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Spin, Charge, and math xmlns="http://www.w3.org/1998/Math/MathML" display="inline">mi>η/mi>/math>-Spin Separation in One-Dimensional Photodoped Mott Insulators

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## Spin, charge and $\eta$ -spin separation in one-dimensional photo-doped Mott insulators

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We show that effectively cold metastable states in one-dimensional photo-doped Mott insulators described by the extended Hubbard model exhibit spin, charge and  $\eta$ -spin separation. Namely, their wave functions in the large on-site Coulomb interaction limit can be expressed as  $|\Psi\rangle = |\Psi_{\text{charge}}\rangle|\Psi_{\eta-\text{spin}}\rangle$ , which is analogous to the Ogata-Shiba states of the doped Hubbard model in equilibrium. Here, the  $\eta$ -spin represents the type of photo-generated pseudoparticle (doublon or holon).  $|\Psi_{\text{charge}}\rangle$  is determined by spinless free fermions,  $|\Psi_{\text{spin}}\rangle$  by the isotropic Heisenberg model in the squeezed spin space, and  $|\Psi_{\eta-\text{spin}}\rangle$  by the XXZ model in the squeezed  $\eta$ -spin space. In particular, the metastable  $\eta$ -pairing and charge-density-wave (CDW) states correspond to the gapless and gapful states of the XXZ model. The specific form of the wave function allows us to accurately determine the exponents of correlation functions. The form also suggests that the central charge of the  $\eta$ -pairing state is 3 and that of the CDW phase is 2, which we numerically confirm. Our study provides analytic and intuitive insights into the correlations between active degrees of freedom in photo-doped strongly correlated systems.

Introduction-Doping charge carriers into strongly correlated insulators provides a pathway to produce intriguing emergent phenomena such as high- $T_c$  superconductivity [1, 2]. In equilibrium, the doping concentration can be chemically controlled. An alternative nonequilibrium way of introducing charge carriers is *photo-doping*, where electrons are excited across the gap [3-7]. The photo-doping of Mott insulators creates novel pseudoparticle excitations such as doublons and holons (in the single-band case), while the equilibrium system can host only one type of charge carrier. Such additional degrees of freedom can lead to intriguing properties and nonthermal phases. Important examples include photoinduced insulator-metal transitions [8-13] and charge density waves [14–16], and the control of magnetic [17, 18] and superconducting orders [19-26].

In systems with a large Mott gap, the life-time of the photo-doped pseudoparticles becomes exponentially enhanced [27–33]. In such a situation, an intraband cooling of the photo-doped pseudoparticles may occur, while their density remains approximately constant. This results in a metastable steady state (a pseudoequilibrium state) [19, 34–41], analogous to the case of photo-doped semiconductors [42-44], see Fig. 1(a). It has been shown that such metastable states can host unique phases such as  $\eta$ -pairing [38, 40], chiral superconducting phases [45], and exotic spin/orbital orders [18, 39, 46]. Since different types of charge carriers are present in photo-doped systems, it is crucial to understand the correlations between the active degrees of freedoms. However, the metastable states of photo-doped strongly correlated systems have been mainly studied numerically so far [34-41, 47], and analytical or intuitive insights are limited.

Here we reveal the nature of the metastable states and the correlations between the active degrees of freedom in photo-doped one-dimensional Mott insulators. We show that the wave functions of the metastable states in the limit of large on-site Coulomb interaction exhibit spin, charge and  $\eta$ -spin separation, see Fig. 1(b). The  $\eta$ -spin represents the type of pseudoparticle: doubly occupied site (doublon) or empty site (holon). Our results provide a comprehensive understanding of the character of the photo-induced metastable phases in one-dimensional systems and reveal the similarities and differences between photo-doped and chemically-doped systems.

*Results*– We focus on the one-dimensional extended Hubbard model,

$$\hat{H} = -t_{\rm hop} \sum_{i,\sigma} (\hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i+1,\sigma} + h.c.) + \hat{H}_U + \hat{H}_V, \qquad (1)$$

and assume that electrons are excited across the Mott gap via photo-excitation. Similar setups can be considered with cold atoms [19].  $\hat{H}_U = U \sum_i (\hat{n}_{i\uparrow} - \frac{1}{2})(\hat{n}_{i\downarrow} - \frac{1}{2})$  is the on-site interaction and  $\hat{H}_V = V \sum_i (\hat{n}_i - 1)(\hat{n}_{i+1} - 1)$ is the nearest-neighbor interaction.  $\hat{c}_{i\sigma}^{\dagger}$  is the creation operator of a fermion with spin  $\sigma$  at site i,  $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$ ,  $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ , and  $t_{hop}$  is the hopping parameter. When the Mott gap is large enough, the recombination time of the created doublons and holons becomes exponentially long [27–32]. Thus, intraband relaxation due to scattering events and coupling to the environment is expected to bring the system into a (intraband thermalized) steady state with a fixed number of doublons and holons, see

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FIG. 1. (a) Schematic picture of the photo-doing and intraband cooling processes that result in a metastable state of the large-gap Mott insulator. UHB (LHB) stands for upper (lower) Hubbard band. (b) The wave function of the metastable state in the limit of  $U \rightarrow \infty$  can be expressed as a direct product of the charge wave function, the spin wave function in the squeezed space and the  $\eta$ -spin wave function in the squeezed space. The green shaded circles in the charge wave function represent spinless fermions, while "h" and "d" stand for a holon and a doublon, respectively.

Fig. 1(a). As previously discussed, such a quasi-steady state can be described with the effective Hamiltonian obtained by a Schrieffer-Wolff transformation [48] from the original Hamiltonian (1) [19, 34–40, 47], see also the Supplemental Material (SM) [49]. This effective Hamiltonian explicitly conserves the number of doublons and holons. Up to  $\mathcal{O}(t_{hop}^2/U)$ , it takes the form

$$\hat{H}_{\text{eff}} = \hat{H}_U + \hat{H}_{\text{kin}} + \hat{H}_V + \hat{H}_{\text{spin,ex}} + \hat{H}_{\text{dh,ex}} + \hat{H}_{U,\text{shift}} + \hat{H}_{3-\text{site}}, \quad (2)$$

where  $\hat{H}_{\rm kin} = -t_{\rm hop} \sum_{\langle i,j \rangle,\sigma} \hat{\bar{n}}_{i,\bar{\sigma}} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.)\hat{\bar{n}}_{j,\bar{\sigma}} - t_{\rm hop} \sum_{\langle i,j \rangle,\sigma} \hat{n}_{i,\bar{\sigma}} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.)\hat{n}_{j,\bar{\sigma}}$  represents the hopping of a doublon or a holon,  $\bar{\sigma}$  is the opposite spin of  $\sigma$ , and  $\hat{\bar{n}}_{i,\sigma} = 1 - \hat{n}_{i,\sigma}$ . The other terms are proportional to  $J_{\rm ex} \equiv \frac{4t_{\rm hop}^2}{U}$ .  $\hat{H}_{\rm spin,ex} = J_{\rm ex} \sum_{\langle i,j \rangle} \hat{s}_i \cdot \hat{s}_j$  is the spin exchange term, and  $\hat{H}_{\rm dh,ex} = -J_{\rm ex} \sum_{\langle i,j \rangle} [\hat{\eta}_i^x \hat{\eta}_j^x + \hat{\eta}_i^y \hat{\eta}_j^y + \hat{\eta}_i^z \hat{\eta}_j^z]$  is the exchange term for doublons and holons on neighboring sites. Here the spin operators are  $\hat{\mathbf{s}} = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} \hat{c}^{\dagger}_{\alpha} \sigma_{\alpha\beta} \hat{c}_{\beta}$  with  $\sigma$  denoting the Pauli matrices, and we introduced the  $\eta$ -spin operators as  $\hat{\eta}_i^+ = (-)^i \hat{c}_{i\downarrow}^{\dagger} \hat{c}_{i\uparrow}^{\dagger}, \hat{\eta}_i^- = (-)^i \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}$  and  $\hat{\eta}_i^z = \frac{1}{2} (\hat{n}_i - 1)$  [50–52].  $\hat{H}_{U,\text{shift}}$  describes the shift of the local interaction and  $\hat{H}_{3-\text{site}}$  represents three-site terms such as correlated doublon hoppings, see SM [49]. In equilibrium (without

doublons), the model corresponds to the *t-J* model when  $\hat{H}_{3-\text{site}}$  is neglected [53]. In the following, we denote the model without  $\hat{H}_{3-\text{site}}$  by  $\hat{H}_{\text{eff2}}$ . When V = 0,  $\hat{H}$ ,  $\hat{H}_{\text{eff}}$  and  $\hat{H}_{\text{eff2}}$  host an SU(2) symmetry of the doublon-holon sector [50, 54] that corresponds to the spin SU(2) symmetry via a particle-hole (Shiba) transformation [55].

We consider an effectively cold system with arbitrary filling, whose state is described by the ground state of the effective Hamiltonian for a given number of doublons and holons, i.e., we assume that the system is thermalized into the lowest energy state for the given constraint. We show that the corresponding wave function can be expressed as the direct product of the charge, spin and  $\eta$ -spin wave functions in the limit of  $J_{\rm ex} \to 0$ with  $V/J_{\rm ex} = \text{const}$ , similar to the Ogata-Shiba state of the doped Hubbard model in equilibrium [56, 57]. To be more specific, we set the system size to L and the number of singly occupied sites to  $N_s$ , so that the number of doublons and holons (the number of  $\eta$  spins) is  $N_{\eta} = L - N_s$ . Now we introduce the Hilbert space

$$\mathcal{H}' = \left\{ |\mathbf{r}\rangle |\boldsymbol{\sigma}\rangle |\boldsymbol{\eta}\rangle \equiv \left(\prod_{r \in \mathbf{r}} \hat{c}_r^{\dagger}\right) |\mathrm{vac}\rangle |\boldsymbol{\sigma}\rangle |\boldsymbol{\eta}\rangle$$
$$: \#\mathbf{r} = \#\boldsymbol{\sigma} = N_s \text{ and } \#\boldsymbol{\eta} = N_{\eta} \right\}.$$
(3)

Here  $\mathbf{r}, \boldsymbol{\sigma}$  and  $\boldsymbol{\eta}$  are sets of space, spin and  $\eta$ -spin indices,  $\hat{c}_r^{\dagger}$  is a creation operator of a spin-less fermion (SF), and # indicates the number of elements.  $\eta$  takes the values  $\uparrow$  or  $\downarrow$  and  $\mathbf{r} = \{r_{N_s}, \cdots, r_1\}$  with  $L \geq r_{N_s} > r_{N_s-1} > \cdots > r_1 \geq 1$ . We identify this Hilbert space with the original Hilbert space using the unitary transformation  $\hat{U}: \mathcal{H} \to \mathcal{H}'$  defined by

$$\hat{U}\left(\left(\prod_{i=1}^{N_s} \hat{c}^{\dagger}_{r_i,\sigma_i}\right) \left(\prod_{j=1}^{N_{\eta}} \hat{a}^{\dagger}_{\bar{r}_j,\eta_j}\right) |\text{vac}\rangle\right) = \left(\prod_{r \in \mathbf{r}} \hat{c}^{\dagger}_r\right) |\text{vac}\rangle |\boldsymbol{\sigma}\rangle |\boldsymbol{\eta}\rangle.$$
(4)

Here,  $\bar{\mathbf{r}} = \{\bar{r}_{N_{\eta}}, \cdots \bar{r}_{1}\}$  with  $L \geq \bar{r}_{N_{\eta}} > \bar{r}_{N_{\eta}-1} > \cdots > \bar{r}_{1} \geq 1$ ,  $\mathbf{r} \cup \bar{\mathbf{r}} = \{L, L-1, \cdots, 1\}$ ,  $\hat{a}^{\dagger}_{\bar{r},\uparrow} = (-)^{\bar{r}} \hat{c}^{\dagger}_{\bar{r}\downarrow} \hat{c}^{\dagger}_{\bar{r}\uparrow}$  and  $\hat{a}^{\dagger}_{\bar{r},\downarrow} = 1$ . With this identification,  $|\mathbf{r}\rangle$  is the basis of SF and  $|\boldsymbol{\sigma}\rangle (|\boldsymbol{\eta}\rangle)$  is the basis of the squeezed spin  $(\eta$ -spin) space. Note that the  $\eta$ -spin configuration represents the sequence of doublons and holons. As shown below, Hamiltonians ruling the  $\sigma$  and  $\eta$  spaces are not fully symmetric due to the staggering of the doublons.

The wave function in the limit of  $J_{\text{ex}} \to 0$  can be constructed by degenerate perturbation theory [57]. For  $J_{\text{ex}} = V = 0$ , the eigenstates of  $\hat{H}_{\text{eff}}$  are degenerate with respect to the configurations of spins and  $\eta$ -spins. This is because  $\hat{H}_{\text{kin}}$  never exchanges the positions of spins or those of doulons and holons. Specifically, one can show that  $\hat{U}\hat{H}_{\text{kin}}\hat{U}^{\dagger} = -t_{\text{hop}}\sum_{\langle i,j \rangle} (\hat{c}_{i}^{\dagger}\hat{c}_{j} + \text{h.c.}) ~(\equiv \hat{H}_{0,\text{SF}})$ . This means that in the representation of  $\mathcal{H}'$  the ground state for  $J_{\text{ex}} = V = 0$  can be described as  $|\Psi_{\text{SF}}^{\text{GS}}\rangle|\Psi_{\sigma,\eta}\rangle$ , where  $|\Psi_{\rm SF}^{\rm GS}\rangle$  is the ground state of  $\hat{H}_{0,\rm SF}$  and  $|\Psi_{\sigma,\eta}\rangle$  is an arbitrary spin and  $\eta$ -spin wave function. The remaining spin/ $\eta$ -spin degeneracy of  $2^{N_s} \cdot 2^{N_\eta}$  is lifted by the terms of  $\mathcal{O}(J_{\rm ex})$ . Within lowest-order degenerate perturbation theory, the wave function of the spin and  $\eta$ -spin is obtained by the  $\mathcal{O}(J_{\rm ex})$  terms projected to  $|\Psi_{\rm SF}^{\rm GS}\rangle|\boldsymbol{\sigma}\rangle|\boldsymbol{\eta}\rangle$ . In the resultant projected Hamiltonian, the squeezed spin and  $\eta$ -spin spaces are decoupled, and the corresponding Hamiltonians become (SQ stands for squeezed space)

$$\begin{split} \hat{H}_{\rm spin}^{\rm (SQ)} &= J_{\rm ex}^s \sum_i \hat{\mathbf{s}}_{i+1} \cdot \hat{\mathbf{s}}_i, \\ \hat{H}_{\eta-{\rm spin}}^{\rm (SQ)} &= -J_X^\eta \sum_j (\hat{\eta}_{j+1}^x \hat{\eta}_j^x + \hat{\eta}_{j+1}^y \hat{\eta}_j^y) + J_Z^\eta \sum_j \hat{\eta}_{j+1}^z \hat{\eta}_j^z, \end{split}$$

with  $J_{\text{ex}}^{\text{s}} = (\tilde{x} - \tilde{x}')J_{\text{ex}}$ ,  $J_{\chi}^{\eta} = (\tilde{y} - \tilde{y}')J_{\text{ex}}$  and  $J_{Z}^{\eta} = -(\tilde{y} - \tilde{y}')J_{\text{ex}} + 4\tilde{y}V$ . Here  $\tilde{x}, \tilde{x}', \tilde{y}$  and  $\tilde{y}'$  are the renormalization factors determined by  $|\Psi_{\text{SF}}^{\text{GS}}\rangle$ . With  $n_s = N_s/L$  and  $n_\eta = N_\eta/L$  and in the limit  $L \to \infty$  they can be expressed as

$$\tilde{x} = n_s - \frac{\sin^2(\pi n_s)}{\pi^2 n_s}, \ \tilde{x}' = \frac{\sin(2\pi n_s)}{2\pi} - \frac{\sin^2(\pi n_s)}{\pi^2 n_s}, \tilde{y} = n_\eta - \frac{\sin^2(\pi n_\eta)}{\pi^2 n_\eta}, \ \tilde{y}' = \frac{\sin(2\pi n_\eta)}{2\pi} - \frac{\sin^2(\pi n_\eta)}{\pi^2 n_\eta}.$$

Here  $\tilde{x}$  and  $\tilde{y}$  are the contributions from the 2-site terms of  $\mathcal{O}(J_{\text{ex}})$ , while  $\tilde{x}'$  and  $\tilde{y}'$  are those from the 3-site terms. Note that  $\hat{H}_{\eta-\text{spin}}^{(\text{SQ})}$  becomes the ferromagnetic Heisenberg model  $(J_X^{\eta} = -J_Z^{\eta} > 0)$  for V = 0. Thus, the wave function (in  $\mathcal{H}'$ ) takes the form

$$|\Psi\rangle = |\Psi_{\rm SF}^{\rm GS}\rangle |\Psi_{\sigma}^{\rm GS}\rangle |\Psi_{\eta}^{\rm GS}\rangle, \qquad (5)$$

where  $|\Psi_{\sigma}^{\text{GS}}\rangle$  is the ground state of  $\hat{H}_{\text{spin}}^{(\text{SQ})}$  and  $|\Psi_{\eta}^{\text{GS}}\rangle$  is that of  $\hat{H}_{\eta-\text{spin}}^{(\text{SQ})}$ . For more details, see SM [49]. The form of  $|\Psi_{\text{SF}}^{\text{GS}}\rangle$  and  $|\Psi_{\sigma}^{\text{GS}}\rangle$  is independent of the ratio of doublons and holons, and, in particular, these states are the same as those in the equilibrium doped Hubbard model at the doping level  $n_{\text{holes}} = n_{\eta}$  [56, 57]. This implies that the effects of photo-doping and chemical doping on the spins are essentially the same, which is consistent with previous numerical analyses [40, 58, 59].

Now we focus on half filling and discuss the implications of the exact form of the wave function for the origin of the different phases. The  $\eta$ -spin sector hosts the phase transition between the gapless and gapful phases of the XXZ model, which is controlled by the ratio between  $J_{\text{ex}}$  and V. As seen below, these states are characterized by the behavior of the correlation functions of the  $\eta$ -spins, i.e.  $\chi_{\eta,a}(r) \equiv \langle \hat{\eta}^a(r) \hat{\eta}^a(0) \rangle$ . Namely, the gapless phase corresponds to the  $\eta$ -pairing phase, where the pair correlation  $\chi_{\eta-\text{pair}} \equiv \chi_{\eta,x}$  is dominant. On the other hand, the gapful phase corresponds to the CDW phase, where the charge correlation  $\chi_{\text{charge}} \equiv \chi_{\eta,z}$  is dominant. True long-range order (LRO) is realized at V = 0 for



FIG. 2. Phase diagram of the photo-doped one-dimensional Mott insulator described by  $\hat{H}_{\rm eff}$  in the limit  $J_{\rm ex} \to 0$ . The phase boundary (black solid line) corresponds to an SU(2) symmetric point of  $\hat{H}_{\eta-{\rm spin}}^{\rm (SQ)}$ , i.e.  $V/J_{\rm ex} = \frac{\tilde{y}-\tilde{y}'}{2\tilde{y}}$ . The horizontal dashed line indicates the phase boundary for the system described by  $\hat{H}_{\rm eff2}$ .

the  $\eta$ -pairing phase [60], while a LRO CDW is realized at  $n_{\eta} = 1$  and  $V > \frac{J_{ex}}{2}$ . Apart from these limits, we have quasi-long-range orders (power law decay of correlations). Note that the appearance of  $\eta$ -pairing in nonthermal states has been recently discussed [22, 26, 38, 61–63] in relation with the photo-induced superconducting-like phases [20, 64-67]. Furthermore, we emphasize that LRO is realized in the squeezed  $\eta$ -spin space for the CDW phase, which is reminiscent of the string order in the Haldane phase [68]. The phase transition occurs at the SU(2) point of  $\hat{H}_{\eta-\text{spin}}^{(SQ)}$   $(J_X^{\eta} = J_Z^{\eta} > 0)$ , see Fig. 2. For  $\hat{H}_{eff2}$  (without  $\hat{H}_{3-site}$ ),  $\Delta (\equiv J_Z^{\eta}/J_X^{\eta})$  and thus the phase boundary are independent of the filling, which consistently explains a previous numerical result [40]. On the other hand, for  $H_{\text{eff}}$ , the ratio  $\Delta$  depends on the filling due to the effects of the 3-site term  $\tilde{y}'$ . In particular, the 3-site term is found to favor the  $\eta$ -pairing phase.

The exact form of the wave function allows us to evaluate the asymptotic behavior of the correlation functions analytically or numerically. Here we extend the analyses for spin correlations of the equilibrium Hubbard model [69, 70]. Since the spin correlations of the metastable state are the same as those for the equilibrium Hubbard model, i.e.  $\langle \hat{s}^a(r) \hat{s}^a(0) \rangle \propto$  $\cos(\pi n_s r) r^{-\frac{3}{2}} (\ln r)^{\frac{1}{2}}$ , we focus on the  $\eta$ -spin correlation functions  $\chi_{\eta,a}(r)$ . Note that despite the apparent similarity between the squeezed spin and  $\eta$  space there are crucial differences in the pairing correlations. Using expression (5), the correlation functions are expressed as

$$\chi_{\eta,a}(r) = \sum_{m=2}^{r+1} \bar{Q}_{\rm SF}^r(m) \chi_{\eta,a}^{\rm (SQ)}(m-1).$$
 (6)

Here  $\bar{Q}_{\rm SF}^r(m) = \langle \hat{n}_0 \hat{n}_r \delta(\sum_{l=0}^r \hat{n}_l - m) \rangle_{\rm SF}$ , which is determined by  $|\Psi_{\rm SF}^{\rm GS}\rangle$ , is the probability that the system has *m* doublons or holons in [0, r].  $\chi_{\eta, a}^{({\rm SQ})}(m) = \langle \hat{\eta}^a(m) \hat{\eta}^a(0) \rangle_{\eta-{\rm spin},{\rm squeezed}}$  is the correlation function in



FIG. 3. (a)(b) Asymptotic behavior analytically obtained for (a)  $\chi_{charge}$  and (b)  $\chi_{\eta-pair}$ . The dashed line at  $\Delta = \frac{1}{2}$ in (a) is the boundary of different expressions. The thick green line corresponds to the SDW, the thick blue line to the CDW with LRO and the thick red line to the  $\eta$ -pairing phase with LRO. (c)(d) Numerically evaluated correlation functions for (c) the  $\eta$ -pairing phase and (d) the CDW phase using Eq. (6) and the iTEBD results for the XXZ model (blue circles). The corresponding points are indicated with crosses in panels (a)(b). We also show the correlations estimated by the conjecture  $\chi_{\eta-pair} \simeq n_{\eta}^2 \chi_{\eta}^{(SQ)}(rn_{\eta})$  as well as the fit with  $C_1 r^{-2} + C_2 r^{-\frac{1}{2} - \frac{1}{\alpha}} \cos(\pi n_{\eta} r)$ .

the squeezed  $\eta$ -spin space. Numerically,  $\bar{Q}_{\rm SF}^r(m)$  and  $\chi_{\eta,a}^{(SQ)}(m)$  can be efficiently evaluated in the thermodynamic limit. We use the expression for the Fourier components and perform an inverse Fourier transformation to obtain  $Q_{\rm SF}^r(m)$  [49, 70], while the infinite time-evolving block decimation (iTEBD) [71] for the XXZ model can be used to calculate  $\chi_{\eta,a}^{(SQ)}(m)$ . Moreover, we can also gain analytic insights using the knowledge of the asymptotic behavior of the correlation functions of the XXZ model [72–74] and the moments of  $\bar{Q}_{\rm SF}^r(m)$  up to the second one [69]. The former can be expressed with  $\alpha \equiv 1 - \frac{1}{\pi} \arccos(\Delta)$ , which is a control parameter of the Tomonaga-Luttinger liquid, and the latter indicates that most of the weight of  $\bar{Q}_{\rm SF}^r(m)$  is at  $rn_{\eta}$ . From these facts, if the asymptotic form of  $\chi_{\eta}^{(SQ)}(m)$  is  $(-)^m f(m)$ with f(m) being a smooth function, one can prove that

$$\sum_{m=2}^{r+1} \bar{Q}_{\rm SF}^r(m)(-)^m f(m) \simeq \left\{ \sum_{m=2}^{r+1} \bar{Q}_{\rm SF}^r(m)(-)^m \right\} f(\overline{\langle m \rangle}).$$
(7)

Here  $\overline{\langle m \rangle} = n_{\eta}r + 1$ . If  $\chi_{\eta}^{(SQ)}(m) \simeq f(m)$ , the equa-



FIG. 4. Central charge of the ground state of  $\hat{H}_{\text{eff2}}$  for  $J_{\text{ex}} = 0.4$  and the indicated values of  $n_{\eta}$ . To evaluate the central charge, we apply Eq. (8) to the iTEBD results with  $D \in [200, 1600]$ . The red shaded area indicates the stability region of the  $\eta$ -pairing phase for  $J_{\text{ex}} \to 0$ , while the blue shaded area shows that of the CDW phase. The inset plots the relation between  $S_E$  and  $\xi_D$  and the corresponding linear fits.

tion without  $(-)^m$  is satisfied. See SM for the detailed meaning of the equality  $\simeq$  and the derivation. Since we have  $\{\sum_{m=2}^{r+1} \bar{Q}_{\rm SF}^r(m)(-)^m\} \propto \frac{\cos(\pi n_\eta r)}{r^{\frac{1}{2}}}$  [69, 75] and  $\sum_{m=2}^{r+1} \bar{Q}_{\rm SF}^r(m) = n_\eta^2$  (in leading order in r), one can obtain the asymptotic form of the correlation functions. Equation (7) shows that the decay of  $\eta$ -spin correlations in real space originates from that in the squeezed space and the contribution from the intercalated singlyoccupied sites. The latter is determined by  $|\Psi_{\rm SF}^{\rm GS}\rangle$ , and has a different impact depending on whether the correlation functions in the squeezed space are staggered or not. In particular, the pairing correlation is not affected by the SF background, while the charge correlations can be affected like the spin correlations.

The asymptotic forms obtained analytically for  $\chi_{\text{charge}}$ and  $\chi_{\eta-\text{pair}}$  are summarized in Figs. 3(a)(b). The magnitude relation of the exponents of these correlation functions changes at the SU(2) point of  $\hat{H}_{\eta-\text{spin}}^{(SQ)}$ . Note that this SU(2) symmetry is an emergent symmetry in the squeezed space, which is absent in the original Hamiltonian. For  $0 < n_{\eta} < 1$ ,  $\chi_{\text{charge}}$  shows an exponent of 1/2in the CDW phase due to the contribution from the SF part, although it shows LRO in the squeezed space. On the other hand, the analytic argument based on Eq. (7)does not allow to make exact statements for the components decaying faster than  $\mathcal{O}(\frac{\ln r}{r^2})$ . To analyze this point, we numerically evaluate the correlation functions, see Figs. 3(c)(d). Firstly, our results verify the conjecture  $\chi_{\eta-\text{pair}}(r) \simeq n_{\eta}^2 \chi_{\eta,x}^{(\text{SQ})}(rn_{\eta})$  and its applicability even in the CDW regime, where  $\chi_{\eta-\text{pair}}(r)$  decays exponentially, see Fig. 3(c). Secondly, Fig. 3(d) shows that Eq. (7) is practically applicable for the leading and the sub-leading terms of  $\chi_{\text{charge}}$  decaying faster than  $\mathcal{O}(\frac{\ln r}{r^2})$ , i.e.  $\chi_{\text{charge}}(r) \simeq C_1 r^{-2} + C_2 r^{-\frac{1}{2} - \frac{1}{\alpha}} \cos(\pi n_\eta r).$ 

The expression (5) also provides valuable insights into the physical nature of the metastable phases. One important quantity that characterizes one-dimensional systems is the central charge (c), which counts to the number of gapless degrees of freedoms [72]. In equilibrium, the doped Hubbard model exhibits c = 2, because of the massless modes both in the spin and charge sectors [76, 77]. On the other hand, the exact form of the wave-function (5) suggests that the metastable state possesses three degrees of freedoms. The wave functions of the charge and spin sectors are those of gapless states (i.e. doped free fermions and the isotropic Heisenberg model), while that of the  $\eta$ -spin sector corresponds to the gapless state or the gapful state of the  $\eta$ -XXZ model for the  $\eta$ -pairing state and the CDW state, respectively. Thus, one naturally expects that c = 3 in the *n*-pairing state and c = 2 in the CDW state. To confirm this, we perform iTEBD simulations on the effective model  $\dot{H}_{eff2}$ for various cut-off dimension (D) and extract c from the relation [78]

$$S_E = \frac{c}{6}\ln(\xi_D) + s_0.$$
 (8)

Here  $S_E$  is the entanglement entropy,  $s_0$  is a constant and  $\xi_D$  is the correlation length evaluated from the second-largest eigenvalue of the transfer matrix, see SM. In Fig. 4, we show the central charge for  $\hat{H}_{\rm eff2}$  with  $J_{\rm ex} = 0.4$ , which is extracted using Eq. (8) and the linear fit of the iTEBD results [see the inset of Fig. 4]. The results indeed confirm the above expectation. We emphasize that the emergence of a c = 3 state in the Hubbard model is hardly expected in equilibrium and reflects the metastable nature of the state.

Conclusion – We showed that the additional degrees of freedom activated by photo-doping lead to peculiar types of quantum liquids absent in equilibrium. In particular, we revealed the intriguing structure of the correlations between active degrees of freedom in photo-doped onedimensional strongly correlated systems, i.e. the spincharge- $\eta$ -spin separation. Our results open a new avenue for studying metastable states in one-dimensional systems and raise interesting questions. Firstly, in contrast to the equilibrium Hubbard model, the weak coupling regime is not well-defined, and the relation between the lattice model and the corresponding conformal field theory is not clear. Construction of the field theory for the metastable states is an important future task. Secondly, we provide a rigorous basis for the future development of a bosonization approach [79, 80]. With such an approach, one can better understand the spectral features of the photo-doped systems and the implications of the spin-charge- $\eta$ -spin separation for dynamical properties. Thirdly, various concepts developed for one-dimensional systems in equilibrium can be extended to understand the physics of metastable states. For example, extending the spin incoherent Luttinger liquids [81] may be helpful for understanding effectively cold, but not ultracold systems.

Finally but not least, our analytical and intuitive insights provide a useful reference for the study of photodoped Mott insulators in higher dimensions, where the separation of spin, charge and  $\eta$ -spin is not expected, but a crossover from high-dimensional to one-dimensional behavior can occur in anisotropic systems.

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