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Born-Oppenheimer and fixed basis models for vibrations in a metal lattice and phonon fluctuations

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Last year we presented results on a model for Karabut's collimated x-rays which seemed to give good agreement with experiment. When writing up the model for publication, we found an error, which forced us to pursue a different version of the model. The issue in the earlier model was that phonon-nuclear coupling based on the relativistic interaction by itself is insufficient to allow for coherent energy exchange between vibrations and nuclear excitation with as much up-conversion as seems to occur in the Karabut experiment. In the new model, we combine phonon-nuclear interactions with electron-phonon interactions to increase the fractionation power of the combined system.

In order to implement the model, we require a description of phonon fluctuations in a metal lattice, formulated in a way so as to be consistent with our phonon-nuclear coupling models. While this might seem to be straightforward, we found that a new formulation of the electron-phonon problem for metals was needed.

At issue is deciding what constitutes phonon exchange. In the literature this problem was attacked in the early years following the development of quantum mechanics making use of phonon exchange in the Bloch picture. In our work, the question arose as to how this relates to the notion of phonon exchange in the Born-Oppenheimer picture, since in this case what seems to be a philosophical difference between the two pictures ends up leading to a difference in how phonon fluctuations are modelled. One can find in the literature a derivation of the Bloch picture model starting from a Born-Oppenheimer picture, so that it is understood how the Bloch picture comes about in the first place starting from a Born-Oppenheimer model.

In a sense, phonon exchange in the Born-Oppenheimer picture is a much weaker effect than in the Bloch picture, so we felt that it was important to understand how the Born-Oppenheimer picture works in the context of phonons in metals. In the new model, the ability of the system to fractionate a large quantum is determined by the level of phonon fluctuations that arise due to dynamical interactions with the electronic degrees of freedom, and this can be readily identified within the Born-Oppenheimer picture. So, we first carried out a general (and formal) Born-Oppenheimer analysis of the problem, which gives very general results (which are easy to understand, but hard to implement to obtain quantitative results). Then we reduced the model in a fixed basis approximation, which results in a model that looks similar to a Bloch picture model, but has a different electron-phonon interaction (one that is well known in the literature). Although to be consistent we should use fixed basis electronic wavefunctions consistent with the Born-Oppenheimer approximation, based on the extensive literature in the Bloch picture it seems clear that one can in some cases extend analyses similar to the Bloch picture to this new model.

In the end we obtain expressions for the phonon dispersion relation that are closely related to the Bloch picture results, but which distinguish between contributions from screening and from phonon exchange; these parts can be understood in terms of the longitudinal dielectric constant. We also obtain expressions for the matrix elements associated with the off-diagonal sector Hamiltonians associated with phonon fluctuations. These latter parameters can then be used to evaluate coherent energy exchange under conditions where a large quantum is fractionated.