Supplemental Material: Effect of impurity on the doping-induced in-gap states in a Mott insulator

Cheng-Ping He,[1] Shun-Li Yu,[1,2] Tao Xiang,[3,4,5,*] and Jian-Xin Li[1,2,†]

[1]*National Laboratory of Solid State Microstructures and School of Physics, Nanjing University, Nanjing 210093, China*
[2]*Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*
[3]*Institute of Physics, National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing,*
[4]*Department of Physics, University of Chinese Academy of Sciences, Beijing 100190, China*
[5]*Beijing Academy of Quantum Information Sciences, Beijing 100193, China*

I. CALCULATION METHOD BASED ON THE CLUSTER PERTURBATION THEORY

We use the cluster perturbation theory (CPT) to carry out the calculations. The CPT is an approximation method based on the exact diagonalization of finite clusters and treating the intercluster coupling as a perturbation [1–9]. Hence, it can treat much larger lattice systems than the exact diagonalization, which is important for our detailed spectral analysis. In CPT, the whole system is divided into identical clusters which constitute a superlattice (see Fig. S1), so the Hamiltonian is rewritten as,

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

where H' is the cluster Hamiltonian obtained by cutting the hopping terms between different clusters, and V contains the inter-cluster hopping terms. In the superlattice, the site i in the original lattice is represented by two new indices (c,α), where c is the index of the cluster and α labels the site in each cluster. By using the Lanczos exact diagonalization technique, the Green's function $\boldsymbol{G}'^{c}$ for the cluster c can be calculated from its definition

$$\begin{aligned} G'^{c}_{\alpha\sigma,\beta\sigma'}(\omega) = &\langle\Omega^c| c^{c}_{\alpha\sigma} \frac{1}{\omega - H'_c + E^c_0 + i\eta} c^{c\dagger}_{\beta\sigma'} |\Omega^c\rangle \\ &+ \langle\Omega^c| c^{c\dagger}_{\alpha\sigma} \frac{1}{\omega - H'_c - E^c_0 + i\eta} c^{c}_{\beta\sigma'} |\Omega^c\rangle, \end{aligned} \tag{2}$$

where E^c_0 is the energy of the ground state $|\Omega^c\rangle$ and η is the Lorentzian broadening. The Green's function $\boldsymbol{G}_{cpt}(\omega)$ for the whole system is calculated from

$$\boldsymbol{G}^{-1}_{cpt}(\omega) = \boldsymbol{G}'^{-1}(\omega) - \boldsymbol{V}. \tag{3}$$

Here, $\boldsymbol{G}_{cpt}(\omega)$, $\boldsymbol{G}'(\omega)$ and $\boldsymbol{V}$ are $2N_s \times 2N_s$ matrices, where $N_s = N_c \times N$ is the number of the whole lattice sites with N_c the number of clusters and N the number of sites in each cluster. In Eq. (3), $\boldsymbol{G}'(\omega)$ and $\boldsymbol{V}$ are defined by

$$G'_{c\alpha\sigma,c'\beta\sigma'}(\omega) = \delta_{cc'} G'^{c}_{\alpha\sigma,\beta\sigma'}(\omega) \tag{4}$$

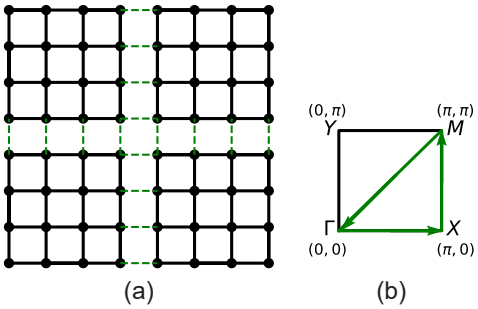

FIG. S1. (Color on line) (a) Tiling of the square lattice with 16-sites, the inter-cluster hopping terms denoted by the green dashed lines are treated as perturbations in CPT. (b) Path in the momentum space along which we present our results for the two-dimensional system in the main text.

and

$$V_{c\alpha\sigma,c'\beta\sigma'} = -t\delta_{c\neq c'}\delta_{\langle c\alpha,c'\beta\rangle}\delta_{\sigma\sigma'}, \tag{5}$$

where $\langle c\alpha, c'\beta\rangle$ means that (c,α) and (c',β) are two inter-cluster nearest-neighbor sites. The local density of states (LDOS) at the site $i = (c,\alpha)$ is given by

$$A_i(\omega) = -\frac{1}{\pi}\sum_{\sigma} \mathrm{Im} G_{cpt,i\sigma,i\sigma}(\omega). \tag{6}$$

In order to obtain the momentum-space spectral function, we transfer $\boldsymbol{V}$ from the real space into the momentum space to get a $2N \times 2N$ matrix $\boldsymbol{V}(\tilde{k})$ with $\tilde{k}$ the momentum in the first Brillouin zone of the superlattice, and the Green's function of the superlattice is given by

$$\boldsymbol{G}^{-1}_{cpt}(\omega,\tilde{\boldsymbol{k}}) = \boldsymbol{G}'^{c-1}(\omega) - \boldsymbol{V}(\tilde{\boldsymbol{k}}). \tag{7}$$

The Green's function of the original lattice can be calculated by a periodization procedure

$$G_{\sigma,\sigma'}(\omega,\boldsymbol{k}) = \frac{1}{N}\sum_{\alpha,\beta}[G_{cpt}]_{\alpha\sigma,\beta\sigma'}(\omega,\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta)}, \tag{8}$$

where $\boldsymbol{k}$ is the momentum in the original first Brillouin zone.

* txiang@iphy.ac.cn
† jxli@nju.edu.cn

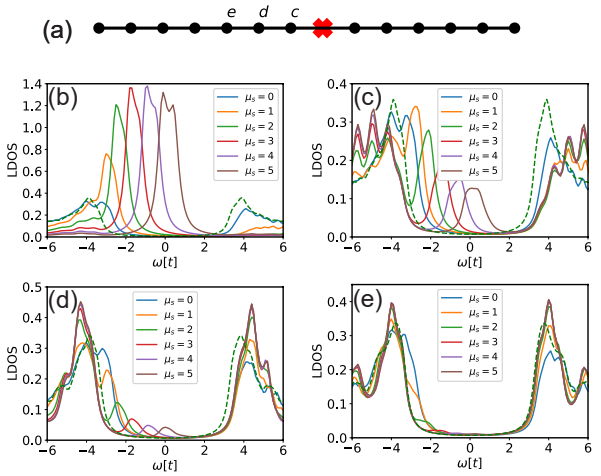

FIG. S2. (a) A 14-site cluster with an impurity at the red cross site. (b)-(e) LDOS at impurity site (b) and the sites with the same labels in (a) for different impurity potential μ_s.

Then, the momentum-space spectral function is given by

$$A(\omega, \boldsymbol{k}) = -\frac{1}{\pi} \sum_{\sigma} \mathrm{Im} G_{\sigma,\sigma}(\omega, \boldsymbol{k}). \tag{9}$$

II. LDOS IN THE ONE-DIMENSIONAL HUBBARD MODEL WITH ONE IMPURITY

In Fig.S2, we show the local density of states of in-gap states in a one-dimensional Hubbard model calculated using the cluster perturbation theory.

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