Comment on "Violation of Anderson's Theorem for the Sign-Reversing s-Wave State of Iron-Pnictide Superconductors"

In Ref. [1], Onari and Kontani studied the nonmagnetic impurity effects on the sign-changing s-wave state ($s_{\pm}$) in the Fe-based superconductors and claimed (1) the orbital-less model such as a band basis model has no impurity pair-breaking effect in the unitary limit, and (2) however, the presence of an orbital degree of freedom (ODF) can make the impurity pair-breaking effect as strong as in the nodal-gap superconductors—therefore, taking into account of the ODF is essential to describe the correct impurity effects. In this Comment, we point out that claims (1) and (2) are incorrect conclusions and show that both the band basis model and the orbital basis model have the same pair-breaking effect and the presence or absence of the ODF is irrelevant for the impurity effects.

The authors of Ref. [1] showed that the $\mathcal{T}$ matrix in the band basis $\hat{\mathcal{T}}^b$ always becomes band diagonal when the impurity potential strength $I \rightarrow \infty$; hence, the pair-breaking interband scattering process vanishes. We argue that this is a pathological artifact of the band basis $\mathcal{T}$ matrix $\hat{\mathcal{T}}^b$ in the $I \rightarrow \infty$ limit and can be cured by subtracting and adding the bare impurity potential $\hat{I}^b$ before and after taking the $I \rightarrow \infty$ limit. With the suggested regularization process, the infinite constant term is absorbed into the chemical potential, and the diagonal and off-diagonal terms in the regularized $\hat{\mathcal{T}}^b_{\rm reg} = \hat{\mathcal{T}}^b - \hat{I}^b$ always become the same order in I; hence, there is a pair breaking in the band basis $\mathcal{T}$ matrix for all values of I.

In the following, we show the physical equivalence of the band basis and the orbital basis models by mapping the five-orbital model of Ref. [1] into a minimal two-band model of Ref. [2]. First, the orbital basis impurity potential $\hat{I}^o = I\delta(r)\delta_{j,l}$ used in Ref. [1] has an overall momentum independence due to $\delta(r)$. The unitary transformation of $\hat{I}^b(k,q) = \hat{U}^\dagger(k)\hat{I}^o\hat{U}(q)$ adds some degree of momentum dependence, but the overall momentum independence of $\hat{I}^o$ continues to survive in $\hat{I}^b$, hence making the intraband and interband scattering terms in $\hat{I}^b$ equal strength on average.

Next, the mapping of the particle-hole asymmetric orbital model of Ref. [1] to the particle-hole symmetric band model of Ref. [2] requires the definition of the renormalized impurity potential $I_{\rm eff}$ due to the particle-hole asymmetry. The particle-hole asymmetry yields nonzero $g_3(\omega)$, which enters only in the combination of $(I^{-1} - g_3)$, and hence it renormalizes only the bare impurity potential I to the effective one $I_{\rm eff}$ as $I^{-1}_{\rm eff} = (I^{-1} - g_3)$ [3]. We can easily read off $g_3(\omega = 0) \approx 1\ {\rm eV}^{-1}$ from the fact that $I = 1$ eV produced the maximum impurity scattering effect (i.e., $I_{\rm eff} = \infty$) in Ref. [1]. Now we can read $I_{\rm eff}(I = 1, \infty, -2, -1\ {\rm eV}) = \infty, -1, -1/1.5$, and $-1/2$ eV, respectively, and the mysterious nonmonotonic relation between the pair-breaking effect and the values of I in Ref. [1] is easily understood.

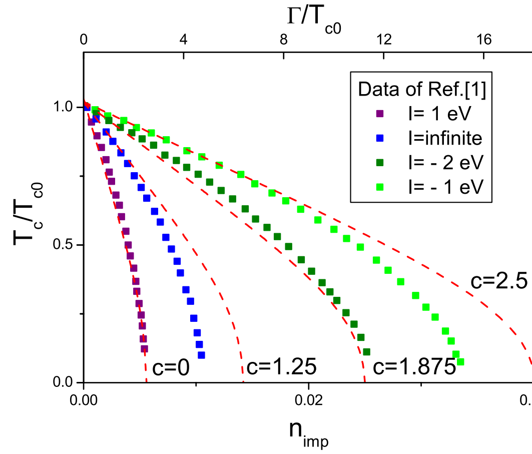

FIG. 1 (color online). Comparison of normalized T_c data for the $s_{\pm}$-wave state from two model calculations. Symbols are the data from Ref. [1] (bottom x axis with $n_{\rm imp}$), and dashed lines are the calculations with the two-band model [2] (upper x axis with Γ/T_{c0}).

With the above obtained $I_{\rm eff}(I)$ and choosing $\pi N_{\rm tot} = 0.8/{\rm eV}$ as a fitting parameter, we calculated the T_c suppression due to the nonmagnetic impurities for the $s_{\pm}$-wave state by using the two-band model of Ref. [2], where the impurity potential strength is parameterized by the phase shift parameter c defined as $\frac{1}{c} = \pi N_{\rm tot} I_{\rm eff}$, so we have $|c|(I = 1, \infty, -2, -1\ {\rm eV}) = 0, 1.25, 1.875$, and 2.5, respectively. Figure 1 shows the comparison between our calculations and the results of the five-orbital model of Ref. [1]. Two data sets closely track each other and demonstrate that the pair-breaking effect of the five-orbital model of Ref. [1] is not due to the ODF. However, it is true that the orbital basis formalism [1] is advantageous to avoid the pathological artifact in $I \rightarrow \infty$ limit since it does not need an extra regularization.

This work was supported by Grants No. NRF-2010-0009523 and NRF-2011-0017079 funded by the National Research Foundation of Korea.

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Received 2 December 2010; published 23 June 2011
DOI: 10.1103/PhysRevLett.106.259701
PACS numbers: 74.20.Rp, 74.62.En, 74.70.Xa

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[2] Y. Bang, H. Y. Choi, and H. Won, Phys. Rev. B **79**, 054529 (2009).
[3] This implies that the particle-hole asymmetry can always be absorbed into the renormalized impurity potential $I_{\rm eff}$ and then be ignored for all practical purposes.

