Pseudo-quantum criticality in electron liquids exhibited in expanded alkali metals

Hideaki Maebashi and Yasutami Takada
Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
maebashi@issp.u-tokyo.ac.jp

It is well known that the compressibility κ of the homogeneous electron gas provides vitally important information on determining the exchange-correlation kernel, a fundamental quantity in the density functional theory. A notable feature of κ is its divergence at r_s = 5.25 with r_s the Wigner-Seitz radius of electrons, resulting in singular long-range fluctuations in the electronic polarization. Usually, singular fluctuations in the response function at zero temperature invoke continuous quantum phase transition. In the electron gas, however, there is no true phase transition owing to the fact that the polarization function in this case represents response to a total of external and induced charges, making it acausal. This singularity which does not induce any phase transition leads to a new concept of pseudo-quantum criticality.

In considering the actual valence electrons in solids or liquids, we should include not only the above-mentioned effects of the electron-electron Coulomb interaction but also those of the electron-ion interaction. Basically, the latter effects are complicated to treat due to the complex nature of an ion composed of a nucleus and core electrons surrounding it. But they can be described by employing another important concept or pseudopotential, taking into account the core-valence orthogonality which makes the valence electrons exclude from the core region.

These two concepts manifest themselves in the problem of the Coulombic screening in alkali metals [1]; the pseudo-quantum criticality combined with the exclusion effect of valence electrons makes the observable phenomena intriguing, in which an important role is played by the emergence of a short-range attractive part in the screened Coulomb interaction between ions. In this talk, we predict the decrease of the equilibration distance between ions against the increase of r_s, provided that the condition of $2r_c < r_s < 4r_c$ is satisfied with r_c the ion-core radius. This prediction is in good quantitative agreement with the recent experiment on expanded liquid Rb exhibiting that an average distance between nearest-neighbor ions decreases with the increase of the Wigner-Seitz radius of ions [2].

[1] H. Maebashi and Y. Takada, cond-mat/0706.4001.
[2] K. Matsuda, K. Tamura, and M. Inui, Phys. Rev. Lett. **98**, 096401 (2007).