

Highlights

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Mobility of Holstein Polaron at Finite Temperature: An Unbiased Approach

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We present the first unbiased results for the mobility μ of a one-dimensional Holstein polaron obtained by numerical analytic continuation combined with diagrammatic and worldline Monte Carlo methods in the thermodynamic limit. We have identified for the first time several distinct regimes in the λ - T plane including a band conduction region, incoherent metallic region, an activated hopping region, and a high-temperature saturation region. We observe that although mobilities and mean free paths at different values of λ differ by many orders of magnitude at small temperatures, their values at T larger than the bandwidth become very close to each other.

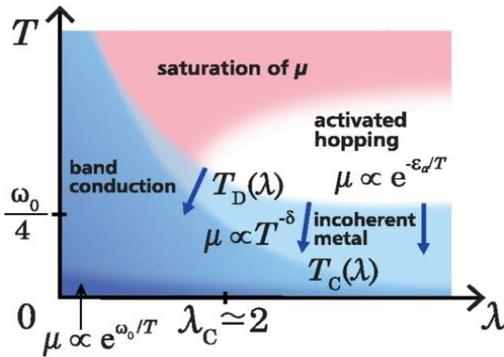


Figure 1 Transport regimes of polaron. Schematic phase diagram showing the four different regimes of polaron mobility μ in the plane of λ - T (λ : EPC strength, T : temperature). Here, the unit of energy is $t=1$, and ω_0 is the phonon frequency. Arrows show the direction of shift of the borderlines between different regimes when the phonon frequency decreases.

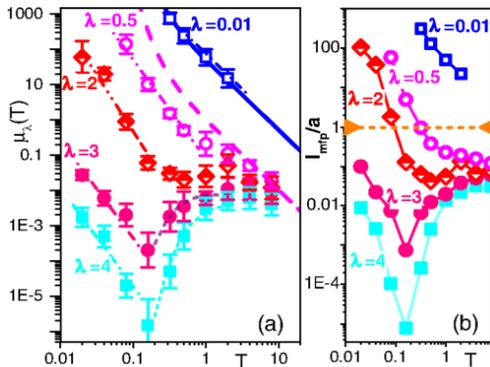


Figure 2 Temperature dependence of mobility and MFP at $\omega_0 = t$. (a) dc mobility $\mu_\lambda(T)$ (in units of ea^2/\hbar). Unbiased numeric values at $\lambda=0.01$ (open squares), $\lambda=0.5$ (open circles), $\lambda=2$ (semifilled diamonds), $\lambda=3$ (filled circles), and $\lambda=4$ (filled squares). Solid bold ($\lambda=0.01$) and dashed bold ($\lambda=0.5$) lines in the top part of the figure show the results obtained by the Boltzmann approach [1]. Fit of the mobility by the activation law is shown for $T>0.2$ at $\lambda=3$ (short-dash line) and $\lambda=4$ (dotted line). Linear dash-dot-dot lines are fits of the low-temperature contribution of mobility, for all the values of λ , by a power law $\mu \sim T^{-6}$. (b) MFP, in units of the lattice parameter a , vs temperature.

[1] G. De Filippis, V. Cataudella, A. de Candia, A. S. Mishchenko, and N. Nagaosa, Phys. Rev. B 90, 014310 (2014).