Universal relations for hybridized s- and p-wave interactions from spin-orbital coupling

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In this work, we study the universal relations for 1D spin-orbital-coupled fermions near both s- and p-wave resonances using effective field theory. Since the spin-orbital coupling mixes different partial waves, a contact matrix is introduced to capture the non-trivial correlation between dimers. We find the signature of the spin-orbital coupling appears at the leading order for the off-diagonal components of the momentum distribution matrix, which is proportional to $1/q^3$ (q is the relative momentum). We further derive the large frequency/momentum behavior of the Raman spectroscopy, which serves as an independent measurable quantity for contacts. We finally give an explicit example of contacts by considering a two-body problem.

Introduction. – In ultracold atomic gases, a series of universal relations was established to set up a bridge between the short distance two-body correlations and the macroscopic thermodynamic properties [1–7]. These relations are connected by a set of key parameters called the contacts that have already been examined in experiments [8–12]. Later, the universal relations were also studied in higher partial-wave systems [13–18], low-dimensional systems [19–29], laser-dressed systems [30, 31], and were taken into account three-body correlations [32–36].

Recent experimental realization of the spin-orbital coupling (SOC) in ultracold gases [37–41] also leads to interesting few- and many-body physics [42–45]. Especially, the universal relations for the spin-orbital coupled Fermi gases attract many attentions [46–50]. Since the SOC breaks the rotational symmetry, it would mix different partial waves at the two-body level. it is interesting to study the universal relations for systems with one-dimensional (1D) SOC with both s- and p-wave interactions. Experimentally, a system with overlapping resonances of s- and p-wave has been realized in ^{40}K atoms using the optical control [51], where in principle additional SOC can be engineered directly.

Motivated by these developments, in this work, we study the universal relations for a 1D Fermi gas with hybridized s- and p-wave interactions from SOC. Importantly, we find that the q^{-3} tail in the spin-mixing (off-diagonal) terms of the momentum distribution matrix is a direct manifestation of SOC induced strong interplay of s- and p-wave interactions, which can be observed through time-of-flight measurement. Further, we study the Raman spectroscopy and also find the spin-mixing term of the Raman spectroscopy matrix is a useful experimental probe that can be used to detect the hybridization of s- and p-wave interactions. In the end, we calculate the contacts in two-body bound states as an explicit example of the contact matrix [52, 53] in the hybridized s- and p-wave Fermi gases. It is found that there is a peak for the two-body hybridized contact of s- and p-wave near the degenerate point of s- and p-wave scattering lengths, indicating a strong interplay between s- and $p-$wave dimers as expected.

Model. – We consider a fermion system with an s-wave interaction between atoms with spin $\uparrow$ and $\downarrow$, together with a p-wave interaction between two spin-$\uparrow$ fermions. Without SOC, the interesting few- and many-body physics have been studied in [54–58]. After adding the SOC, the effective 1D Lagrangian is given by ($\hbar = 1$ throughout the paper)

$$\begin{aligned}\hat{L} =& \sum_k \Psi_k^\dagger \left(i\partial_t - \mathcal{H}_k^0\right)\Psi_k + \sum_{Q;\alpha=S,P}\frac{\varphi_{Q,\alpha}^\dagger\varphi_{Q,\alpha}}{g_\alpha}\\ &-\frac{1}{2\sqrt{L}}\sum_{Q,k}\left[\varphi_{Q,s}^\dagger\left(\Psi_{\frac{Q}{2}+k}^T S\Psi_{\frac{Q}{2}-k}\right)+\text{H.c.}\right]\\ &-\frac{1}{2\sqrt{L}}\sum_{Q,k}k\left[\varphi_{Q,p}^\dagger\left(\Psi_{\frac{Q}{2}+k}^T P\Psi_{\frac{Q}{2}-k}\right)+\text{H.c.}\right].\end{aligned} \tag{1}$$

Here L is the system size. We have defined $\Psi_k = (\psi_{k,\uparrow}, \psi_{k,\downarrow})^T$, where $\psi_{k,\sigma}$ is the field operator for the fermionic atoms with momentum k. The single-particle Hamiltonian is $\mathcal{H}_k^0 = \frac{(k+k_0\sigma_z)^2}{2m} + \Omega\sigma_x$, where atoms in the state $|\uparrow\rangle$ are coupled to the state $|\downarrow\rangle$ by the Raman laser with the strength Ω, and $2k_0$ is the momentum transfer during the two-photon processes. $\varphi_{Q,S}$ ($\varphi_{Q,P}$) is the field operator of the $s(p)$-wave dimer with momentum Q. Note that although we have introduced dimer field for convenience, the Lagrangian contains no dynamics of dimers and is essentially single-channel. The generalization to two-channel models is straightforward and gives the same universal relations to the leading order. Inter-

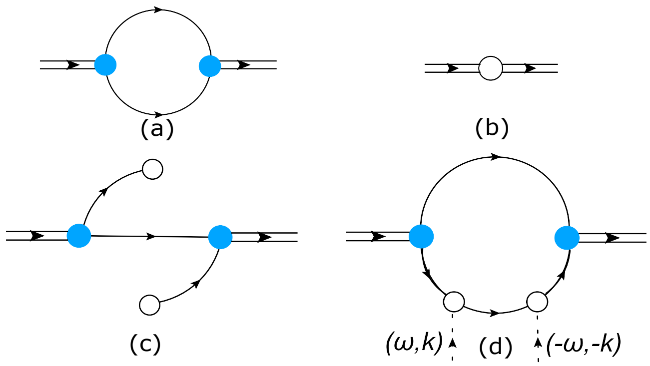

FIG. 1. (a) Diagrams for the matrix elements of the dimer-atom interaction operator. (b) Diagrams for the matrix elements of the dimer local operator $\varphi^\dagger_\alpha(R)\varphi_\beta(R)$. (c) Diagram for the matrix elements of the operator $\psi^\dagger_\sigma(R+x)\psi_{\sigma'}(R)$. (d) Diagram for the matrix element of $\int dt\ e^{i\omega t-ikx}\int dx\mathcal{T}\mathcal{O}_{\sigma 3}(R+x,t)\mathcal{O}^\dagger_{\sigma' 3}(R,0)$ ($\sigma=\uparrow,\downarrow$). The single line denotes the atom propagator matrix G, the double lines denote the matrix elements of the dimer propagator martrix $D_{\alpha\beta}$ with $\alpha,\beta=S,P$, the blue dot represents the interaction vertex: $-i\alpha$ or $-i\beta$, and the open dot represents the insertion of operators.

action vertexes S and P can be related to Pauli matrices σ_j as $S=i\sigma_y$, $P=\frac{1}{2}(1+\sigma_z)$, which is equivalent to

$$\frac{1}{2}\Psi^T_{Q/2+k}S\Psi_{Q/2-k}=\psi_{Q/2+k,\uparrow}\psi_{Q/2-k,\downarrow}, \tag{2}$$

$$\Psi^T_{Q/2+k}P\Psi_{Q/2-k}=\psi_{Q/2+k,\uparrow}\psi_{Q/2-k,\uparrow}. \tag{3}$$

To regularize the possible divergence, we impose a momentum cutoff at $k\sim\Lambda$. The bare interaction parameter g_S and g_P can be related to the physical scattering lengths by

$$a_s=-\frac{2}{mg_S},\qquad \frac{1}{a_p}=\frac{4}{mg_P}+\frac{2\Lambda}{\pi}, \tag{4}$$

where a_s (a_p) is the 1D s(p)-wave scattering length.

With above renormalization relation of g_P, the scattering amplitude of the model (1) is finite. Explicitly, the non-trivial part of the scattering amplitude is from the renormalization of the dimer Green's function $D_{\alpha\beta}(E_0,Q)=\left\langle\varphi_{Q,\alpha}(E_0)\varphi^\dagger_{Q,\beta}(E_0)\right\rangle$. Here the expectation is under the real-time path-integral with the Lagrangian (1). As shown in Fig. 1(a), the inverse of the dimer propagator matrix is given by

$$D^{-1}(E_0,Q)=\begin{pmatrix}(ig_S)^{-1}-\Pi_{SS}(E_0,Q) & -\Pi_{SP}(E_0,Q)\\ -\Pi_{PS}(E_0,Q) & (ig_P)^{-1}-\Pi_{PP}(E_0,Q)\end{pmatrix}, \tag{5}$$

where the polarization bubble reads

$$\Pi_{\alpha\beta}(E_0,Q)=-\int\frac{dpdp_0}{(2\pi)^2}\frac{p^{l_\alpha+l_\beta}}{2}\times\mathrm{Tr}\left[G^T(p_0,Q/2+p)\alpha G(E_0-p_0,Q/2-p)\beta^\dagger\right], \tag{6}$$

where $\alpha,\beta\in\{S,P\}$ and we have defined $l_S=0$ and $l_P=1$. Tr denotes the trace over the spin degrees of freedom. G is the time-ordered Green's function matrix for fermions defined as $G_{\sigma\sigma'}(\omega,k)=\left\langle\psi_\sigma(\omega,k)\psi^\dagger_{\sigma'}(\omega,k)\right\rangle$. We have

$$[G^{-1}(\omega,k)]_{\sigma\sigma'}=-i[(\omega+i0^+)\delta_{\sigma\sigma'}-(\mathcal{H}^0_k)_{\sigma\sigma'}]. \tag{7}$$

The integral in (5) can be carried out analytically and we present the result with $Q=0$ in the supplementary material [59]. Here, for simplicity, we only present result for small k_0 and Ω:

$$D^{-1}(E_0,0)\approx\begin{pmatrix}-\frac{ma_s}{2}+\frac{m}{2\sqrt{-mE_0}} & \frac{\sqrt{m}k_0\Omega}{8(-E_0)^{3/2}}\\ \frac{\sqrt{m}k_0\Omega}{8(-E_0)^{3/2}} & \frac{m-a_pm\sqrt{-mE_0+k_0^2}}{4a_p}\end{pmatrix}. \tag{8}$$

We have assumed $E_0<0$ and kept terms up to the k_0^2 and Ω order. The result shows all divergence can be absorbed by the renormalization relation (4). Especially, the off-diagonal terms Π_{SP} and Π_{PS} are proportional to $k_0\Omega$ and thus finite, indicating the physics is universal. This is due to a non-trivial SOC, we need both Ω and k_0 to be non-zero. In contrast, for the higher partial-wave systems in higher dimension, additional divergence may appear and new renormalization relations are needed.

Contact matrix. – For a dilute atomic gas system described by (1), we expect universal behaviors governed by two-body physics when we focus on physics at some momentum scale k that satisfies $\Lambda\gg k\gg\max\{k_F,\sqrt{mT}\}$. Here k_F is the Fermi momentum determined from the density of fermions and T is the temperature.

Theoretically, Operator Product Expansion (OPE) is an ideal tool to explore such universal physics [4, 5]. One can expand the product of two operators as

$$\mathcal{O}_i(x+R)\mathcal{O}_j(R)|_{x\to 0}=\sum_n C^k_{ij}(x)\mathcal{O}_k(R), \tag{9}$$

where $\{\mathcal{O}_i\}$ is a set of local operators and $C^k_{ij}(x)$ are expansion functions. After the Fourier transform, this gives the major contribution at large momentum. There is a similar expansion in time direction.

For cold atom system with only $s-$ or $p-$wave interaction, it is known that the leading order contribution is from contact operators $\sim\varphi^\dagger_S(R)\varphi_S(R)$ of $\sim\varphi^\dagger_P(R)\varphi_P(R)$. Intuitively, These contact operators count the effective number of dimers in a many-body system. When we turn on SOC, there is a finite correlation between s- and p-wave dimers. We expect the system should be instead governed by the contact operator matrix:

$$\hat{C}_{\alpha\beta}(R) = m^2 \begin{pmatrix} \varphi_S^\dagger(R)\varphi_S(R) & \varphi_S^\dagger(R)\varphi_P(R) \\ \varphi_P^\dagger(R)\varphi_S(R) & \varphi_P^\dagger(R)\varphi_S(R) \end{pmatrix}_{\alpha\beta}, \quad (10)$$

The contact matrix of the system is then defined as $C_{\alpha\beta} = \int dR \left\langle \hat{C}_{\alpha\beta}(R) \right\rangle$. The idea of a matrix form contact was introduced in [52, 53, 60]. We now derive the universal relations for the momentum distribution and Raman spectral by matching their asymptotic behaviors with contact operators.

Momentum tail. – Physically, we know that SOC should make spin $\uparrow$ and $\downarrow$ different. Hence, we consider the momentum distribution matrix $n_{\sigma'\sigma}(q) = \langle \psi_{q,\sigma}^\dagger \psi_{q,\sigma'} \rangle = \int dx dR e^{-iqx} \langle \psi_\sigma^\dagger(R+x)\psi_{\sigma'}(R) \rangle / L$, where q is the relative momentum. This correspond to consider $\mathcal{O}_i = \psi_\sigma^\dagger$ and $\mathcal{O}_j = \psi_{\sigma'}$ in (9).

To determine the coefficient of OPE, we take the matrix elements for both sides of (9). Usually, one considers both in-coming and out-going states with two fermions. However, in our model (1), two fermions can only interact by firstly combining to dimers and we could equivalently consider a single incoming dimer $|I_{\alpha_i}\rangle = \int dt dR\ e^{i(E_0 t - QR)} \varphi_{\alpha_i}^\dagger(R,t)|0\rangle$ and a single outgoing dimer $\langle O_{\alpha_o}| = \int dt dR\ e^{-i(E_0 t - QR)} \langle 0| \varphi_{\alpha_o}(R,t)$. Here E_0/Q is the total energy/momentum.

We firstly consider the matrix element of the contact operator matrix, which is expected to be the right-hand side of the OPE equation (9). The corresponding digram is shown in Fig. 1(b):

$$\begin{aligned} \frac{C_{\alpha\beta}}{m^2} &= \int dR \langle O_{\alpha_o}| \varphi_\alpha^\dagger(R)\varphi_\beta(R) |I_{\alpha_i}\rangle \\ &= D_{\alpha_o\alpha}(E_0,Q) \times D_{\beta\alpha_i}(E_0,Q). \end{aligned} \quad (11)$$

where E_0 is the total energy, Q is the total momentum. This is to be matched with the matrix element of $\psi_\sigma^\dagger(R+x)\psi_{\sigma'}(R)$. The non-trivial interaction effect comes from the diagram shown in Fig. 1(c). After the Fourier transform, we get the momentum distribution matrix as

$$\begin{aligned} n(q) = &\sum_{\alpha,\beta=S,P} (-i)^2 D_{\alpha_o\alpha}(E_0,Q) D_{\beta\alpha_i}(E_0,Q) \int_{-\infty}^{\infty} \frac{dp_0}{2\pi} \\ &\times q^{l_\alpha + l_\beta} G(E_0-p_0,q)\beta^\dagger G^T(p_0,Q-q)\alpha G(E_0-p_0,q). \end{aligned} \quad (12)$$

Keeping every element up to the first order in the $1/q$ expansion, we have the momentum distribution matrix:

$$n(q) \sim \begin{pmatrix} \frac{C_{PP}}{q^2 L} & \frac{C_{SP}}{q^3 L} \\ \frac{C_{PS}}{q^3 L} & \frac{C_{SS}}{q^4 L} \end{pmatrix}. \quad (13)$$

Recall that the effective Lagrangian (1) is different from that in the laboratory frame by a momentum shift. For sub-leading terms, this momentum shift would modify the coefficient, as in [48, 50]. However, the leading order result (13) is free from such complications. Moreover, note that this derivation here can also be carried out for systems without SOC, which leads to the same result (13). However, in that case, we have $C_{SP} = C_{PS} = 0$ due to the reflection symmetry. The SOC here plays a role of breaking the rotational symmetry and making C_{SP}/C_{PS} finite.

Experimentally, we could measure each components separately and extract their leading-order behaviors. As an example, for the off-diagonal terms, we could measure the momentum of fermions in $|\pm x\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$. This gives

$$n_{++}(q) - n_{--}(q) = n_{\downarrow\uparrow}(q) + n_{\uparrow\downarrow}(q) \sim \frac{C_{PS} + C_{SP}}{q^3 L}.$$

Similarly, measuring in $|\pm y\rangle$ basis gives $C_{PS} - C_{SP}$.

Raman spectroscopy. – The Raman spectroscopy can be used as an important experimental tool in cold atom systems. When the transfer momentum and frequency is large, the Raman spectroscopy can also be related to the contacts. We consider applying a Raman coupling with frequency $\omega > 0$ and momentum k to transfers fermions from the internal spin state $|\sigma\rangle$ ($\sigma = \uparrow, \downarrow$) into a third spin state $|3\rangle$. The Hamiltonian reads $H_c = \sum_\sigma \Omega_\sigma \int dx\ e^{i(kx-\omega t)} \mathcal{O}_{\sigma 3}(x,t) + \text{H.c.}$, where $\mathcal{O}_{\sigma 3}(x,t) \equiv \psi_3^\dagger(x,t)\psi_\sigma(x,t)$. The transition rate function $R(\omega,k)$ to $|3\rangle$ is given by the Fermi golden rule, which is related to the imaginary part of the time-ordered two-point correlation function [61, 62]:

$$R(\omega,k) = 2\pi \sum_{\sigma\sigma'} \Omega_\sigma \Omega_{\sigma'}^* \Gamma_{\sigma\sigma'}^R(\omega,k). \quad (14)$$

$$\begin{aligned} \Gamma_{\sigma\sigma'}^R(\omega,k) = &\frac{1}{\pi} \text{Im} \int dR \int dt\ e^{i\omega t} \int dx\ e^{-ikx} \\ &\times i \left\langle \mathcal{T} \mathcal{O}_{\sigma 3}(R+x,t) \mathcal{O}_{\sigma' 3}^\dagger(R,0) \right\rangle, \end{aligned} \quad (15)$$

where $\mathcal{T}$ is the time-ordering operator. We thus study the OPE of $\mathcal{O}_{\sigma 3}$ and $\mathcal{O}_{\sigma' 3}^\dagger$. The diagram is shown in Fig. 1(d):

$$\begin{aligned} &\Gamma_{\sigma\sigma'}^R(\omega,k) \\ &= \frac{1}{\pi} \text{Im}\ i \sum_{\alpha,\beta=S,P} (-i)^2 D_{\alpha_o\alpha}(E_0,Q) D_{\beta\alpha_i}(E_0,Q) \\ &\int \frac{dp dp_0}{(2\pi)^2} p^{l_\alpha + l_\beta} G_0(E_0 - p_0 + \omega, p+k) \\ &\left[G(E_0-p_0,p)\beta^\dagger G^T(p_0,Q-p)\alpha G(E_0-p_0,p) \right]_{\sigma\sigma'}, \end{aligned} \quad (16)$$

Matching Eq. (16) with Eq. (11), we have the Raman transfer rate in high-frequency and large-momentum

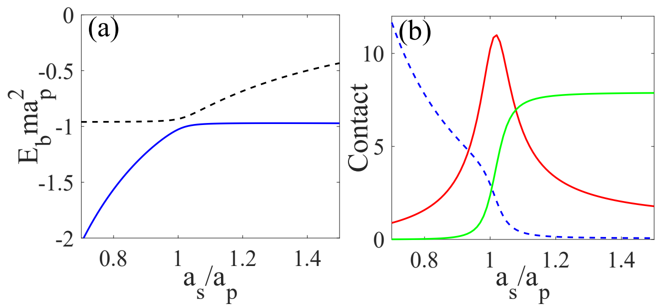

FIG. 2. (a) Dimensionless two-body banding energy versus a_s/a_p. The black dashed curve denotes $E_b^{(+)}ma_p^2$ and the blue solid curve denotes $E_b^{(-)}ma_p^2$. (b) Dimensionless two-body contacts versus a_s/a_p. The red solid curve denotes $C_{SP}a_p^2$, the blue dashed curve denotes $C_{SS}a_p^3$, and the green solid curve denotes $C_{PP}a_p$. Here, we choose the SOC parameters as $k_0a_p = 0.2$ and $m\Omega a_p^2 = 0.3$.

limit:

$$\Gamma^R(\omega, k) = \frac{2m}{\pi\sqrt{4m\omega - k^2}} \times \begin{pmatrix} \frac{2m\omega C_{PP}}{(k^2-2m\omega)^2} & \frac{k\left(k^2-6m\omega\right)C_{SP}}{(k^2-2m\omega)^3} \\ \frac{k\left(k^2-6m\omega\right)C_{PS}}{(k^2-2m\omega)^3} & \frac{2\left[4(m\omega)^2+4k^2m\omega-k^4\right]C_{SS}}{(k^2-2m\omega)^4} \end{pmatrix}. \tag{17}$$

Here we have assumed $\omega > k^2/(4m)$. Taking the limit of $k = 0$ leads to the high-frequency tail of the radio-frequency spectral $\Gamma^{rf}_{\sigma\sigma'}(\omega) = \Gamma^R_{\sigma\sigma'}(\omega, 0)$. This result provides an individual experimental observable to determine different contacts by tuning Ω_σ (14). The Raman spectroscopy, together with the momentum distribution, serves as a non-trivial check for the universal relations in the hybridized system (1).

Other universal relations. – Other universal relations, including the adiabatic relations and thermodynamical relations, are discussed in the supplementary material. Here we only briefly comment on the adiabatic relations. The traditional $s/p-$wave contacts corresponds to the change of energy when varying a_s or $-1/a_p$, which can be seen from taking derivative with g_α in the Lagrangian (1). However, there is no direct $s-$ and $p-$wave dimer mixing in (1) and thus no adiabatic relation for C_{SP} or C_{PS}. On the other hand, we could consider a non-spherical potential between atoms where microscopic mixing terms $\delta_{SP}\varphi^\dagger_{Q,S}\varphi_{Q,P}$ + H.c. exist in the action. In this case, the off-diagonal components of the contact matrix correspond to varying δ_{SP}.

Contacts in two-body bound states. – To give an explicit example of contact matrix in the hybridized s- and $p-$wave system, we now perform a calculation for the two-body bound state. Generally, the binding energy E_b with momentum Q is given by solving $\det(D^{-1}(E_0, Q)) = 0$. We consider the case with small SOC strength where we could use (8).

We focus on $Q = 0$ with both $a_s > 0$ and $a_p > 0$. For $\Omega = 0$, there is both an s-wave bound state with binding energy $E_b^{(s)} = -1/(ma_s^2)$ and a p-wave bound state with binding energy $E_b^{(p)} = -1/(ma_p^2) + k_0^2/m$. Here the presence of k_0 is because $Q = 0$ corresponds to a center-of-mass momentum $2k_0$ for the p-wave bound state in the laboratory frame. When we turn on finite but small Ω, the binding energies receive important correction only near the resonance with $1/(a_s^0)^2 = 1/(a_p^0)^2 - k_0^2$. We then approximate

$$D^{-1}(E_b, 0) \approx \begin{pmatrix} I_1\left(E_b - E_b^{(s)}\right) & K_\Omega \\ K_\Omega & I_2\left(E_b - E_b^{(p)}\right) \end{pmatrix}. \tag{18}$$

with $I_1 = \frac{m^2a_s^3}{4}$, $I_2 = \frac{m^2a_p}{8}$ and $K_\Omega = \frac{k_0\Omega m^2(a_s^0)^3}{8}$. Then the binding energy can be derived as

$$2E_b^{(\pm)} = E_b^{(p)} + E_b^{(s)} \pm \sqrt{(E_b^{(p)})^2 - 2E_b^{(p)}E_b^{(s)} + (E_b^{(s)})^2 + \frac{4K_\Omega^2}{I_1I_2}}. \tag{19}$$

The contacts C_{SS} and C_{PP} can be derived by taking derivation with a_s or $-1/a_p$. To calculate C_{SP} or C_{PS}, we apply the trick by adding the additional δ_{SP} terms, and set them to be zero after taking derivatives.

The explicit formula for all contacts are given in the supplementary material. A plot for $E_b^{(\pm)}$ and contacts for $E_b^{(-)}$ are shown in Fig. 2. Away from the degenerate point, $E_b^{(\pm)}$ approaches $E_b^{(s)}$ or $E_b^{(p)}$. Consequently, for the diagonal components of the contact matrix, we have $C_{SS} \approx 0$ for $a_s/a_p \gg 1$ and $C_{PP} \approx 0$ for $a_s/a_p \ll 1$. Near the degenerate point $a_s/a_p \sim 1$, we see a peak for C_{SP}, indicating a large mixing between s- and $p-$wave dimers as expected.

Discussions. – In this work, we have derived the momentum tail and the Raman spectroscopy for hybridized s- and p-wave interactions from spin-orbital coupling in 1D. We find new contacts appear at the leading order of certain observables due to the mixing between different partial waves.

We finally comment on the generalization to higher-dimensional systems with 1D (NIST) SOC. In higher dimensions, firstly, we have the additional quantum number $m = -1, 0, 1$ in 3D or $m = \pm 1$ in 2D for p-wave dimers. Depending on whether their resonance split, we may have a larger contact matrix. To the leading order, the off-diagonal components of the momentum distribution should again correspond to the off-diagonal contacts and should be proportional to $1/q^3$. On the contrary, the scaling of Raman spectral would change (by a factor of $\sim \omega^{(D-1)/2}$ for large ω), due to the difference of the density of state.

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