPS in the high-velocity limit, while predicting a higher stopping power around the Bragg peak. Significant differences are observed between the models at higher density (c and d).

We directly compare theories over a wide range of parameters in Fig. 3. The plot shows the ratio of LP to MD theory (top row) and BPS to MD (bottom row) for D^3He protons (left) and DT αs (right) over several orders of magnitude in density and temperature. The LP and MD theories disagree around the Bragg peak, with the Li-Petrasso theory giving a higher stopping power by around $20-30\%$. This causes the vertical bands at $20-30$ keV for D^3He protons, and around $1-2$ keV for the DT-αs. The MD and BPS theories agree well over most ICF-relevant plasma conditions. At high density and modest or low temperature (upper left of the plots) all of the three theories disagree substantially, by factors of $2\times$ or more. We note this is a challenging regime with strong coupling and degeneracy effects, and the BPS theory, in particular, does not include an effective temperature correction for electron-degenerate plasmas or strong-coupling effects. Across these comparisons we only consider the instantaneous stopping power, a more detailed investigation of the impact of scattering effects is not considered here.

IV. CONCLUSION

In this paper we discuss several modifications to the parameterization of the LP stopping-power theory that are either physically motivated or used to extend the range of applicability. Some of these modifications are already in use in evaluations or computational implementations but have not been described previously in the literature. They include a corrected treatment of the collective-effects stopping power (Section II A), a more general form of the Coulomb logarithm (Section II B), a physical treatment of the relative velocity u (Section II C), and a generally-applicable effective temperature for electron degenerate plasmas (Section II D). This modified LP theory can be used in modeling, diagnosing, and understanding ICF and high-energy-density plasmas. The modified theory exhibits a higher stopping power near the Bragg peak than the originally published LP theory and other theories such as MD and BPS, typically by $20-30\%$, while the high-velocity limit is in better agreement with MD and BPS than the original LP. This is attributed primarily to the modified collective effects treatment.

Based on this work we conclude that the higher stopping power calculated near the Bragg peak in the modified LP theory is physically motivated based on the derivation and inputs to the model, and therefore measurements near the Bragg peak should be able to distinguish between the LP theory and other models such as MD and BPS. These results therefore corroborate the interpretation of recently-published experimental results, especially those of Cayzac et al.[27] and Frenje et al.[25], which found that the LP model overestimates dE/dx near the Bragg peak by tens of percent when the particles lose a small fraction of their initial energy. In other regimes, especially the high-velocity limit for low or modest density plasmas, the modified LP theory agrees well with MD and BPS. The effect on the total range of charged particles, which is particularly important for fusion self-heating, has an additional complication from scattering effects which is worthy of additional study both theoretically and experimentally. Theoretical study of charged-particle stopping power is also an active area of study, and we encourage work including *ab initio* simulations using techniques like time-dependent density-functional theory to estimate the accuracy and range of validity for simple stopping-power theory.

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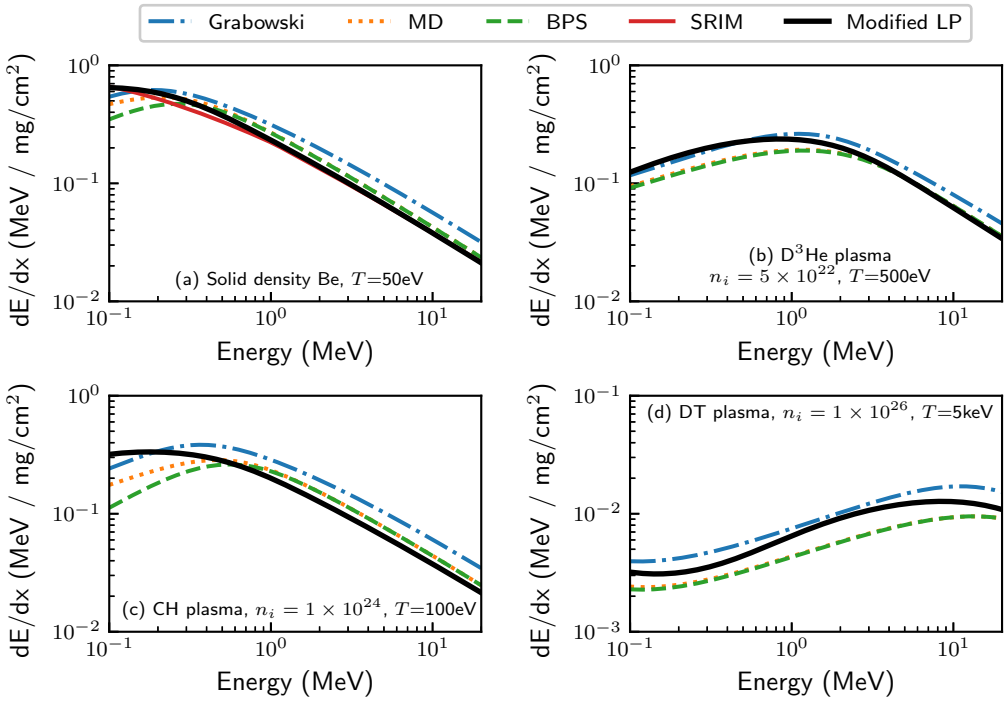

FIG. 2. Comparison of several stopping theories for protons slowing in various ICF-relevant plasmas. **(a)** Fully-ionized solid-density Be at 50eV (WDM regime), **(b)** in a D^{3}He plasma at 500 eV, **(c)** in a CH plasma at 10^{24}/cc and 100eV, relevant to dense shells, and (d) in a high-density and hot DT plasma, relevant to ignition targets.

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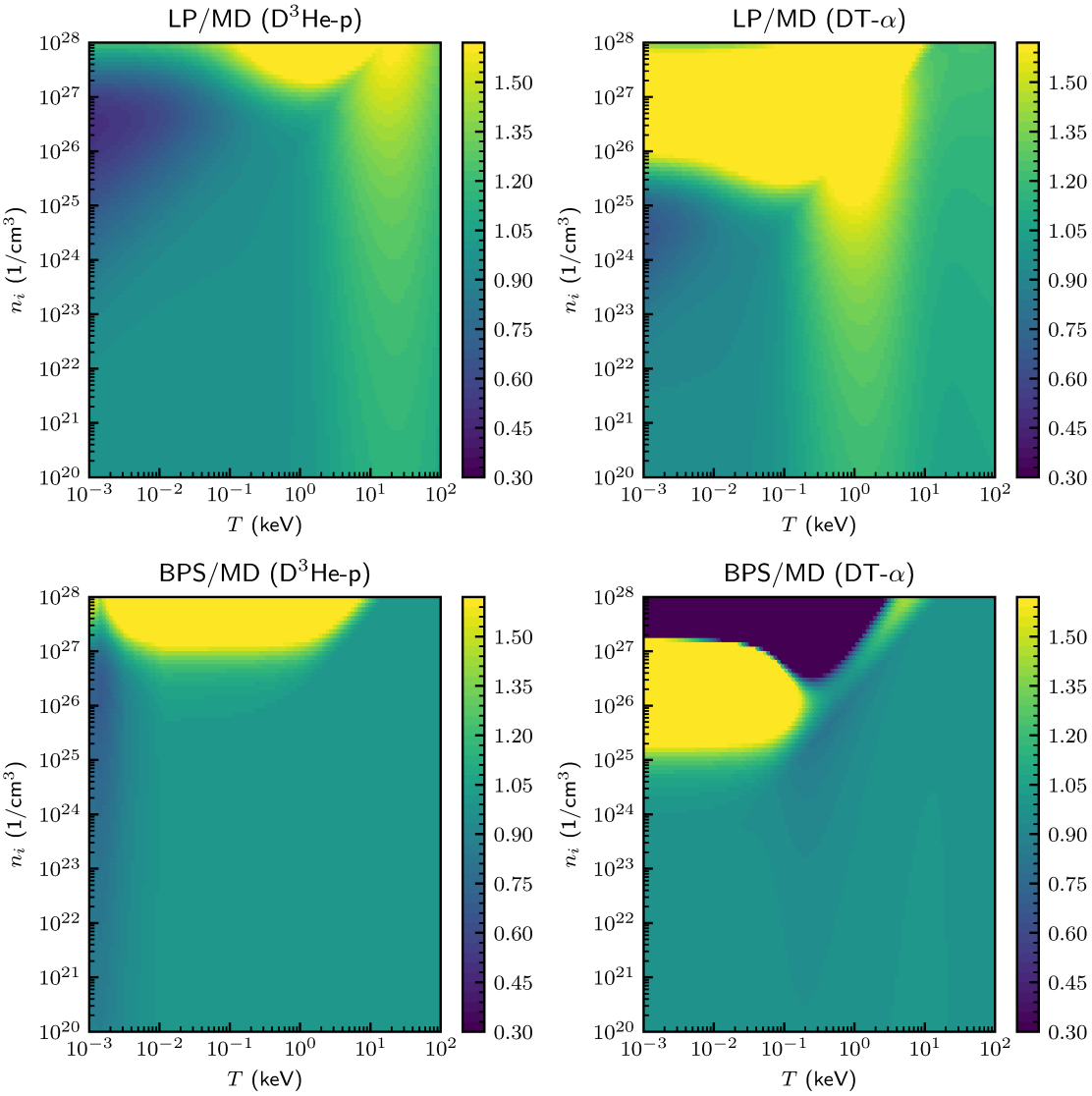

FIG. 3. Ratio of stopping powers for D^3He-p (14.7 MeV, left) and DT-α (3.5 MeV, right) slowing in a DT plasma at various densities and temperatures ($T = T_e = T_i$). Top row: ratio of LP and MD theories, bottom row: ratio of BPS and MD.

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