Ab initio heat dynamics in phonon-based dark matter detectors

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The search for dark matter (DM) is at present one of the most exciting areas of research in Cosmology and Particle Physics. The lack of results for traditional high-mass DM candidates has driven attention to lighter candidates. Recent theoretical work has suggested that such DM may have a relatively strong interaction with polar semiconductors [1]henceforth called the target-, so that a single optical phonon is created. These phonons could be theoretically collected into a superconductor, from now on referred to as the collector, for subsequent detection using transition edge sensors (TES)-i.e. a detection architecture known as quasiparticle-trapassisted TES, or QET [3]-; so that phonon-based detectors can be considered (see Fig. 1). However, the rapid decay of this phonon due to intrinsic scattering or the target-collector interface scattering can severely hinder the collected signal or render it below detectable levels. Therefore, phonon dynamics is a limiting factor for the devices' design, making its understanding essential for the optimization of any instrument. Nonetheless, there exist packages to model phonon transport in similar setups [4], they rely on tabulated data or isotropic approximation, limiting their transferability and/or accuracy.

In this work, we have developed tools for the computation of phonon dynamics within the target of a cryogenic phonon-based DM detector allowing for the obtaining of collected thermal signal (phonons) for an Al_2O_3 -Al system (target-collector); the developed tools are supplemented with *ab initio* phonon data which allows for the simulation of any pair of materials.

Though arbitrary initial states (single phonon) are allowed, we have selected our initial states based on DM-phonon scattering rates (see Fig. 2) calculated using phonon spectra together with DarkELF [2]. Following the choice of the initial state we obtain the gross flux crossing the target collector interface using a simplified model without spatial resolution, as developed by Swartz et al. [5], together with a full band diffusive mismatch model [6] to obtain the mode-dependent transmission coefficient for such a model. The simplified model allows us to check different approaches to the collision operator, showing not only that mode coupling in the scattering is essential, but that linearized and full collision operators provide essentially the same results for our kind of systems (i.e. differences smaller than 0.01%)[see Fig. 3]. This simplified model also allows us to qualitatively investigate the effect that several initial parameters have over the collected signal, namely, the initial phonon state, the isotopic purity of the sample, and/or its volume; showing, for instance, a clear dependence on the collected signal in the initial phonon energy for all the studied target volumes, with higher energies providing better signals. Finally, we have developed an energy deviational Monte Carlo solver [7] which allows us, not only, to obtain more accurate results but also to model spatial effects over the signal.

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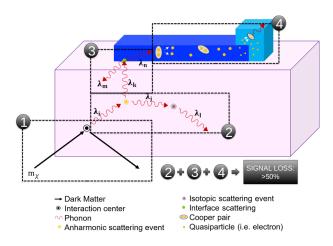
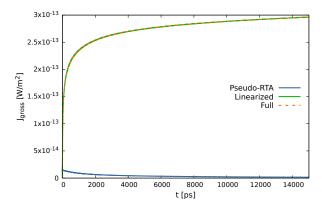


Fig. 1. Sketch of the physical processes within the DM phonon based detector. The related and individual processes—(1) DM -target interaction, (2) phonon downconversion, (3) interface scattering, and (4) pair breaking diffusion and detection—that affect the detected signal are indicated with black-dashed boxes.



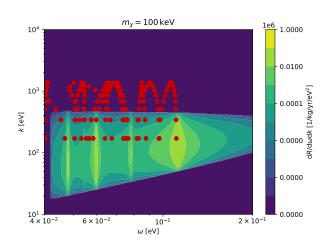


Fig. 2. Spectral and momentum decomposition of DM-phonon scattering rate per unit target mass for Al_2O_3 in the $\langle 0001 \rangle$ direction. Available points for a Γ -centered $17 \times 17 \times 17 q$ -mesh are given as reference.

Fig. 3. Gross heat flux computed with Swartz's model [5] traversing the interface as function of time, for $Al_2O_3\langle 0001\rangle$ - $Al\langle 111\rangle$ system at 0.01 K using different approaches for the collision operator. Interface scattering is computed using the diffusive mismatch model. Here, pseudo-RTA refers to an incomplete linearized operator (almost diagonal, that is similar to the relaxation time approximation one), which does not properly model the mode coupling due to the scattering.