Comment on “Continuum Lowering and Fermi-Surface Rising in Strongly Coupled and Degenerate Plasmas”

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In a recent *Letter*, Hu [1] reported photon absorption cross-sections in strongly coupled, degenerate plasmas from quantum molecular dynamics (QMD). The *Letter* claims that the K-edge shift as a function of plasma density computed with simple ionization potential depression (IPD) models are in violent disagreement with the QMD results. The QMD calculations displayed an increase in K-edge shift with increasing density while the simpler models yielded a decrease. This *Comment* shows that the claimed large errors reported by Hu for the widely used Stewart-Pyatt (SP) model [2] stem from an invalid comparison of disparate physical quantities and is largely resolved by including well-known corrections for degenerate systems.

Hu correctly attributed the increased K-edge shift to degeneracy effects in the QMD calculations but absent in the SP model. Hu failed, however, to apply the well-known Pauli-blocking effect [3], which is routinely included in degenerate plasmas simulations together with the IPD contribution [4]. Thus, the error by Hu was to compare directly in his Fig. 3 the K-shell binding energy, E_{1s}, with the K-edge photon ionization feature, E_K. These quantities are in principle distinct and are approximated in degenerate systems by [4]

$$\begin{aligned} E_{1s} &= E_{1s}^{o} - E_C \\ E_K &= E_{1s} + E_{Fermi} \end{aligned} \tag{1}$$

where E_{1s}^{o} is the binding energy for an isolated ion, E_C is the IPD due to the plasma environment, and E_{Fermi} is the Fermi energy to account for Pauli blocking. As written, all quantities in Eq. (1) are greater than or equal to zero.

To ascertain the validity of the customary SP model for degenerate system, calculations of Eq. (1) were performed for carbon plasmas with the semi-classical Thomas-Fermi (TF) model [5], which provide the average ion charge state and Fermi energy. The average charge is used to compute quantum mechanical quantities unavailable from the TF model;

E_{1s}^{o} is obtained from a hydrogenic variational scheme [6] and E_C from the SP model. A second set of calculations were performed using a fully quantum mechanical ion-sphere plasma description, Purgatorio [7], which directly provides E_{1s} and E_{Fermi}.

These E_K calculations are compared in Fig. 1 with those from QMD. The plots include a constant additive correction to force agreement with experimental values at the lowest density as was done for the QMD results [1]. The results from Purgatorio, a model conceptually similar to the single-ion-in-a-box [1], are as expected in good agreement with QMD. The figure also shows that the combined TF and SP model yields reasonable agreement with the QMD results.

Contrary to the claims by Hu [1], a correctly implemented Stewart-Pyatt model yields K-edge shifts in qualitative agreement with the QMD calculations. Note that non-degenerate systems (e.g.; Orion [8] and LCLS [9] IPD experiments) allow photon absorption at the bottom of the continuum band with negligible Pauli blocking. Nevertheless, experimental determination of the IPD can be obscured by fluctuations [4,10].

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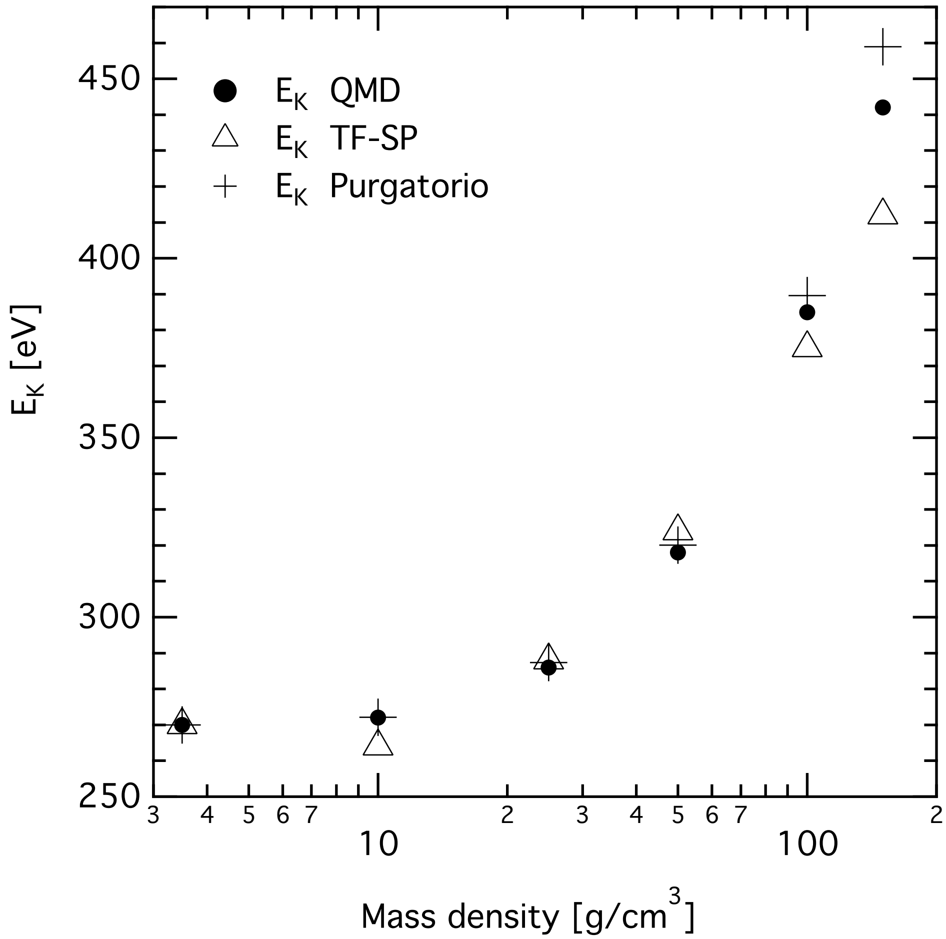

Fig 1. K-edge photon absorption feature, E_K, as a function of mass density from QMD, TF-SP model, and Purgatorio for carbon plasmas at the conditions used in the QMD calculations [Fig. 3 in Ref. 1].