While the impurity-induced nanoscale electronic disorder has been extensively reported in the underdoped iron pnictides, its microscopic origins remain elusive. Recent scanning tunneling microscopy (STM) measurements reveal a dimer-type resonant structure induced by cobalt doping. These dimers are randomly distributed but uniformly aligned with the antiferromagnetic a axis. A prevalent explanation is that the structural transition results from the fluctuations of incipient AFM order [14, 15]. Alternatives include the key role of orbital degrees of freedom [16] and, in particular, the proposal that the structural transition originates from the pocket density-wave (PoDW) order in parent compounds, a “hidden” order responsible for orbital ferromagnetism.

Recent scanning tunneling microscopy (STM) experiments observe the nematic-type electronic formations developing around dopant atoms [9, 18]. These formations appear as “dimer resonances,” with two neighboring peaks separated by ∼6−8 lattice spacings. Importantly, the dimers are oriented along the a axis of the pnictides’ unidirectional AFM order. In this Rapid Communication, we show that both the appearance of dimer resonances and their size and orientation provide a direct insight into the electronic structure and correlations in iron pnictides. In this regard, the properties of such dimers can serve as a diagnostic tool to unravel the nature of the underlying microscopic ground state and the sequence of Fermi-surface reconstructions left in the wake of various itinerant density-wave (DW) orderings [19].

These are our main results: The dimer resonance [9, 18] is a consequence of a type of “reconstructed” nesting [20] characterized by the wavevector \( \vec{q}_n \approx (0.4\pi, 0) \). Such nesting tendency is manifest in our detailed calculations within the three orbital model [21], where \( \vec{q}_n \) — associated with the short axis of the elliptical electron pocket — emerges as a prominent feature of the reconstructed band structure, itself occasioned by the transition from the paramagnetic phase to the PoDW. Specifically: i) In the paramagnetic phase, the Fermi pocket is far from any nesting at \( \vec{q}_n \). Consequently, no resonances appear; ii) As a PoDW is formed, the electron pocket is itself deformed while, simultaneously, sections of the reconstructed hole pockets become flatter as the PoDW order parameter increases. This gives rise to the “reconstructed” nesting at \( \vec{q}_n \); iii) \( \vec{q}_n \) is perpendicular to the PoDW, producing the real-space dimer pattern breaking the \( C_4 \) symmetry. The resonant pattern arises when randomly distributed dopant impurities induce two peaks in the local density of states (LDOS), both their separation and direction set by \( \vec{q}_n \); iv) When a PoDW and a SDW coexist, two nesting vectors \( \vec{q}_n \approx (0.4\pi, 0) \) and \( \vec{q}_b \approx (0, 0.4\pi) \) emerge from the reconstructed pockets. With \( e_y \) and \( e_x \) coupled to the inner and outer hole pockets, \( h_2 \) and \( h_1 \), respectively, the susceptibility near \( \vec{q}_n \) remains much larger than its counterpart near \( \vec{q}_b \). Again, the \( C_4 \) symmetry is broken resulting in dimer patterns observed in [9, 18].

We now supply the details behind the above physical picture. Experiments and theoretical calculations indicate that iron pnictides contain four disconnected Fermi-surface pockets (Fig. 1) [22, 23]. Additional parts of the Fermi surface are present in some materials [23] but this is not important for the physics discussed here. When two hole pockets closely match two electron pockets, as is the case in many iron pnictide parent compounds [23], the geometric nesting favors the formation of two DWs [17]. The PoDW partially gaps \( e_y \) and one hole pocket and induces a structural transition, while \( e_x \) and the remaining hole pocket form the partially gapped SDW. The theory [17] naturally explains the proximity of the two transitions and accounts for the observed orbital ferromagnetism.

While geometric nesting tendencies are important [22], they are not the complete story: The orbital content of the Fermi pockets must be considered as well [24]. Here, we start with a simplified geometric model allowing for an
Within a detailed numerical follow-up employing three-orbital content \[21\], known to capture the main features of real materials \[22\]. We model the Fermi pockets as:

\[ \epsilon_{e_x}(k_x) = \frac{(k_x - \pi)^2}{2m_a} + \frac{k_y^2}{2m_b} - \epsilon_0; \]

\[ \epsilon_{e_y}(k_y) = \frac{(k_y - \pi)^2}{2m_b} - \epsilon_0; \]

\[ \epsilon_{e_z}(k_x) = \epsilon_{e_y}(k_x \leftrightarrow k_y + \pi); \]

with \( m_a > m > m_b \), so that the two DWs are partially gapped when order parameters \( \Delta_{PoDW} \) and \( \Delta_{SDW} \) are small. \( e_y \) and \( e_z \) bands are related by 90° rotation. To simplify the analytic calculation, we assume that \( h_1 \) and \( h_2 \) are isotropic and have the same dispersion relations.

![FIG. 1. (Color online) Fermi pockets in the unfolded Brillouin zone of iron pnictides. Two hole pockets \( h_1 \) and \( h_2 \) are centered at the \( \Gamma = (0,0) \) point. The elliptical electron pockets \( e_x \) and \( e_y \) are centered at \( M_1 = (\pi,0) \) and \( M_2 = (0,\pi) \), respectively. \( h_1, h_2, e_x, \) and \( e_y \) pockets exhibit strong nesting tendencies in many parent compounds. Here, we propose that the resonant electronic structure arises due to the "reconstructed" nesting with the wave vector \( \vec{q}_a \), the shorter axis of the \( e_y \) pocket.

It is known that static charge/spin susceptibilities contain peaks around the nesting vectors \( M_1 = (\pi,0) \) and \( M_2 = (0,\pi) \) in the above noninteracting model, implying a tendency to DW formation in moderately correlated iron pnictides \[22\]. Initially, by ignoring the orbital content at the Fermi level within \[22\], we can determine the analytic form for such geometric susceptibility at \( T = 0 \), within a single elliptical electron pocket \[1\]:

\[ \chi(q_x, q_y) = 2 \int \frac{d^2k}{(2\pi)^2} \frac{n_f(\epsilon(k_x)) - n_f(\epsilon(k_y))}{\epsilon(k_y - \epsilon(k_x)) - \epsilon(\vec{q}) + i0^+} \]

\[ = \left\{ \begin{array}{ll}
\frac{\sqrt{m_a m_b}}{4\pi} & \text{if } \frac{q_x^2}{2m_a} + \frac{q_y^2}{2m_b} < 4\epsilon_0, \\
\frac{\sqrt{m_a m_b}}{4\pi} \left[ 1 - \sqrt{1 - \frac{4\epsilon_0}{\frac{q_x^2}{2m_a} + \frac{q_y^2}{2m_b}}} \right] & \text{if } \frac{q_x^2}{2m_a} + \frac{q_y^2}{2m_b} > 4\epsilon_0.
\end{array} \right. \]

\( \chi(\vec{q}) \) is effectively a constant for \( \vec{q}/2 \) within the pocket, and decreases slowly as \( \vec{q}/2 \) moves outside. Consequently, \( \chi(q) \) contains only an unremarkable ridge instead of a peak, implying no resonance around \( \vec{q}_a \) in the normal state of such a simple geometric model. These features of geometric nesting are echoed in a realistic calculation with full orbital content \[22, 25\]:

\[ \chi(\vec{r}, \vec{r}') = \langle \rho(\vec{r}) \rho(\vec{r}') \rangle = \sum_{\alpha, \beta} \langle d^\dagger_{\alpha}(\vec{r}) d_{\alpha}(\vec{r}) d^\dagger_{\beta}(\vec{r}') d_{\beta}(\vec{r}') \rangle \]

\[ = - \frac{2}{N^2} \sum_{\vec{k}_i, \mu, \nu, \vec{q}} \langle d^\dagger_{\mu}(\vec{k}_i) d_{\mu}(\vec{k}_i + \vec{q}) d^\dagger_{\nu}(\vec{k}_i + \vec{q}) d_{\nu}(\vec{k}_i) \rangle \;
\]

\[ \langle d_{\mu}(\vec{k}_i) d_{\nu}(\vec{k}_i + \vec{q}) \rangle = \frac{2}{N} \sum_{\vec{k}_i, \mu, \nu} \frac{\langle \mu, \vec{k}_i + \vec{q}, \nu, \vec{k}_i \rangle}{\epsilon_{\mu}(\vec{k}_i + \vec{q}) - \epsilon_{\nu}(\vec{k}_i) + i0^+} \exp \left( ik_2 - \vec{k}_1 \right) \]

where \( \alpha, \beta \) denote \( d \) orbitals and \( \mu \)'s are the band indices. In the paramagnetic phase, the Green’s function \( \langle d_{\mu}(\vec{k}_i, \omega_n) d^\dagger_{\nu}(\vec{k}_j, \omega_n) \rangle \) is finite only if \( \vec{k}_i = \vec{k}_j \) and \( \mu_i = \mu_j \) and thus Eq. (2) gives

\[ \chi(q) = 2 \frac{N}{N} \sum_{\vec{k}_i, \mu, \nu} \left| \frac{\langle \mu, \vec{k}_i + \vec{q}, \nu, \vec{k}_i \rangle}{\epsilon_{\mu}(\vec{k}_i + \vec{q}) - \epsilon_{\nu}(\vec{k}_i) + i0^+} \right| . \]

The factor of 2 in (2) is due to spin and \( n_f(\epsilon) \) is the Fermi distribution function. Again, we find nesting peaks at \( (\pi,0) \) and \( (0,\pi) \) but no enhanced structure near \( \vec{q}_a \).

The situation changes once the DW order is established. Within a PoDW, which is the leading DW instability of Ref. \[17\], the electron pocket \( e_y \) couples with one of the hole pockets; in the following, we assume this is \( h_2 \). The reconstructed Fermi surface is shown in Fig. 2.

![FIG. 2. (Color online) As PoDW order develops, the Fermi surface reconstructs, and \( e_y \) and the inner hole pocket \( h_2 \) are deformed. The curvature along \( e_y \) decreases, leading to the "reconstructed" nesting at \( q_0 \), the short axis of the \( e_y \) pocket. This reconstructed nesting is absent in the paramagnetic phase, but becomes pronounced as \( \Delta_{PoDW} \) increases.](image)
optimizes nesting. For $\Delta_{PoDW} \ll \Delta_{opt}$, $\chi$ increases by
\[
\delta \chi(q_a) = \chi_{PoDW}(q_a) - \chi_{para}(q_a)
\approx \frac{\sqrt{2m_a m_b}}{\pi} \left( \frac{m_a - m_b}{m_a + m_b} \right)^{1/2} \left( \frac{\Delta}{\epsilon_0} \right)^2 \frac{m(m + m_a)}{(m - m_b)^2},
\]
while, for $\Delta_{PoDW} = \Delta_{opt}$,
\[
\delta \chi(q_a) \approx \frac{1}{\pi} \left( \frac{\Delta k}{v_F^l \beta} \right)^{1/4}
\]
$\Delta k$ is width of the reconstructed pocket, $v_F$ is the Fermi velocity $\parallel \tilde{x}$, $\tilde{k} = q_a/2$, and $\beta = (\partial^2 \epsilon / \partial k^2)_{k_x = q_a/2, k_y = 0}$.

\[\begin{align*}
\Delta k &\approx \sqrt{e_0 m_a - m_b} \left( m + m_b \right) (m + m_a) \\
v_F &= \frac{2e_0}{\sqrt{m_a m_b (m + m_a)}} \\
\beta &= \left( \frac{1}{m} + \frac{1}{m_a} \right) \frac{m_a + m_b}{32e_0 m_b (m - m_a)} \left[ 1 - \frac{1}{4} \left( \frac{m_a - m}{m + m_b} \right)^2 \right].
\end{align*}\]

\[\text{FIG. 3. (Color online) Left: Feynman diagrams for } \chi^c \text{ in the PoDW phase. All other diagrams cancel out. Right: } \chi^c(\tilde{k}) \text{ with } \Delta_{PoDW} = 20 \text{meV in the realistic three-orbital model. The original peaks at } (0, \pm \pi) \text{ in the paramagnetic phase are suppressed by finite } \Delta_{PoDW}. \text{ Instead, } \chi^c(\tilde{k}) \text{ contains a plateau centered at } q_a \approx (\pm 0.4 \pi, 0), \text{ breaking the } C_4 \text{ symmetry. This plateau arises from the “reconstructed” nesting at } q_a.\]

Again, we fortify the above picture with the realistic calculation of charge susceptibility $\chi^c(q)$ within the three orbital model. In the PoDW state, $\langle d_{\mu \dagger}(k_i, \omega_n) d_{\lambda}(k_j, \omega_m) \rangle$ is finite only if $\mu_i = \mu_j$ and $k_i = k_j$ or $(\mu_i, \mu_j) = (e_y, h_2)$ and $k_i = k_j + (0, \pi)$. Figure 3 displays Feynman diagrams contributing to $\chi^c(\tilde{k})$. Additional diagrams, composed of one normal and one anomalous Green’s function, break time reversal symmetry and cancel out upon summation over $\tilde{k}$. $\chi^c$ is calculated within the three-orbital model and is shown in Fig. 3. Evidently, a high plateau around $(\pm 0.4 \pi, 0)$ arises due to the “reconstructed nesting” at vector $q_a$. This is qualitatively consistent with the results in Eq. (6) for the simple model [1]. In addition, the original peaks at $\tilde{M}_2 = (0, \pm \pi)$ are suppressed due to the formation of a PoDW.

At low $T$, Ref. [17] predicts the coexistence of a PoDW and a SDW, and therefore, leads to two “reconstructed” nesting vectors, $q_a$ and $q_b$, related by $90^\circ$ rotations. If $\Delta_{PoDW} \neq \Delta_{SDW}$, the $C_4$ symmetry is already broken by this unequal pairing. In Ref. [17], $\Delta_{PoDW} > \Delta_{SDW}$ and this naturally leads to $\chi(q_a) > \chi(q_b)$. When $\Delta_{PoDW} = \Delta_{SDW}$, the difference between $\chi(q_a)$ and $\chi(q_b)$ could still arise from the distinct orbital content of Fermi pockets. To illustrate the effect of orbital content, we assume $[23]$
\[\begin{align*}
h_1 &= \cos(\theta) d_{yx} + \sin(\theta) d_{xz} \\
h_2 &= \cos(\theta) d_{xz} - \sin(\theta) d_{yx} \\
e_x &= d_{yx}, \quad e_y = d_{xz},
\end{align*}\]
where $\theta$ is the polar angle at the Fermi pocket.

\[\begin{align*}
\delta \chi &= \int \frac{d\tilde{k}}{(2\pi)^2} \left( \cos^2 \theta(\tilde{k} + \tilde{q}) - \sin^2 \theta(\tilde{k} + \tilde{q}) \right) \\
u^2(\tilde{k} + \tilde{q})v^2(\tilde{k}) &\left( k_i n_f(\lambda(\tilde{k})) - n_f(\lambda(\tilde{k} + \tilde{q})) / \lambda(\tilde{k} + \tilde{q}) - \lambda(\tilde{k}) \right).
\end{align*}\]

The vertex factors $\cos^2 \theta(\tilde{k} + \tilde{q})$ and $\sin^2 \theta(\tilde{k} + \tilde{q})$ come from the orbital component of the charge density $\rho(\tilde{r})$ when calculating $\chi(q_a)$ and $\chi(q_b)$, respectively.

\[u^2(\tilde{k}) = \frac{1}{2} \left( 1 + \frac{(\epsilon_h(\tilde{k}) - \epsilon_c(\tilde{k} + \tilde{M}))}{2} \right)\]

\[v^2(\tilde{k}) = 1 - u^2(\tilde{k}).\]
$n_f$ is the Fermi function, and $\lambda$ is the energy of the reconstructed, partially gapped fermions. The other diagrams give similar contributions, with different vertices.

It is now difficult to get an analytic expression for $\delta \chi$ even within the model (1). However, for $\Delta_{PoDW} = \Delta_{SDW}$ in (4) and at $T = 0$, 

$$\delta \chi \approx \frac{1}{\pi^2} \left( \frac{\Delta k}{\nu_f \beta} \right)^{1/2} \left( \frac{m \sigma m_b (m - m_b) (m_a + m)}{m (m_a + m_b)} \right),$$  

(14)

with $\delta k$, $v_f$ and $\beta$ from Eqs. (1)-(3). The anisotropy is determined by the choice of coupling between the $e$ and $h$ pockets: $\chi(q_{e} + \vec{M}_2) > \langle \langle \rangle \rangle \chi(q_{e} + \vec{M}_1)$ when $e_y$ and $e_x$ couple to $h_2(h_1)$ and $h_1(h_2)$, respectively [20].

Again, we follow up with the realistic calculation of $\chi^{\nu} (q)$ based on the three-orbital model. The results are displayed in Fig. 5. The peaks at the nesting vectors $\vec{M}_1$ and $\vec{M}_2$ are suppressed due to the PoDW and SDW. Evidently, $\chi (\vec{k})$ breaks the $C_4$ symmetry, as expected.

STM experiments reveal an anisotropic electronic dimer structure developing when the iron pnictide is doped with cobalt [18]. Our theory of reconstructed nesting can account for this phenomenon, by considering the impurity-induced quasiparticle interference in the parent compounds. First, the local potential of the cobalt atom is $H_{imp} = \sum_{\sigma, \alpha} (V_s^\alpha + \sigma V_m^\alpha) d_\alpha (\vec{r}) d_\alpha (\vec{r})$, where $V_s$ and $V_m$ are the nonmagnetic and the magnetic parts of the impurity potential, respectively, and are given for each orbital $\alpha$ in [24]. The LDOS with a single impurity is:

$$\rho(E, \vec{r}) = -\frac{1}{\pi} \sum_{\sigma, \alpha, \sigma} G_{\alpha \alpha, \sigma} (i \omega \rightarrow E + i0^+, \vec{r}, \vec{r}')$$

$$G_\sigma (i \omega, \vec{r}, \vec{r}') = G_0 (\vec{r}, \vec{r}') + G_0 (\vec{r}, \vec{r}) V_{imp} G_0 (\vec{r}, \vec{r}')$$

(15)

$$V_{imp} = H_{imp} (1 - G_0 H_{imp})^{-1}$$

(16)

$G_0$ is the bare Green’s function matrix in orbital space.

Figure 6 shows the LDOS on a $10 \times 10$ square lattice, centered around the cobalt impurity. Note the pronounced peaks at $\vec{r} = (\pm 3a, 0)$, giving rise to the anisotropic dimer structure, observed in [18]. The dimer’s size is tied to the magnitude of the “reconstructed” nesting vector $q_{\nu} \approx (0.4\pi, 0)$. Since the cobalt impurity potential is repulsive, LDOS is small at the impurity site and large when $\vec{r} = (\pm a^{1/2} \pi/0.4\pi, 0) \approx (\pm 3a, 0)$. Therefore, the size of the dimer is $6a$, close to $8a$ of Ref. [18]. In addition, the $C_4$ symmetry is broken — even if $\Delta_{PoDW} = \Delta_{SDW}$ — due to the different orbital components within each pocket. The charge susceptibility, therefore, peaks along the direction perpendicular to PoDW, and results in the $a$-axis orientation of the dimer.

In summary, we have shown that the anisotropic electronic dimer structure can be understood based on the “hidden” PoDW order in parent compounds. This order induces a “reconstructed” nesting vector $q_{\nu}$, at which the charge susceptibility $\chi(q_{\nu})$ develops pronounced peaks. Furthermore, the $C_4$ symmetry is genetically broken due to the orbital components. The dimer, therefore, points along the $a$ axis of AFM order, in accordance with experiments. More generally, our results accentuate the potential of local probes as diagnostic tools in unraveling the patterns of various forms of order in iron pnictides.

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