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Development of orbital and spin fluctuations in Fe-based superconductors based on the self-consistent vertex correction (SC-VC) method

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To achieve unified understanding of the whole phase diagram of Fe-based superconductors, we analyze the multiorbital Hubbard model going beyond the random phase approximation (RPA). The 2nd-order non-magnetic structure transition at $T_{\rm S}(> T_{\rm N})$, nematic order as well as large softening of shear modulus C_{66} indicate the strong orbital fluctuations in the normal state. However, only the spin fluctuations develop within the RPA. To resolve this discrepancy, we develop the self-consistent vertex correction (SC-VC) method beyond the RPA, and find the mutual development of orbital and spin fluctuations due to the Aslamazov-Larkin VC, which describes the Kugel-Khomskii type spin-orbital coupling [1]. We find that (i) both the antiferro-orbital and ferro-orbital (=nematic) fluctuations develop for $J/U > 0.17$ by including the self-energy correction (=SC-VΣ method): Both fluctuations contribute to the s-wave superconductivity, and the nematic fluctuations are the origin of the structure transition and the softening of C_{66}. (ii) The coexistence of orbital and spin fluctuations can induce the loop-shape nodes on the electron-pockets in $BaFe_2(As,P)_2$, as well as (impurity-induced) smooth $s_{\pm} \to s_{++}$crossover with high $T_{\rm c}$ [2,3]. Also, the horizontal node on the z^2-orbitlal hole-pocket predicted by RPA is filled by the inter-orbital fluctuations due to the VC, consistently with laser ARPES and other bulk experiments of 122 compounds. (iii) The same orbital nematic fluctuations are obtained in a simple two-orbital model for $Sr_3Ru_2O_7$, not only by the SC-VC method [4] but also by the two-dimensional RG method [5]. Therefore, the VC is expected to be the origin of novel orbital physics in various multiorititat d- and f-electron systems.

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