Supplementary Material for: "Realization of metallic state in 1T-TaS_2 with persisting long-range coherence of charge density wave"

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Here, we show the details of the cluster perturbation theory for the theoretical calculations of the single-particle spectral weight in the main text.

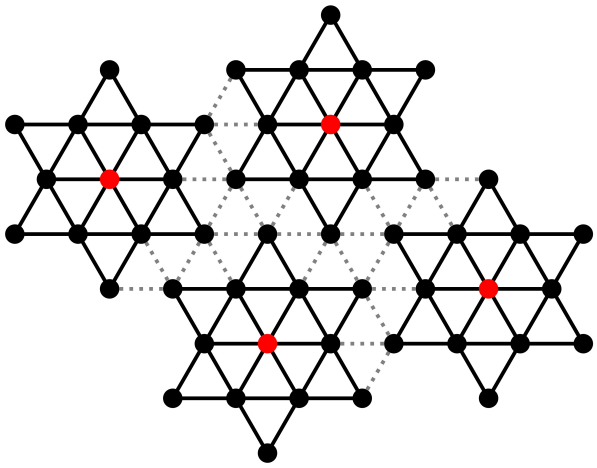

FIG. 1. Tiling of the triangular lattice with 13-site clusters. The nearest-neighbor hoppings within a cluster are represented by solid lines, and intercluster hoppings by dashed lines. Here, each site represents a David star in 1T-TaS_2, and the red sites are the David stars where the K^+ cations are located in the theoretical calculations.

In the main text, the computational technique for our calculation of the single-particle spectral weight $A_i(\omega)$ on site i is based on the cluster perturbation theory (CPT), which has been successfully applied to many strongly correlated systems [1–7]. As shown in Fig. 1, in the CPT calculations, we divide the original lattice into identical 13-site clusters which constitute a superlattice. Then, the lattice Hamiltonian is written as

$$H = H' + V, \tag{1}$$

where H' is the cluster Hamiltonian, obtained by severing the hopping terms between different clusters, and V contains the intercluster hoppings. The CPT method is based on a strong-coupling perturbation expansion of the one-body operators V linking the individual clusters[1]. At the lowest order of this expansion, the Green's function $\boldsymbol{G}$ of the original lattice can be expressed (in matrix form) as

$$\boldsymbol{G}(\tilde{\boldsymbol{k}},\omega) = \boldsymbol{G}'(\omega)[1 - \boldsymbol{V}(\tilde{\boldsymbol{k}})\boldsymbol{G}'(\omega)]^{-1}, \tag{2}$$

where $\boldsymbol{G}'$ is the cluster Green's function, and $\tilde{\boldsymbol{k}}$ is the wavevector in the Brillouin zone (BZ) of the superlattice. $\boldsymbol{G}'$ is independent of $\tilde{\boldsymbol{k}}$, while $\boldsymbol{V}$ is frequency independent. The cluster Green's function $\boldsymbol{G}'$ is calculated by the exact diagonalization method with the Lanczos algorithm, and it has the following expression,

$$\begin{aligned} G'_{\mu\nu}(\omega) = &\langle 0|c_\mu \frac{1}{\omega - H + E_0 + i\eta} c_\nu^\dagger|0\rangle \\ &+ \langle 0|c_\nu^\dagger \frac{1}{\omega + H - E_0 + i\eta} c_\mu|0\rangle, \end{aligned} \tag{3}$$

where E_0 is the energy of the ground state $|0\rangle$, and η is a small real number introduced in the calculation to shift the poles of the Green's function away from the real axis. Here, μ and ν denote both the site and spin degrees of freedom in a cluster. The spectral function of the local single-particle excitation is given by

$$A_{\mu\mu}(\omega) = -\frac{1}{\pi}\sum_{\tilde{\boldsymbol{k}}} G_{\mu\mu}(\tilde{\boldsymbol{k}},\omega). \tag{4}$$

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