Highlights

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Crossover from Super- to Subdiffusive Motion and Memory Effects in Crystalline Organic Semiconductors

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The transport properties at finite temperature of crystalline organic semiconductors are investigated, within the Su-Schrieffer-Heeger model, by combining an exact diagonalization technique, Monte Carlo approaches, and a maximum entropy method. The temperature-dependent mobility data measured in single crystals of rubrene are successfully reproduced: a crossover from super- to subdiffusive motion occurs in the range $150 \leq T \leq 200$ K, where the mean free path becomes of the order of the lattice parameter and strong memory effects start to appear. We provide an effective model, which can successfully explain features of the absorption spectra at low frequencies. The observed response to slowly varying electric field is interpreted by means of a simple model where the interaction between the charge carrier and lattice polarization modes is simulated by a harmonic interaction between a fictitious particle and an electron embedded in a viscous fluid.

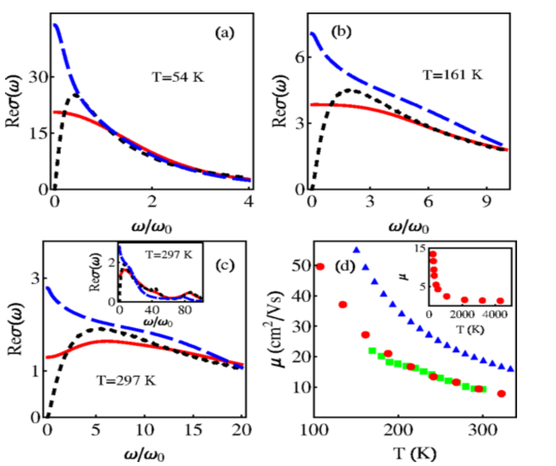

Figure 1 [(a)–(c)] OC, in units of $a^2\, e^2/\hbar$, in different approximations: exact results (solid red line), Boltzmann (long-dashed blue line), and adiabatic (short-dashed black line) approaches. (d) Temperature dependence of the mobility in rubrene [1] (green squares) compared with exact results (red circles) and Boltzmann approach (blue triangles). In the inset is mobility (exact results in units cm^2/Vs) in a wider range of temperatures.

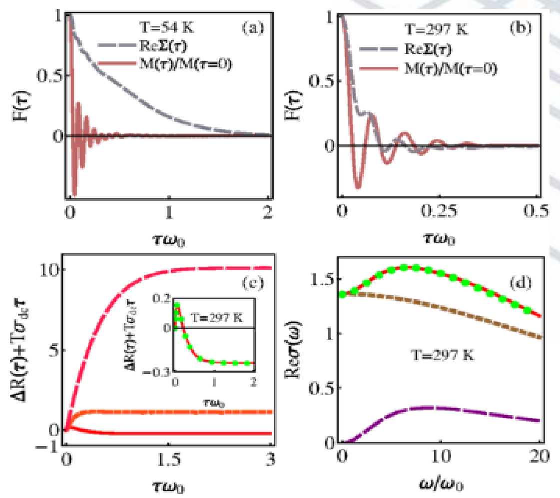

Figure 2 [(a) and (b)] Comparison between current operator relaxation function and memory function at two temperatures; $F(\tau)$ stands for the dimensionless quantities $\mathrm{Re}\Sigma(\tau)$ and $M(\tau)/M(\tau{=}0)$. (c) Relaxation function of the polarization at different temperatures; in the inset is a comparison with the model (green circles). (d) $\mathrm{Re}\sigma(\omega)$: exact results (red solid line); Drude-Lorentz contribution (DLC) (long-dashed purple line), and note that the mobility of DLC is zero; Drude contribution (DC) (short-dashed brown line); DCL+DC (green circles).

[1] V. Podzorov, E. Menard, J. A. Rogers, and M. E. Gershenson, Phys. Rev. Lett. 95, 226601 (2005).