Reply to "Comment on 'Attractive forces between ions in quantum plasmas: Failure of linearized quantum hydrodynamics' "

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This is the last of a series of three papers. In the first [Phys. Rev. E **87**, 033105 (2013)], the same authors presented a critical analysis of the prediction of "novel attractive forces" between protons in dense hydrogen put forward by Shukla and Eliasson in a recent Letter [Phys. Rev. Lett. **108**, 165007 (2012)]. Based on *ab initio* density functional theory (DFT) calculations and general considerations, it was shown that no such force exists. In the second of the three papers [Phys. Rev. E **87**, 037101 (2013)], Shukla, Eliasson, and Akbari-Moghanjoughi (SEA) rejected this analysis. SEA did not discuss our arguments but claimed that the discrepancy between their quantum hydrodynamic model (QHD) and DFT is due to a failure of the latter. It is the purpose of the present Reply to demonstrate that this claim is incorrect because DFT is more accurate than QHD, by construction.

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In our original paper [1], we tested the predictions of Shukla *et al.* [2] for dense hydrogen, and we came to the following two main conclusions: (1) The prediction of a "novel attractive proton-proton potential" is wrong and (2) this error arises from a failure of the linearized quantum hydrodynamics (LQHD) model applied by the authors outside its applicability range. This conclusion was based on a comparison with our density functional (DFT) simulation results. In their Comment [3], Shukla, Eliasson, and Akbari-Moghanjoughi (SEA), in fact, have come to very similar conclusions about the validity of the LQHD. At the same time there appears to be a misunderstanding about the physical basis of DFT that apparently has led SEA to misinterpret our results. For the benefit of the reader we, therefore, give a brief comparison of the two methods below, critically assessing their respective strengths and weaknesses.

To begin with, DFT and the Kohn-Sham equations [4] have been derived rigorously from the N-particle Schrödinger equation of a system of interacting electrons moving in the external potential of the nuclei. For practical computations, an approximation has to be applied to the exchange-correlation energy functional $E_{\rm XC}[n]$. As correctly pointed out by SEA, the development of improved functionals $E_{\rm XC}[n]$ is still a matter of active current research. The role of $E_{\rm XC}[n]$ is to account for the exchange-correlation effects of the interacting electrons. All the single-particle quantum mechanical effects, however, are fully accounted for by solving the Kohn-Sham equations, which are formally equivalent to a single-particle Schrödinger equation for particles moving in an effective potential $v_{\rm eff}([n];r)$ that is determined self-consistently. Thus, as denoted in Table I, DFT correctly captures all quantum effects. It becomes accurate at high densities, i.e., in the weak coupling limit, when the mean interparticle distance $\bar{r}$ is much less than the Bohr radius $a_{\rm B}$ (the scale of the local field) [5], i.e., the Brueckner parameter $r_s = \bar{r}/a_{\rm B}$ is much less than one. At lower densities its accuracy is determined by the

TABLE I. Comparison of key properties and limitations of standard density functional theory (DFT) and (linearized) quantum hydrodynamics (L)QHD. Points (8) and (9) apply to LQHD only. $E_{\rm XC}$: exchange-correlation functional, $r_s = \bar{r}/a_{\rm B}$, is the quantum coupling (Brueckner) parameter, where $\bar{r}$ denotes the mean interparticle distance and $a_{\rm B}$ is the Bohr radius. n_0 is the unperturbed density and δn is the induced density response.

	Property	DFT	QHD, LQHD
(1)	Quantum diffraction effects	Included for Kohn-Sham states	Approximate, via Bohm potential ("quantum recoil") [3]
(2)	Quantum coherence effects, e.g., quantum interference	Included for Kohn Sham states	Missing (no phase information)
(3)	Spin effects, Pauli principle	Approximate via $E_{\rm XC}$	Approximate, via ideal equation of state ("Fermi pressure") [3]
(4)	Many-particle effects	Approximate via $E_{\rm XC}$	Missing (standard formulation) corrections derived from $E_{\rm XC}$ [2,6][a]
(5)	Accessible temperature	$T = 0$ [b]	$T = 0$
(6)	Accessible density	No restriction	Weak coupling, $r_s \lesssim 1$ Incomplete: misses Friedel oscillations
(7)	Resolvable length scales	No restriction	$l >$ several $\bar{r}$
(8)	Strength of perturbation	No restriction	Weak, $\lvert\delta n\rvert < n_0$ (LQHD)
(9)	Computational effort	Large	Low, semianalytical (LQHD)

[a]These references used a simplified version of $E_{\rm XC}$ from DFT.
[b]Extensions to finite temperature exist.

exchange-correlation functional E_{XC}. For hydrogen reliable expressions for $E_{\mathrm{XC}}[n]$ exist, which were discussed in Ref. [1], allowing for accurate calculations of the proton potential in a dense jellium background. In particular, bound states between protons and Friedel oscillations are correctly reproduced.

Compared to DFT, QHD and LQHD contain three important additional approximations [7]: (i) Instead of a set of general complex wave functions, QHD and LQHD solve for real-valued hydrodynamic quantities, thereby losing access to quantum interference effects (2), in contrast to the statements of SEA [3]; (ii) as any hydrodynamic theory, QHD averages over a finite volume containing many particles, thereby losing the capability to resolve scales on the order of the mean interparticle distance $\bar{r}$, cf. point (7), where the relevant length scale was determined in Ref. [1]; and (iii) SEA correctly note that QHD is a free electron theory, i.e., it does not contain electron-electron correlation effects and can only be applied to high densities, $r_s \lesssim 1$ (indicated by the shaded area in Fig. 1 of Ref. [1]), cf. point (6) in Table I. Surprisingly, in their Letter [2], Shukla and Eliasson extended their claim of the attractive potential to the low-density value of $r_s \sim 26$, supporting it by numerical data. Comparing their data to DFT simulations we demonstrated [1] that no "novel" potential minimum other than that caused by bound states or Friedel oscillations exists.

In conclusion, even though DFT is—obviously—not an exact theory, as correctly pointed out by SEA, it is nonetheless generally more accurate than QHD (with or without linearization) by construction. Therefore, a "failure of DFT" [3] to reproduce predictions of linearized quantum hydrodynamics (LQHD) is a serious indication of the failure of the latter.

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[1] M. Bonitz, E. Pehlke, and T. Schoof, this issue, Phys. Rev. E **87**, 033105 (2013).
[2] P. K. Shukla and B. Eliasson, Phys. Rev. Lett. **108**, 165007 (2012); **108**, 219902(E) (2012); **109**, 019901(E) (2012).
[3] P. K. Shukla, B. Eliasson, and M. Akbari-Moghanjoughi, preceding paper, Phys. Rev. E **87**, 037101 (2013).
[4] R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods* (Cambridge University Press, Cambridge, UK, 2005).
[5] As in Ref. [1], the plasma density n is characterized by the common Brueckner parameter, $r_s = \bar{r}/a_{\mathrm{B}}$, where a_{B} denotes the Bohr radius and $\bar{r}$ the mean interparticle distance which is related to the density by $4\pi\bar{r}^3/3 = n^{-1}$.
[6] N. Crouseilles, P.-A. Hervieux, and G. Manfredi, Phys. Rev. B **78**, 155412 (2008).
[7] This is in agreement with the recent analysis in S. V. Vladimirov and Yu. O. Tyshetskiy, Phys. Usp. **54**, 1243 (2011).