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# Exploring Pair Density Waves and Superconductivity in the Emery Model using Density-Matrix Renormalization Group

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**ABSTRACT**

*Pair density waves (PDWs) are a distinct state of matter in superconducting systems characterized by a spatially oscillating superconducting order parameter, in contrast to traditional uniform superconductors. The Emery model includes a negative electron hopping term tpp between nearby oxygen sites. By changing the direction of oxygen-oxygen hopping, kinetic frustration may be achieved, which in turn changes the local model parameters by reducing the Cu-Cu antiferromagnetic exchange and increasing the charge transfer energy. Our findings show that at low doping levels, there is a ground state that is very close to a PDW, with superconducting, charge, and spin density wave correlations that are reciprocal. The system exhibits a unique d-wave superconductivity as the attractive $V_{pp}$ increases.*

**Keywords**: Spin, Density wave, Emery model, Matrix, Superconductivity

## I.INTRODUCTION

Superconductivity is an intriguing quantum mechanical phenomena in which some materials demonstrate zero electrical resistance and the ejection of magnetic fields when chilled below a crucial temperature. Superconductivity, discovered in mercury by Heike Kamerlingh Onnes in 1911, has since become a fundamental aspect of condensed matter physics. The Bardeen-Cooper-Schrieffer (BCS) theory elucidates the microscopic mechanism of superconductivity, positing that at low temperatures, electrons form Cooper pairs that traverse a crystal lattice without scattering, enabling resistance-free current flow. These electron pairs aggregate into a macroscopic quantum state, resulting in a superconducting phase defined by a consistent pairing amplitude across the material. Recent investigations have revealed intricate superconducting states, such as pair density waves (PDWs), which complicate and enhance our comprehension of superconductivity.

Pair density waves represent a situation wherein the superconducting order parameter displays a spatially varied pattern instead of being uniform across the material. This indicates that the amplitude or phase of the superconducting pairs fluctuates regularly in space. PDWs exemplify a spatially modulated superconducting phase characterized by oscillations in the order parameter, akin to the spatial modulations observed in a charge density wave concerning electron density. In the context of PDWs, the modulation transpires in the density of Cooper pairs rather than in the charge density itself. Pair density waves have been detected in some high-temperature superconductors, like cuprates, where intricate interactions among charge, spin, and lattice degrees of freedom foster an environment favorable to such atypical pairing.

The notion of pair density waves is a notable divergence from the conventional BCS framework of superconductivity, wherein the order parameter is often considered to be uniform. PDWs introduce a layer of complexity by including a periodic structure inside the superconducting phase. This modulated structure can coexist with other forms of order, such as charge density waves (CDWs) or spin density waves (SDWs), resulting in complex and detailed phase diagrams. Comprehending these coexisting orders is essential for a profound understanding of the mechanisms behind unconventional superconductivity, especially in systems where robust electron correlations are significant, such as cuprates and iron-based superconductors.

The investigation of PDWs has intensified due to their potential to elucidate some perplexing phenomena shown by high-temperature superconductors, particularly the pseudogap phase in cuprates. The pseudogap is a phase characterized by the emergence of a partial energy gap above the superconducting transition temperature, and its characteristics have been the focus of much discussion for decades. Certain theoretical models propose that PDWs may account for the pseudogap, indicating that a modified superconducting order might persist even above the superconducting transition point. This implies that PDWs may serve as a prelude to uniform superconductivity, offering a novel viewpoint on the interaction between superconductivity and other types of order in these materials.

The theoretical basis for comprehending PDWs entails expanding the BCS theory to incorporate spatial changes in the pairing amplitude. This can be accomplished by employing principles from the Ginzburg-Landau theory, wherein the superconducting order parameter is permitted to fluctuate spatially. Within this perspective, the establishment of a PDW state may be perceived as an equilibrium between the kinetic energy of the Cooper pairs and the potential energy linked to spatial modulations. This method elucidates the potential emergence of PDWs from the rivalry among superconducting, magnetic, and charge-ordered states. Furthermore, microscopic theories, like the mean-field approach to the Hubbard model and the t-J model, have been utilized to investigate the stabilization of PDW states in certain materials due to high correlations.

Experimentally, detecting pair density waves is a tough endeavor due to the nuanced nature of their spatial modulations. Techniques such as scanning tunneling microscopy (STM), X-ray scattering, and nuclear magnetic resonance (NMR) have proved pivotal in detecting signs of PDWs. For instance, STM can disclose variations in the density of states, which may signify an underlying PDW order. In cuprate superconductors such as Bi2Sr2CaCu2O8+x (BSCCO), scanning tunneling microscopy (STM) investigations have demonstrated evidence of spatially modulated pairing consistent with the notion of pair density waves (PDWs). Likewise, resonant X-ray scattering has been employed to identify spatial modulations in the superconducting state, providing more evidence of PDW events. The experimental results have reinforced the theoretical predictions and underscored the significance of PDWs in the intricate phase behavior of unconventional superconductors.

One of the fascinating elements of PDWs is their possible association with topological properties and exotic quasiparticles. The periodic variation in the pairing amplitude can induce spatially changing phase shifts, potentially resulting in topological defects such as vortices and solitons. These flaws may be linked to Majorana bound states, which are significant for their prospective uses in quantum computing owing to their non-Abelian statistics and resilience to local perturbations. Consequently, PDWs enhance our comprehension of superconducting phases and facilitate the investigation of novel forms of topological matter. The interaction between topology and PDW states is a dynamic field of study, with consequences for both basic physics and practical applications.

Moreover, PDWs provide a distinctive insight into the characteristics of the superconducting gap structure. In conventional superconductors, the superconducting gap is often isotropic (s-wave symmetry) or has a defined angular dependency (d-wave or p-wave). In a PDW condition, the gap function might exhibit spatial periodicity, resulting in a more complex gap structure. The spatial modulation of the gap can produce atypical characteristics in the electronic spectrum, including supplementary gap nodes or mini-gaps, which can be investigated using spectroscopic methods like as angle-resolved photoemission spectroscopy (ARPES). Comprehending the gap structure of PDW states is essential for correlating theoretical models with experimental findings and for clarifying the pairing mechanisms in high-temperature superconductors.

The identification of pair density waves signifies a transformation in our comprehension of superconductivity, broadening the framework beyond uniform phases to encompass spatially variable superconducting states. This transition is integral to a comprehensive initiative aimed at elucidating the intricate phase diagrams of correlated electron systems, wherein conflicting interactions generate a spectrum of unusual phases. PDWs illustrate how intricate many-body interactions may generate novel quantum states of matter that defy traditional understanding. Through the examination of PDWs, researchers aspire to elucidate the fundamental principles that regulate high-temperature superconductivity, hence facilitating advancements in the development of novel materials with improved superconducting characteristics.

## II.MATERIALS AND METHOD

This research examines the creation of the same or a different SC state following doping in the PDW or SC states, as well as matching pairing symmetry, using the DMRG and Emery model on the square lattice. The basic plaquette centered at a generic Cu site has signals for the hopping matrix members in the right orbital arrangement the Cu 3d$x^2-y^2$ and $O_{x/y}$ $2p_x/2p_y$ orbitals. The sign of $t_{pp} \equiv t^{\sigma}_{pp} - t^{\pi}_{pp}$ is considered negative, which goes against the conventional choice. Increasing ligand oxygen orbital delocalization energy increases effective charge transfer energy, alters Cu-O magnetic exchange, and changes ground state orbital arrangement local symmetry. The system's local physics and ground state change significantly.

Considering this system's ground state features in respect to $V_{pd}$ and $V_{pp}$, we establish $t_{pd} = 1$ as the energy unit and use a conventional set of constants Ud = 8, Up = 3, Δpd = 3 for cuprates, and negative $t_{pp} = -0.5$.

We consider two-legged cylinders of width $L_y = 2$ and length up to $L_x = 96$

where $L_y$ = the number of unit cells along the $e_1$ and $e_2$ directions, and

$L_x$ = the length in units of 96.

The total of all sites (N) equals $N_u$, the number of unit cells $3L_xL_y + 2L_y$, which is equal to $3N_u + 2L_y$.

The total density of holes in the system is given by $\rho = 1 + \delta$, where $\delta = N_h/N_u$ is the concentration of holes and $N_h$ is the number of holes away from half-filling. With a common truncation error of $\epsilon \sim 10^{-10}$, we retain up to 20,000 states while considering $\delta = 1/12$ and 1/8.

## III.RESULTS AND DISCUSSION

### <u>Pair density wave phase</u>

At vast distances, the SC correlations fade like a power-law, and their periodic oscillations in real space cause its spatial average to disappear. This phase occupies most of the ground state phase diagram.

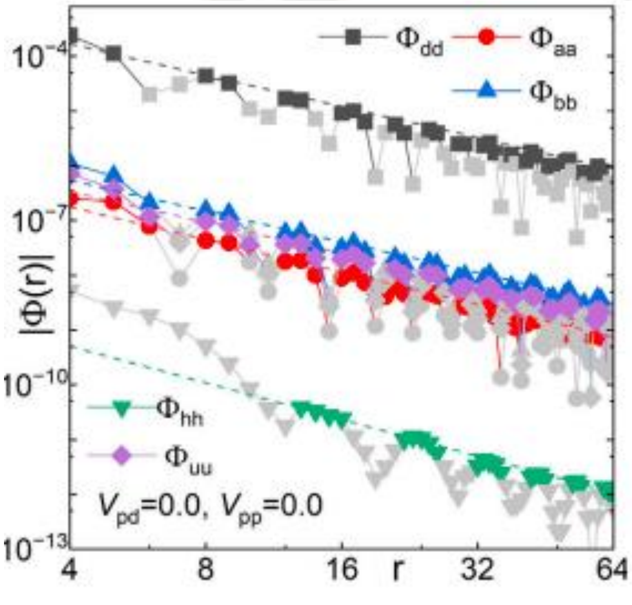


**Figure 1: Superconducting correlations at δ = 1/8 for Φ(r) at $V_{pd} = V_{pp} = 0$**

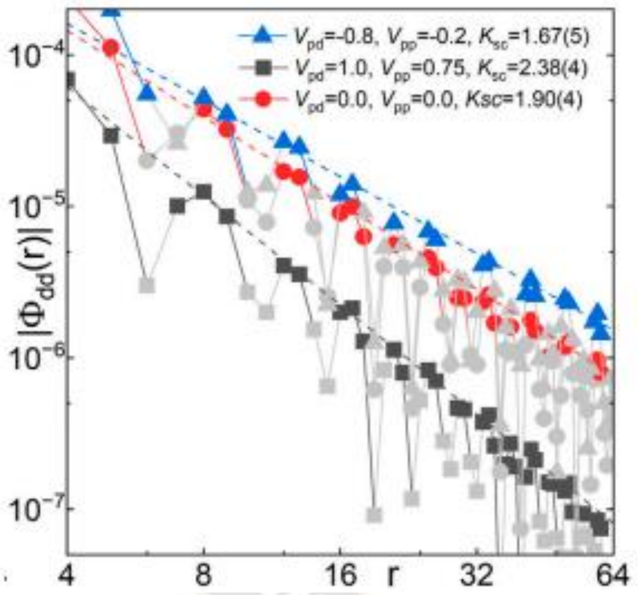


**Figure 2: Differences in $V_{pd}$ and $V_{pp}$ at δ = 1/8 for $\Phi_{dd}(r)$**

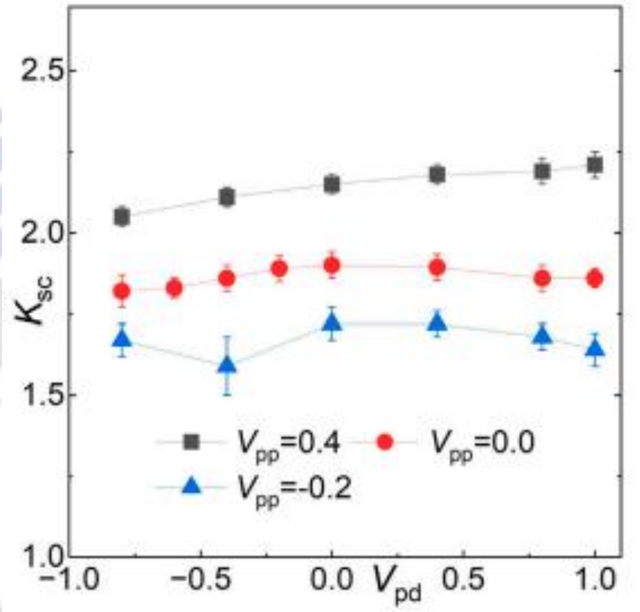


**Figure 3 Variations at δ = 1/8 in the superconducting correlations with respect to the Luttinger exponent $K_{sc}$ and $V_{pd}$ and $V_{pp}$**

### *Superconducting correlations*

We calculated equal-time spin-singlet SC pair-pair correlations to study superconductivity.

$$\Phi_{\alpha\beta}(r) = \langle \hat{\Delta}^{\dagger}_{\alpha}(x_0, y_0)\hat{\Delta}_{\beta}(x_0 + r, y_0)\rangle$$

Here,

$$\hat{\Delta}^{\dagger}_{\alpha}(x, y) = \frac{1}{\sqrt{2}}[\hat{c}^{\dagger}_{(x,y),\uparrow}\hat{c}^{\dagger}_{(x,y)+\alpha,\downarrow} - \hat{c}^{\dagger}_{(x,y),\downarrow}\hat{c}^{\dagger}_{(x,y)+\alpha,\uparrow}]$$

is described as an operator that builds spin-singlet pairs on the bond α = a, b, d, d¯, h, and u. The distance between two bonds in the e1 direction is denoted by r, and the reference bond ($x_0$, $y_0$) has an $x_0 \sim L_x/4$. Each part of the SC correlations has been carefully examined by us. This includes calculations of $\Phi_{aa}$, $\Phi_{ab}$, $\Phi_{bb}$, $\Phi_{dd}(r)$, $\Phi_{dd}\bar{}(r)$, $\Phi_{\bar{d}\bar{d}}(r)$, $\Phi_{hh}$, $\Phi_{uu}$ and $\Phi_{uh}$. The positive $t_{pp}$ example shows strong correlations in $\Phi_{hh}$ and $\Phi_{uu}$, whereas the negative case shows considerable differences.

The geographical distribution of SC correlations, with a focus on $\Phi_{dd}(r)$, has been thoroughly investigated. Figure 4 shows our results for three typical parameter settings. In this case, $\Phi_{dd}(r)$ displays distinct spatial fluctuations as $\Phi_{dd}(r) \sim f(r)\phi_{dd}(r)$ throughout a large area of r. The spatial oscillation is caused by $\phi_{dd}(r)$, whereas f(r) functions as the envelope in this context. The power-law decline of the envelope function $f(r) = A * r^{-Ksc}$ is maintained as we approach larger distances.

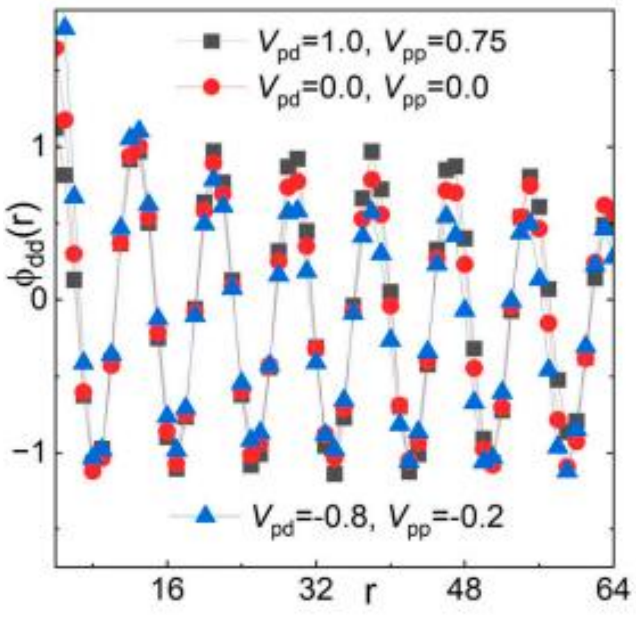


**Figure 4: At δ = 1/8, Normalized functions $\phi_{dd}(r) = \Phi_{dd}(r)/f_{dd}(r)$ portray spatial oscillation of $\Phi_{dd}(r)$**

The previously developed normalized function ϕ(r) captures the spatial oscillation of the SC correlations Φ(r). The fitting function $\phi_{dd}(r) \sim \sin(Qr + \theta)$ is well-aligned with the $\phi_{dd}(r)$ depictions in Figure 4. This pattern is consistent with features seen in the PDW state where the spatial average of ϕ(r) is zero. With a similar wavelength $\lambda_{sc} = 1/\delta$ and $Q \approx 2\pi\delta$, The PDW ordering wavevector appears incommensurate. As an example, when δ = 1/8, λsc is closer to 8, while when δ = 1/12, it's closer to 12.

### *Charge density wave*

We generated the charge density profile for the system, where α is the Cu/Ox/Oy site, to demonstrate its properties (nα(x, y) ⟨n^α(x, y)⟩ and its rung average.

$$\bar{n}(x) = \sum_{y=1}^{L_y} \bar{n}_a(x, y)/L_y$$

The spatial oscillation of nα(x), like in the positive $t_{pp}$ situation investigated by Jiang (2023), is defined by two ordering wavevectors at Q and 2Q, which correspond to wavelengths $\lambda_Q = 1/\delta$ and $\lambda_{2Q} \approx 1/2\delta$, respectively.

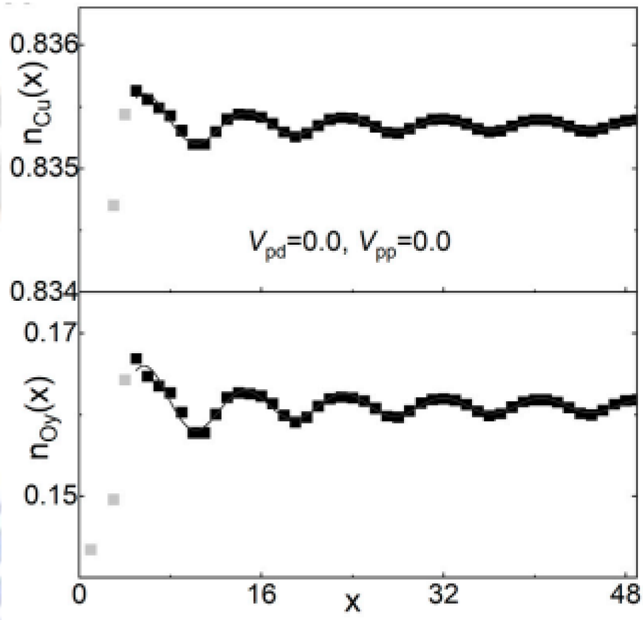


**Figure 5: Measurements at δ = 1/8 Cu and Oy $V_{pd} = V_{pp}$ = 0 are $nC_u(x)$ and $n_{Oy}(x)$**

Fitting the charge density oscillations generated by the cylinder boundaries yields a power-law with an exponent Kc that dominates the spatial decline of the CDW correlation over large distances.

$$n(x) = A_Q * \cos(Qx + \phi_1) * x^{-K_c/2} + A_{2Q} * \cos(2Qx + \phi_2) * x^{-K_c/2} + n_0$$

The amplitudes here are denoted as AQ and A2Q, the phase shifts as ϕ1 and ϕ2, and the mean density as $n_0$.

### *Correlations of Spin-spin*

In order to clarify the ground state's magnetic characteristics, we look at the spin-spin correlation functions $F_\alpha(r)$ ⟨$S_{x0,\ y0} \cdot S_{x0+r,\ y0}$⟩, where α is the Cu/$O_x$/$O_y$ site. Figure 7 shows F(r) instances with two exemplary δ = 1/8 parameter values. In the presence of kinetic frustration, oxygen sites show a substantial relationship, unlike Cu sites. Note that this decays power-law-like over great distances, denoted by $F(r) \sim r^{-Ks}$. For Vpd = $V_{pp}$ = 0, the related Luttinger exponent is around 1.1, while for $V_{pd} = -0.8$ and $V_{pp} = -0.2$, it is approximately 1.3. As can be observed in the figure 7 inset, F(r) displays

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noticeable spatial oscillations ($\lambda_s = 1/\delta$), which are indicative of a PDW state. An ordering wavevector $Q \approx 2\pi\delta$ similar to the SC correlation is produced, which is in tight alignment with $\lambda_{sc}$.

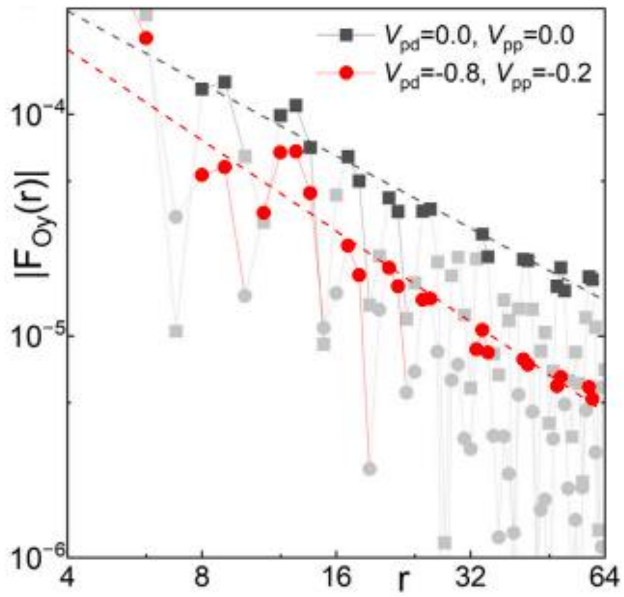


**Figure 6: Magnitude of spin-spin correlation |F(r)| at δ = 1/8, charge density profile, and entanglement entropy**

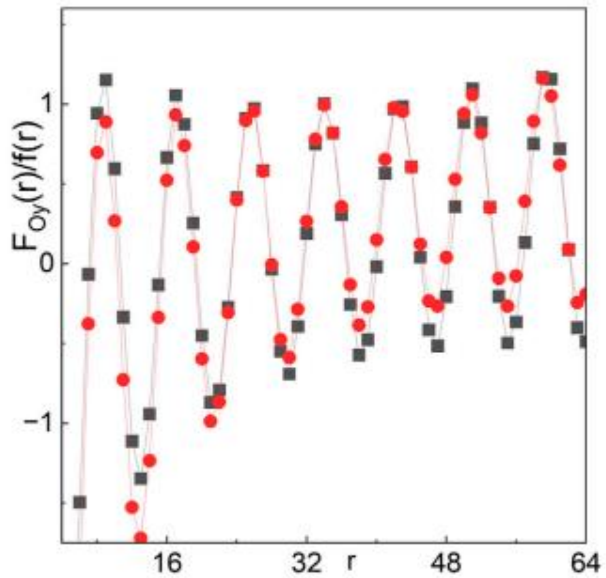


**Figure 7: Entanglement entropy, spin-spin correlation, and charge density profile at δ = 1/8 for Function normalized F(r)/f(r)**

***Entanglement entropy***

Several gapless modes, including charge and spin degrees of freedom, are shown to exist by our studies. The core charge, c, may be used to characterize them. The von Neumann entropy, which is represented as this charge, is: $S(x) = -\mathrm{Tr}\rho_x \ln\rho_x$, where $\rho_x$ is the x-length subsystem's reduced density matrix. For critical systems in one-dimensional space with a conformal field theory, an open system of length $L_x$ has been shown to

$$S(x) = \frac{c}{6}\ln\left[\frac{4(L_x+1)}{\pi}\sin\frac{\pi(2x+1)}{2(L_x+1)}|\sin k_F|\right] + \tilde{A}\frac{\sin[k_F(2x+1)]}{\frac{4(L_x+1)}{\pi}\sin\frac{\pi(2x+1)}{2(L_x+1)}|\sin k_F|} + \tilde{S}$$

A~ and S~ are fitting parameters that rely on the model, whereas $k_F$ denotes the Fermi momentum. Our results indicate a core charge of around c = 2, as seen in Figure 8. We specifically noted $c \approx 1.95$ for $V_{pd} = V_{pp} = 0$ and $c \approx 2.0$ at $V_{pd} = -0.8$ and $V_{pp} = -0.2$ at $\delta = 1/8$. These findings indicate the existence of both a gapless charge mode and a gapless spin mode.

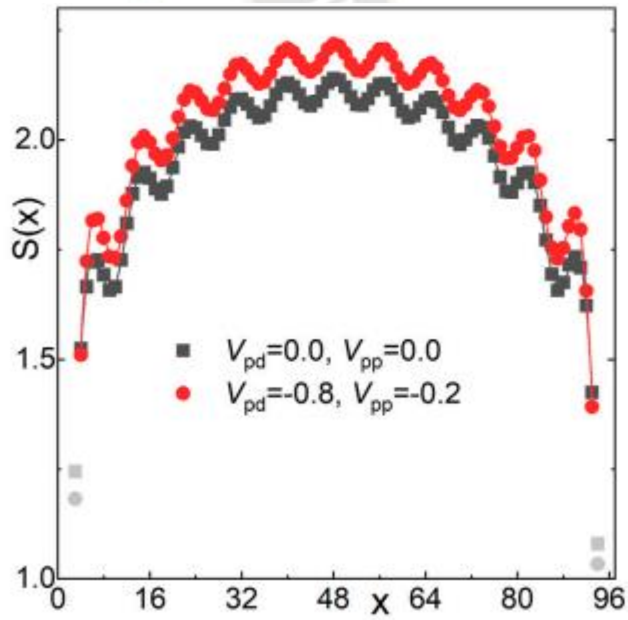


**Figure 8: At δ = 1/8 for Von Neumann entanglement entropy S(x)**

## IV. CONCLUSION

Pair density waves are a cutting-edge area in superconductivity research, providing understanding of the interaction between spatially modulated superconducting order and other types of electronic order. Their research has significant significance for comprehending high-temperature superconductors, the characteristics of the pseudogap phase, and the essential principles behind unusual pairing. The evolution of experimental techniques and theoretical models in the study of PDWs is poised to reveal new enigmas in condensed matter physics and may facilitate practical progress in quantum devices and energy-efficient systems. A comprehensive grasp of PDWs brings us nearer to resolving the enduring enigma of high-temperature superconductivity and to using quantum coherence in novel and inventive manners.

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