Polarons in Jahn-Teller Crystals: Intrinsic Difference between e_g and t_{2g} Electrons

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About a decade ago, Tokura's group made an interesting comparative study of the effective mass m^* between e_g and t_{2g} electrons by measuring the low-temperature electronic specific heat $C_e(T)$ of the manganese oxides $La_{1-x}Sr_xMnO_3$ as well as the titanium ones $La_{1-x}Sr_xTiO_3$ [1]. They have found that the t_{2g} (titanium) system has a larger T-linear coefficient in $C_e(T)$ than the e_g (manganese) one by more than a factor of two, irrespective of x, implying that t_{2g} electrons may be intrinsically much heavier than e_g ones.

Since Mn^{3+} and Ti^{3+} ions are, respectively, considered as typical $E\otimes e$ and $T\otimes t$ Jahn-Teller (JT) centers, we may anticipate that the above experimental result directly reflects an inherent difference in the mathematical structure of JT centers, namely, either $E\otimes e$ or $T\otimes t$. Motivated by this anticipation and as a work subsequent to a previous one of our group for the $E\otimes e$ polarons [2], we have made a comparative study of the polaronic effective mass m^* between the $E\otimes e$ and the $T\otimes t$ JT polarons. A comparison with the conventional Holstein polarons is also made.

If the electron-phonon (el-ph) coupling is weak, it is straightforward to determine the ratio of m^* to the bare band mass m by resorting to second-order perturbation calculation, from which we obtain m^*/m as $1+2\alpha$ for both JT polarons with α the nondimensional el-ph coupling constant in its conventional definition. Exactly the same mass ratio can be reproduced in the Holstein model, if we redefine α in the model in an appropriate way. Thus we see that there is no essential difference in the enhancement of m^* among those three polarons in the small-α limit.

In the limit of $\alpha \rightarrow \infty$, a polaron will be completely localized at a single site, implying $m^*/m = \infty$. For a finite but very large α, the localized polaron will begin to hop between sites, but the hopping in this case is a very rare event. Thus physics connected with such a hopping can be well captured by just considering a two-site system. In fact, by implementing the two-site calculation by exact diagonalization, we can obtain a generic feature of m^*/m in the strong-coupling ($\alpha \rightarrow \infty$) and/or antiadiabatic (the electron hopping integral t much smaller than the local optic phonon energy ω_0) region.

The results of the two-site calculation are shown in Fig. 1. We note that the Holstein polaron (the dotted-dashed curve) is characterized analytically by the relation of $m/m^*=e^{-2\alpha}$, while the $E\otimes e$ polaron (the dashed curve) by $m/m^*=(\pi\alpha/2)^{1/2}e^{-\alpha}$ [2], indicating the much lighter effective mass of the latter system.

Physically the mass enhancement is brought about by the virtual excitation of local phonons in those model Hamiltonians describing the coupling of an electron with local optic phonons. In the Holstein model no restriction is imposed on exciting multiple phonons, but in the $E\otimes e$ JT model there is a severe restriction due to the existence of a conserved quantity intimately related to the SO(2) rotational symmetry in the pseudospin space representing the twofold degenerate orbitals.

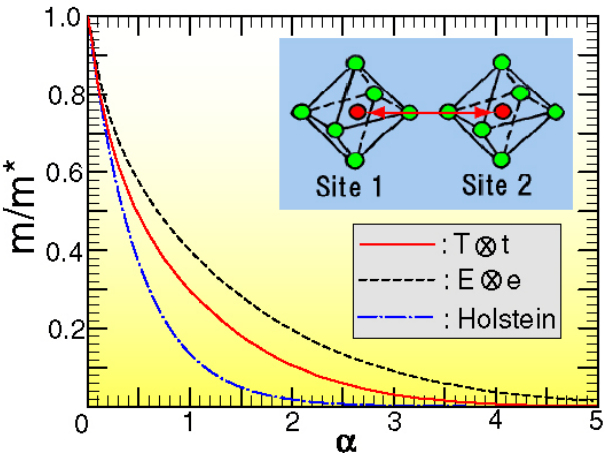

Fig. 1. Inverse of the mass enhancement factor, m/m^*, as a function of α for the $T\otimes t$ (solid curve) and the $E\otimes e$ (dashed curve) JT polarons in comparison with the Holstein one (dotted-dashed curve). All the results are obtained in the strong-coupling and/or antiadiabatic region.

As for the $T\otimes t$ model, no corresponding symmetry exists in the pseudospin space, explaining its difference in m/m^* from the $E\otimes e$ model in Fig. 1. In order to understand its difference from the Holstein model, however, a more detailed analysis is needed. It is well known that the adiabatic potential energy surface for the $T\otimes t$ model contains four equivalent wells for sufficiently large α, but the wells are not isotropic; the vibrational t-mode splits into an a_1-mode and two e-modes (i.e., $t \rightarrow a_1\oplus e$). This fact indicates that the $T\otimes t$ model is a combination of the Holstein and the $E\otimes e$ models, explaining the reason why the result of m/m^* in this model (the solid curve in Fig. 1) comes between those of the Holstein and the $E\otimes e$ models.

Our model is too primitive to make a quantitative comparison with experiment, but we find that, at least in the strong-coupling and/or antiadiabatic region, the difference in the behavior of m^* as a function of α can be ascribed to the presence/absence of rotational symmetry in the pseudospin space representing the internal mathematical structure of each JT center.

References

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