Reply to Comment on "Violation of Anderson’s Theorem for the sign-reversing s-wave state of Iron-Pnictide Superconductors" [arXiv:1012.0414] by Y. Bang

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We explain that the study of impurity effect in iron pnictides [1] are correctly calculated based on the T-matrix approximation, contrary to the Comment by Bang[2]. The replacement $\tilde{T}^b$ with $\tilde{T}^b - \tilde{I}^b$ proposed by Bang breaks the perturbation theory and is therefore erroneous.

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In Ref.[1], we studied the nonmagnetic impurity effect in the multiorbital model for iron pnictide superconductors. In the sign-reversing s-wave state ($s_\pm$), we found that (i) $T_c$ is substantially suppressed by the inter-band impurity scattering, since the T-matrix has large inter-band matrix elements. (ii) This result holds even in the unitary limit, contrary to the claim that (iii) inter-band scattering vanishes in the unitary limit if the bare impurity potential in the band basis $\tilde{T}^b$ is a constant matrix and $\text{det}\{\tilde{T}^b\} \neq 0$ [3]. In iron pnictides, the statement (ii) holds since $\tilde{T}^b$ has large $k$-dependence.

In Ref. [2], Bang complained that the result (iii) is incorrect, that is, he claimed that inter-band scattering exists in the unitary limit even if $\text{det}\{\tilde{T}^b\} \neq 0$. Here, we explain the formalism of the T-matrix approximation when $\tilde{T}^b$ is constant, and point out the error in Ref. [2]. The T-matrix for a single impurity in the band-basis is

$$\tilde{T}^b = (1 - \tilde{I}^b g_{\text{loc}})^{-1} \tilde{g}^b,$$

where $g_{\text{loc}}$ is the local Green function. In the T-matrix approximation, the normal and anomalous self-energies for dilute impurity concentration $n_{\text{imp}} \ll 1$ are given as

$$\Sigma^a_n(i\omega_n) = n_{\text{imp}} \tilde{T}^b(i\omega_n),$$

$$\Sigma^s_n(i\omega_n) = n_{\text{imp}} \tilde{T}^b(i\omega_n)f(i\omega_n)\tilde{T}^b(-i\omega_n),$$

where $f(i\omega_n) \equiv \sum_k \tilde{F}_k(i\omega_n) \ll 1$ is the linearized local anomalous Green function. $\Sigma^a$ is diagrammatically expressed in Fig. 1 (a), which expresses the inter-band scattering of a Cooper pair when $\tilde{T}^b$ has off-diagonal elements, as shown in Fig. 1 (b). In the $s_\pm$-wave state, this inter-band impurity scattering suppresses the superconductivity.

When $\text{det}\{\tilde{T}^b\} \neq 0$, eq. (1) becomes $T^b_{\alpha,\beta} = -1/g_{\text{loc}}^{b,\alpha,\beta}$, $\delta_{\alpha,\beta}$ in the unitary limit ($T \rightarrow \infty$), which is band-diagonal even if $\tilde{T}^b$ is not band-diagonal. Therefore, the pair-breaking due to inter-band scattering is absent in the unitary limit unless det{ $\tilde{T}^b$} = 0 [3].

On the other hand, Fe-ion substitution in iron pnictides induces the orbital-diagonal local impurity potential. Then, $\tilde{P}$ is given as $\tilde{P}_{\alpha k} = U_k U_\alpha^*$, where $U_k$ is the transformation matrix between orbital- and band-bases.

Because of the large $k$-dependence in iron pnictides, $\tilde{T}^b$ is not diagonal even in the unitary limit, and therefore $s_\pm$-wave state is fragile against impurities. This is the main result in Ref. [1].

In Comment[2], Bang seems to claim that the bare impurity potential $\tilde{T}^b$ should be subtracted from the T-matrix $\tilde{T}^b$. If we follow his comment in eq. (3), inter-band scattering of Cooper pair always occurs. However, such subtraction violates the perturbation theory, and induces various unphysical results, for example, the divergence of $\Sigma^a$ for $\tilde{T}^b \rightarrow \infty$ will give the divergence of $T_c$ in the $s_{++}$ wave state. We agree that the real-part of the “normal self-energy”, which becomes $n_{\text{imp}} \tilde{T}^b$ in the Born limit [4], is absorbed by the change in the chemical potential. However, this fact never means that T-matrix is renormalized to $\tilde{T}^b - \tilde{I}^b$, contrary to the claim by Bang.

In the constant $\tilde{I}^b$ model, Bang[2] showed that the T-matrix is not band-diagonal when $\tilde{P} \propto \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, (i.e. det{ $\tilde{P}^b$} = 0) in the unitary limit. However, this is the special case (measure zero probability) in the statement (iii). In contrast, $\tilde{T}^b$ always has off-diagonal elements in multiorbital models since $\tilde{P}^b$ is not constant. Thus, it is better to analyze the multiorbital model for a quantitative study of impurity effects in iron pnictides.

In summary, our studies of impurity effect in iron pnictides[1] are correctly calculated based on the T-matrix approximation, which becomes exact in the dilute limit. The replacement $\tilde{T}^b$ with $\tilde{T}^b - \tilde{I}^b$ in eq. (3), which was proposed by Bang [2], breaks the perturbation theory and is therefore erroneous.
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[2] Y. Bang, arXiv:1012.0414.
[3] Y. Senga and H. Kontani: J. Phys. Soc. Jpn. 77 (2008) 113710; Y. Senga and H. Kontani, New J. Phys. 11, 035005 (2009); M.L. Kulic and O.V. Dolgov, Phys. Rev. B 60 (1999) 13062; Y. Ohashi, J. Phys. Soc. Jpn. 71 (2002) 1978.

[4] In the presence of the electron-hole symmetry, Re$\Sigma^n = \frac{I^h}{1 + (\pi N^\varepsilon)^2}$ for general $I^h$, where $N$ denotes the density of state on the Fermi energy.