# Effect of nearest- and next-nearest neighbor interactions on the spin-wave velocity of one-dimensional quarter-filled spin-density-wave conductors

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We study spin fluctuations in quarter-filled one-dimensional spin-density-wave systems in presence of shortrange Coulomb interactions. By applying a path integral method, the spin-wave velocity is calculated as a function of on-site (U), nearest (V) and next-nearest  $(V_2)$  neighbor-site interactions. With increasing V or  $V_2$ , the pure spin-density-wave state evolves into a state with coexisting spin- and charge-density waves. The spin-wave velocity is reduced when several density waves coexist in the ground state, and may even vanish at large V. The effect of dimerization along the chain is also considered.

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# I. INTRODUCTION

Organic conductors of the tetramethyltetraselena fulvalene (TMTSF) and tetramethyltetrathiafulvalene (TMTTF) salts family often exhibit density-wave (DW) instability at low temperature.<sup>1–3</sup> Recent experiments have shown that a  $2k_F$  spin-density wave (SDW) may coexist with a  $4k_F$  and/or a  $2k_F$  charge-density wave (CDW).<sup>4,5</sup> (The quantity  $k_F$  denotes the one-dimensional Fermi wave vector and  $2k_F$  is the nesting wave vector for the SDW.) Furthermore, these CDW's seem to be of pure electronic origin without any (significant) contribution from the lattice.

This unusual ground state can be understood on the basis of a mean-field theory for a quarter-filled one-dimensional system in the presence of several kinds of Coulomb interaction. Within an extended Hubbard model with on-site (*U*) and nearest-neighbor (*V*) interactions, it has been shown that a  $4k_F$  CDW may coexist with the  $2k_F$  SDW when *V* is strong enough.<sup>6</sup> When the next-nearest-neighbor interaction (*V*<sub>2</sub>) is also taken into account, three different ground states can be stabilized:<sup>7-9</sup> (i) a pure  $2k_F$  SDW at small *V* and *V*<sub>2</sub>, (ii) coexisting  $2k_F$  SDW and  $4k_F$  CDW at large *V*, and (iii) coexisting  $2k_F$  SDW,  $2k_F$  CDW, and  $4k_F$  SDW at large *V*<sub>2</sub>. Although the SDW instability is driven by the on-site repulsive interaction *U*, the nearest- and next-nearest-neighbor interactions play a crucial role for the appearance of CDW's. Following the standard analysis,<sup>10–17</sup> fluctuations around

Following the standard analysis,<sup>10–17</sup> fluctuations around the mean-field ground state have been studied. For a quarterfilled system, commensurability effects with the underlying crystal lattice pin the DW's and produce a gap in the sliding modes.<sup>18</sup> Surprisingly, this gap vanishes at the boundary between the pure  $2k_F$  SDW and the coexisting  $2k_F$  SDW and  $4k_F$  CDW.<sup>19</sup> The spin-wave modes have been studied only within the Hubbard model ( $V=V_2=0$ ).<sup>20</sup> The spin-wave velocity decreases monotonically with increasing *U*, in qualitative agreement with the exact solution of the onedimensional Hubbard model.<sup>21</sup>

In this paper, we study the spin-wave modes in presence of the nearest- and next-nearest-neighbor interactions  $(V, V_2 \neq 0)$ . We consider a one-dimensional system, assuming that long-range order is stabilized by (weak) interchain coupling. Our analysis is based on a functional integral formulation<sup>22-25</sup> that allows a simple treatment of the spinwave modes even in the presence of these interactions. The electron-electron interaction is treated within (Hartree-Fock) mean-field theory, while the SU(2) spin rotation symmetry is maintained by introducing a fluctuating spin-quantization axis in the functional integral. Transverse spin-wave modes then correspond to fluctuations of the spin-quantization axis around its mean-field value.

In Secs. II and III, we extend the derivation of Ref. 25 from the incommensurate to the commensurate case. Previous mean-field results<sup>8</sup> are recovered within a saddle point approximation. Then we derive the effective action of the spin-wave modes and obtain the spin-wave velocity. In Sec. IV, the spin-wave velocity is calculated as a function of V,  $V_2$ , and the dimerization along the chain. Section V is devoted to discussion.

# **II. PATH INTEGRAL FORMULATION**

We consider a one-dimensional electron system at quarter-filling with dimerization along the chain. Within the extended Hubbard model, the Hamiltonian is given by

$$H = H_0 + H_I, \tag{2.1}$$

$$H_0 = -\sum_{\sigma,n,n'} t_{nn'} \psi^{\dagger}_{n\sigma} \psi_{n'\sigma}, \qquad (2.2)$$

$$H_{I} = U \sum_{n} n_{n\uparrow} n_{n\downarrow} + V \sum_{n} (\psi_{n}^{\dagger} \psi_{n}) (\psi_{n+1}^{\dagger} \psi_{n+1}) + V_{2} \sum_{n} (\psi_{n}^{\dagger} \psi_{n}) (\psi_{n+2}^{\dagger} \psi_{n+2}) = -\frac{U}{4} \sum_{n} (\psi_{n}^{\dagger} \sigma_{z} \psi_{n})^{2} + \sum_{n,n'} (\psi_{n}^{\dagger} \psi_{n}) V_{nn'} (\psi_{n'}^{\dagger} \psi_{n'}),$$
(2.3)

where  $\psi_n = (\psi_{n\uparrow}, \psi_{n\downarrow})^t$ ,  $n_{n\sigma} = \psi_{n\sigma}^{\dagger} \psi_{n\sigma}$ , and  $\psi_{n\sigma}^{\dagger}$  is the creation operator of an electron with spin  $\sigma(=\uparrow,\downarrow)$  at the lattice site *n*. The transfer integral in the kinetic term  $H_0$  is defined by

$$t_{nn'} = \begin{cases} t - (-1)^n t_d & \text{for } n' = n+1 \\ t + (-1)^n t_d & \text{for } n' = n-1 \\ 0 & \text{otherwise} \end{cases}$$
(2.4)

where a finite  $t_d$  is due to the dimerization. The interaction Hamiltonian is expressed in terms of the Hubbard interaction U and the density-density interaction  $V_{nn'}$  defined by

$$V_{nn'} = \begin{cases} U/4 & \text{for } n' = n, \\ V/2 & \text{for } n' = n \pm 1, \\ V_2/2 & \text{for } n' = n \pm 2, \\ 0 & \text{otherwise,} \end{cases}$$
(2.5)

where  $V(V_2)$  is the coupling constant for nearest (nextnearest) neighbor-site interaction  $(U, V, V_2 \ge 0)$ .

In order to derive the effective action for the spin-wave modes, we write the partition function Z as a path integral:

$$Z = \int \mathcal{D}\psi^{\dagger} \mathcal{D}\psi \ e^{-\mathcal{S}[\psi^{\dagger},\psi]}, \qquad (2.6)$$

$$S = \int d\tau \left[ \sum_{n} \psi_{n}^{\dagger} (\partial_{\tau} - \mu) \psi_{n} + H[\psi^{\dagger}, \psi] \right], \qquad (2.7)$$

where the action S is a function of the Grassmann variable  $\psi$ .  $\tau$  is a Matsubara time-varying between 0 and 1/T. Following Refs. 23 and 25, we now introduce the new field  $\phi$  defined by

$$\psi_n = R_n \phi_n ,$$
  
$$R_n \sigma_z R_n^{\dagger} = \boldsymbol{\sigma} \cdot \mathbf{n}_n , \qquad (2.8)$$

where  $R_n$  is an SU(2)/U(1) unitary matrix and  $\mathbf{n}_n$  is a unit vector that gives the direction of the spin-quantization axis at site *n* and time  $\tau$  for the field  $\phi$ . Substituting Eq. (2.8) into Eq. (2.7), the action is rewritten as  $S = S_0 + S_I$ , where

$$S_{0} = \int d\tau \Biggl\{ \sum_{n} \phi_{n}^{\dagger} (\partial_{\tau} - \mu + R_{n}^{\dagger} \partial_{\tau} R_{n}) \phi_{n} - \sum_{n,n'} \phi_{n}^{\dagger} R_{n}^{\dagger} t_{nn'} R_{n'} \phi_{n'} \Biggr\}, \qquad (2.9)$$

$$S_{I} = \int d\tau \left\{ -\frac{U}{4} \sum_{n} \rho_{sn}^{2} + \sum_{n,n'} \rho_{cn} V_{nn'} \rho_{cn'} \right\}. \quad (2.10)$$

 $\rho_{cn} = \phi_n^{\dagger} \phi_n$ , and  $\rho_{sn} = \phi_n^{\dagger} \sigma_z \phi_n$  are the charge- and spindensity operators. The quantities  $\sigma_x, \sigma_y$  and  $\sigma_z$  are Pauli matrices. Note that  $S_I$  is invariant under the transformation  $\psi \rightarrow \phi$ , since the interaction is invariant with respect to spin rotations. It is convenient to rewrite the action as

$$S = \int d\tau \Biggl\{ \sum_{n} \phi_{n}^{\dagger} (\partial_{\tau} - \mu - A_{0n}) \phi_{n} \Biggr\}$$
$$- \sum_{n,n'} \phi_{n}^{\dagger} t_{nn'} \exp \Biggl( -i \int_{n}^{n'} dl A_{xl} \Biggr) \phi_{n'} \Biggr\}$$
$$- \frac{U}{4} \sum_{n} \rho_{sn}^{2} + \sum_{n,n'} \rho_{cn} V_{nn'} \rho_{cn'} \Biggr\}, \qquad (2.11)$$

where the SU(2) gauge fields  $A_0$  and  $A_x$  are defined by

$$A_{0n} \equiv -R_n^{\dagger} \partial_\tau R_n \,, \qquad (2.12a)$$

$$\exp\left(-i\int_{n}^{n+\delta} dl A_{xl}\right) \equiv R_{n}^{\dagger}R_{n+\delta} \quad (\delta = \pm 1).$$
(2.12b)

The lattice spacing is taken as unity. Using the Stratonovich-Hubbard identity,<sup>26</sup> the interaction part of the action is rewritten as (note that  $U, V, V_2 > 0$ )

$$\exp\left(-\sum_{n,n'}\int d\tau \rho_{cn}V_{nn'}\rho_{cn'}\right)$$
$$=\int \mathcal{D}\Delta_{c}\exp\left(-\sum_{n,n'}\int d\tau \Delta_{cn}V_{nn'}^{-1}\Delta_{cn'}\right)$$
$$+ 2i\sum_{n}\int d\tau \Delta_{cn}\rho_{cn}\right), \qquad (2.13)$$

$$\exp\left(\frac{U}{4}\sum_{n}\int d\tau\rho_{sn}^{2}\right)$$
$$=\int \mathcal{D}\Delta_{s}\exp\left(-\frac{1}{U}\sum_{n}\int d\tau\Delta_{sn}^{2}+\sum_{n}\int d\tau\Delta_{sn}\rho_{sn}\right),$$
(2.14)

where  $\Delta_{cn}$  and  $\Delta_{sn}$  are (real) auxiliary fields. By using Eqs. (2.13) and (2.14), the final form of the partition function is given by

$$Z = \int \mathcal{D}\Delta_{c}\mathcal{D}\Delta_{s}\int \mathcal{D}\mathbf{n}\int \mathcal{D}\phi^{\dagger}\mathcal{D}\phi \ e^{-(S_{0}+S_{I})}, \quad (2.15)$$

$$S_{0} = \int d\tau \Biggl\{ \sum_{n} \phi_{n}^{\dagger}(\partial_{\tau}-\mu-A_{0n})\phi_{n} -\sum_{n,n'} \phi_{n}^{\dagger}t_{nn'}\exp\Biggl(-i\int_{n}^{n'}dlA_{xl}\Biggr)\phi_{n'}\Biggr\}, \quad (2.16)$$

$$S_{I} = \int d\tau \Biggl\{ \sum_{n} \left[ \frac{1}{U}\Delta_{sn}^{2}-\Delta_{sn}\rho_{sn}-2i\Delta_{cn}\rho_{cn} \right]$$

$$+\sum_{n,n'} \Delta_{cn} V_{nn'}^{-1} \Delta_{cn'} \bigg\}, \qquad (2.17)$$

where  $V_{nn'}^{-1} = V_{n'n}^{-1}$ .

# **III. EFFECTIVE ACTION FOR THE SPIN-WAVE MODE**

In this section, we derive the action corresponding to the spin-wave modes at quarter-filling. First, we reproduce the mean-field result of Ref. 8 within a saddle-point approximation. Then we consider transverse spin fluctuations arising from the dynamics of the spin-quantization axis.

# A. Mean-field solution

The standard mean-field solution is recovered from a saddle-point approximation with  $\mathbf{n} = \hat{\mathbf{z}}$  at each lattice site. One then has  $R_n = 1$  and  $A_0 = A_x = 0$ .

By minimizing the free energy with respect to  $\Delta_{sn}$  and  $\Delta_{cn}$ , we obtain the self-consistent mean-field equations

$$\Delta_{sn} = \frac{U}{2} \langle \rho_{sn} \rangle_{\rm MF}, \qquad (3.1)$$

$$\Delta_{cn} = i \sum_{n'} V_{nn'} \langle \rho_{cn'} \rangle_{\rm MF}. \qquad (3.2)$$

The average  $\langle \; \rangle_{MF}$  is to be calculated with the mean-field action

$$S_{\rm MF} = \beta \sum_{n} \frac{1}{U} \Delta_{sn}^{2} + \beta \sum_{n,n'} \Delta_{cn} V_{nn'}^{-1} \Delta_{cn'} + \int d\tau \Biggl\{ \sum_{n} \phi_{n}^{\dagger} (\partial_{\tau} - \mu - 2i \Delta_{cn} - \Delta_{sn} \sigma_{z}) \phi_{n} - \sum_{n,n'} \phi_{n}^{\dagger} t_{nn'} \phi_{n'} \Biggr\}.$$
(3.3)

At quarter-filling, the mean fields  $\langle \rho_{sn} \rangle_{\rm MF}$  and  $\langle \rho_{cn} \rangle_{\rm MF}$  are periodic with a periodicity of four lattice spacings. They can be written as

$$\langle \rho_{sn} \rangle_{\rm MF} = \sum_{m=0}^{3} S_m e^{imQ_0 n}, \qquad (3.4)$$

$$\langle \rho_{cn} \rangle_{\rm MF} = \sum_{m=0}^{3} D_m e^{imQ_0 n}, \qquad (3.5)$$

where  $Q_0 = 2k_F = \pi/2$ . Since  $\langle \rho_{cn} \rangle_{MF}$  and  $\langle \rho_{sn} \rangle_{MF}$  are real quantities, one finds  $D_0 = D_0^*, D_1 = D_3^*, D_2 = D_2^*$  and  $S_0 = S_0^*, S_1 = S_3^*, S_2 = S_2^*$ . In Eqs. (3.4) and (3.5),  $S_0 = 0$  due to the absence of ferromagnetism and  $D_0 = 1/2$  for a quarter-filled band. From Eqs. (3.1)–(3.5), the final form of the mean-field action is obtained as

$$\begin{split} \mathcal{S}_{\rm MF} &= \beta N \bigg[ -\frac{U}{16} - \frac{U}{2} (|D_1|^2 - |S_1|^2) - \frac{U}{4} (D_2^2 - S_2^2) \\ &- V \bigg( \frac{1}{4} - D_2^2 \bigg) - V_2 \bigg( \frac{1}{4} - 2|D_1|^2 + D_2^2 \bigg) \bigg] \\ &+ \int d\tau \bigg\{ \sum_k \phi_k^{\dagger} \bigg( \partial_\tau - \mu + \frac{U}{4} + V + V_2 - 2t \cos k \bigg) \phi_k \end{split}$$

$$+\left[\sum_{k} \phi_{k}^{\dagger} \left(\frac{U}{2}(D_{1}-S_{1}\sigma_{z})-2V_{2}D_{1}\right)\phi_{k-Q_{0}}+\text{c.c.}\right]$$
$$+\sum_{k} \phi_{k}^{\dagger} \left(\frac{U}{2}(D_{2}-S_{2}\sigma_{z})-2VD_{2}\right)$$
$$+2V_{2}D_{2}-2it_{d}\sin k\phi_{k-2Q_{0}}, \qquad (3.6)$$

where  $\phi_k = (1/\sqrt{N}) \Sigma_n e^{-ikn} \phi_n$  and *N* is the number of lattice sites. The action (3.6) agrees with the mean-field Hamiltonian obtained previously by the conventional method.<sup>8</sup>

# **B.** Fluctuations

In the long-wavelength limit, collective modes can be separated into sliding (charge) modes and spin-wave modes. In this paper, we consider only transverse (acoustic) spinwave modes (i.e., magnons). These modes show up in the fluctuations of the unit vector field **n**. They do not couple to charge modes and gapped spin-wave modes. We shall make the following two approximations: (i) We neglect the coupling to long-wavelength spin fluctuations  $[\Delta_s(q) \text{ with } |q| \leq Q_0]$ . In the Hubbard model  $(V = V_2 = 0)$ , this coupling is known to renormalize the spin-wave velocity by the factor  $[1 - UN(0)]^{1/2}$  in the weak-coupling limit<sup>27</sup> [N(0) is the density of states at the Fermi level]. (ii) We also neglect any possible coupling to spin fluctuations at wave vector  $2Q_0 + q [\Delta_s(2Q_0 + q)]^{28}$ 

When two SDW's coexist in the ground state, our formalism can only yield the "in-phase" modes where the two spin-density waves oscillate in phase. It misses the modes where the oscillations are out-of-phase.<sup>29</sup> These modes are gapped and do not couple to the "in-phase" modes considered in this paper.

Before proceeding with the spin-wave mode analysis, let us discuss the limit of validity of our approach. The spinwave modes will be obtained by expanding about the (Hartree-Fock) mean-field state. Such an approach should hold (at least qualitatively) as long as the interaction is smaller than the bandwidth, i.e.,  $U, V, V_2 \leq 4t$ . Nevertheless, it does not necessary break down in the strong-coupling limit. In the context of the two-dimensional Hubbard model, Schrieffer *et al.* have shown that a random-phase approximation (RPA) analysis of the fluctuations about the mean-field state in the limit  $U \geq t$  agrees with the conclusions obtained from the Heisenberg model with exchange constant J $= 4t^2/U$ .<sup>30</sup>

Another limitation of our approach comes from the analysis of the fluctuations of the unit vector **n**. As will become clear below, the main assumption is that **n** is a slowly varying field, thus allowing a gradient expansion. Whereas this assumption is perfectly valid in the weak-coupling limit  $(U,V,V_2 \leq 4t)$ , it breaks down in the strong-coupling limit. In the latter, one should write  $\mathbf{n} = \mathbf{n}^{\text{slow}} + \cos(n\pi/2)\mathbf{L}_r$  where  $\mathbf{n}^{\text{slow}}$  is a slowly varying field and  $\mathbf{L}_r$  a small perpendicular component  $(\mathbf{L} \cdot \mathbf{n}^{\text{slow}} = 0$  and  $|\mathbf{L}| \leq |\mathbf{n}^{\text{slow}}| \approx 1$ ).<sup>31,23</sup> The effective action of the spin-wave modes,  $S_{\text{eff}}[\mathbf{n}^{\text{slow}}]$ , is then obtained by integrating out both the fermions and the (small) transverse component  $\mathbf{L}_r$ . For  $V=V_2=0$ , this allows to interpolate smoothly between the weak-coupling regime, and the strong-coupling regime which is well described by the Heisenberg model.<sup>23</sup>

Long-wavelength transverse spin fluctuations correspond to fluctuations of the SU(2) gauge fields  $A_0$  and  $A_x$  [Eqs. (2.12a) and (2.12b)], which are rewritten as

$$A_{0n} = \sum_{\nu = x, y, z} A_{0n}^{\nu} \sigma_{\nu}, \qquad (3.7)$$

$$A_{xn} = \sum_{\nu = x, y, z} A_{xn}^{\nu} \sigma_{\nu}.$$
 (3.8)

From Eqs. (2.11), (3.6), (3.7), and (3.8), we write the action of the spin degrees of freedom as

$$S = S_{\rm MF} - \sum_{n} \int d\tau \phi_n^{\dagger} A_{0n} \phi_n$$
$$- \sum_{n,n'} \int d\tau \phi_n^{\dagger} \bigg[ t_{nn'} \exp \bigg( -i \int_n^{n'} dl A_{xl} \bigg) - t_{nn'} \bigg] \phi_{n'} .$$
(3.9)

To order  $O(A_x^2)$  we obtain

$$S = S_{\rm MF} - \sum_{n} \int d\tau \, \phi_{n}^{\dagger} A_{0n} \phi_{n} - \sum_{n,n'} \int d\tau \, t_{nn'} \\ \times \phi_{n}^{\dagger} \left( -\frac{i}{2} (n-n') (A_{xn} + A_{xn'}) - \frac{1}{2} A_{xn}^{2} \right) \phi_{n'} \\ = S_{\rm MF} - \sum_{n} \sum_{\mu=0,x} \sum_{\nu=x,y,z} \int d\tau \, j_{\mu n}^{\nu} A_{\mu n}^{\nu} + S_{x}^{\rm dia},$$
(3.10)

where  $j_{xn}^{\nu}$ ,  $j_{0n}^{\nu}$ , and  $S_x^{\text{dia}}$  are given by

$$j_{xn}^{\nu} = -\frac{i}{2} \sum_{\delta=\pm 1} \delta[t_{n,n+\delta} \phi_n^{\dagger} \sigma_{\nu} \phi_{n+\delta} + t_{n-\delta,n} \phi_{n-\delta}^{\dagger} \sigma_{\nu} \phi_n],$$
(3.11)

$$j_{0n}^{\nu} = \phi_n^{\dagger} \sigma_{\nu} \phi_n, \qquad (3.12)$$

$$S_{x}^{\text{dia}} = \frac{1}{2} \sum_{n,n'} \sum_{\nu,\nu'} t_{nn'} \int d\tau \ \phi_{n}^{\dagger} \sigma_{\nu} \sigma_{\nu'} \phi_{n'} A_{xn}^{\nu} A_{xn}^{\nu'}.$$
(3.13)

The second term of Eq. (3.10) denotes the coupling of the gauge field  $A_{\mu n}^{\nu}$  to the spin current  $(j_{xn}^{\nu})$  and spin density  $(j_{0n}^{\nu})$ . The last term of Eq. (3.10),  $S_x^{\text{dia}}$ , is the diamagnetic contribution.<sup>25</sup>

The effective action of the gauge field is obtained by integrating out the fermions in the partition function. By substituting Eq. (3.10) into Eq. (2.15), one obtains the effective action up to  $O(A^2)$  as

$$\begin{aligned} \mathcal{S}_{\text{eff}}[A^{\nu}_{\mu}] &= \langle \mathcal{S}^{\text{dia}}_{x} \rangle_{\text{MF}} - \sum_{n,\mu,\nu} \int d\tau \langle j^{\nu}_{\mu n} \rangle_{\text{MF}} A^{\nu}_{\mu n} \\ &- \frac{1}{2} \sum_{n,n'} \sum_{\mu,\mu',\nu,\nu'} \int d\tau d\tau' A^{\nu}_{\mu n}(\tau) \\ &\times \Pi_{j^{\nu}_{\mu'}j^{\nu'}_{\mu'}}(n,\tau,n',\tau') A^{\nu'}_{\mu'n'}(\tau'), \end{aligned}$$
(3.14)

where

$$\Pi_{j_{\mu}^{\nu}j_{\mu'}^{\nu'}}(n,\tau,n',\tau') = \langle j_{\mu n}^{\nu}(\tau) j_{\mu' n'}^{\nu'}(\tau') \rangle_{\rm MF}, \quad (3.15)$$

$$\langle \mathcal{S}_{x}^{\text{dia}} \rangle_{\text{MF}} = \frac{1}{2} \sum_{n,n',\nu} t_{nn'} \int d\tau \langle \phi_{n}^{\dagger} \phi_{n'} \rangle_{\text{MF}} (A_{xn}^{\nu})^{2}.$$
(3.16)

The quantity  $\Pi_{j_{\mu}^{\nu}j_{\mu'}^{\nu'}}$  denotes the current-current correlation function in the mean-field state. We note that  $\langle j_{\mu n}^{\nu} \rangle_{\rm MF} = 0$  in the long-wavelength limit<sup>32</sup> and that  $A_{\mu n}^{\nu}$  is of the order  $O(\nabla)$ . To order  $O(\nabla^2)$ , we obtain

$$\begin{split} \mathcal{S}_{\text{eff}} &= -\frac{1}{2} \sum_{\tilde{q}} \left\{ \langle K \rangle_{\text{MF}} \sum_{\nu = x, y, z} |A_{x}^{\nu}(\tilde{q})|^{2} \right. \\ &+ \sum_{\mu, \mu'(=0, x)} \sum_{\nu, \nu'} A_{\mu}^{\nu}(\tilde{q}) A_{\mu'}^{\nu'}(-\tilde{q}) \left. \Pi_{j_{\mu'}^{\nu'} \mu'}^{\nu'}(\tilde{q}) \right\}, \end{split}$$

$$(3.17)$$

$$\langle K \rangle_{\rm MF} = \left\langle -\frac{1}{N} \sum_{n,n'} t_{nn'} \phi_n^{\dagger} \phi_{n'} \right\rangle_{\rm MF},$$
 (3.18)

where  $\langle K \rangle_{\rm MF}$  is the mean value of the kinetic energy per site in the mean-field state.  $\tilde{q} = (q, i\Omega)$  and  $\Omega$  is a bosonic Matsubara frequency. The quantity  $\prod_{j\mu'\mu'} \tilde{q}_{\mu'} \tilde{q}_{\mu'} \tilde{q}_{\mu'} \tilde{q}_{\mu'} \tilde{q}_{\mu'}$  is the Fourier transform of Eq. (3.15) with respect to n and  $\tau$ . In Eq. (3.17), it can be evaluated at  $\tilde{q}=0$  since  $A^{\nu}_{\mu} \propto O(\nabla)$ . Note that  $\prod_{j\mu'\mu'} \prod_{j\mu'\mu'} \prod_{j\mu'\mu'} \prod_{j\mu'\mu'} q_{\mu'} \tilde{q}_{\mu'} = 0$  and  $\prod_{j_0'j_n'} \tilde{q}_{\eta'} \tilde{q}_{\eta'} = 0$ . Taking the continuum limit  $n \to \xi$  (with  $\xi$  a real continuous variable) and writing  $A^{\nu}_{\mu n} = A^{\nu}_{\mu}(\xi, \tau)$ , the effective action (3.17) is rewritten as

$$\begin{split} S_{\text{eff}} &= -\frac{1}{2} \sum_{\tilde{q}} \sum_{\nu=x,y,z} \left\{ \langle K \rangle_{\text{MF}} | A_{x}^{\nu}(\tilde{q})|^{2} + \sum_{\mu} | A_{\mu}^{\nu}(\tilde{q})|^{2} \Pi_{j_{\mu}^{\nu} j_{\mu}^{\nu}} \right\} \\ &= -\frac{1}{2} \int d\xi \, d\tau \bigg\{ (\langle K \rangle_{\text{MF}} + \Pi_{j_{x}^{x} j_{x}^{x}}) \\ &\times \sum_{\nu=x,y} A_{x}^{\nu 2}(\xi,\tau) + \Pi_{j_{0}^{x} j_{0}^{x}} \sum_{\nu=x,y} A_{0}^{\nu 2}(\xi,\tau) \bigg\} \\ &- \frac{1}{2} \sum_{\tilde{q}} \left\{ (\langle K \rangle_{\text{MF}} + \Pi_{j_{x}^{z} j_{x}^{z}}) | A_{x}^{z}(\tilde{q})|^{2} + \Pi_{j_{0}^{z} j_{0}^{z}} | A_{0}^{z}(\tilde{q})|^{2} \right\}, \end{split}$$

$$(3.19)$$

where  $\Pi_{j_{\mu}^{\nu}j_{\mu}^{\nu}} \equiv \Pi_{j_{\mu}^{\nu}j_{\mu}^{\nu}}(\tilde{q}=0)$  and  $\Pi_{j_{\mu}^{x}j_{\mu}^{x}} = \Pi_{j_{\mu}^{y}j_{\mu}^{y}}$ . Here we note the identities  $\langle K \rangle_{\rm MF} + \Pi_{j_{\chi}^{z}j_{\chi}^{z}} = 0$  and  $\Pi_{j_{0}^{z}j_{0}^{z}} = 0$ , which can be deduced from the gauge invariance of Eq. (2.8) (Appendix A). We have verified numerically the validity of these identities. Finally, noting that<sup>33</sup>

$$\sum_{\nu=x,y} A_x^{\nu 2}(\xi,\tau) = \frac{1}{4} (\partial_{\xi} \mathbf{n})^2, \qquad (3.20)$$

$$\sum_{\nu=x,y} A_0^{\nu 2}(\xi,\tau) = -\frac{1}{4} (\partial_{\tau} \mathbf{n})^2, \qquad (3.21)$$

we obtain the following final expression for the effective action of the spin-wave modes<sup>25,31</sup> (Appendix A):

$$S_{\text{eff}} = \frac{1}{2} \int d\xi d\tau \{ \chi(\partial_{\tau} \mathbf{n})^2 + \rho(\partial_{\xi} \mathbf{n})^2 \}, \qquad (3.22)$$

where  $\chi$  and  $\rho$  are the uniform transverse spin susceptibility and the spin stiffness, respectively:

$$\chi = \langle S_{\nu} S_{\nu} \rangle_{\tilde{q}=0}^{\text{MF}} = \frac{1}{4} \Pi_{j_{0}^{\nu} j_{0}^{\nu}} \quad (\nu = x, y), \qquad (3.23)$$

$$\rho = -\frac{1}{4} (\langle K \rangle_{\rm MF} + \prod_{j_x^{\nu} j_x^{\nu}}) \quad (\nu = x, y).$$
 (3.24)

From Eq. (3.22) we deduce the spin-wave velocity

$$v = \left(\frac{\rho}{\chi}\right)^{1/2}.$$
 (3.25)

In the incommensurate case,  $\prod_{j_x^{\nu_j} y_x^{\nu}} \to 0$  in the weak-coupling limit so that  $\rho = -\langle K \rangle_{\rm MF}/4$ .<sup>25</sup> As shown in the following section,  $\prod_{j_x^{\nu_j y_x}}$  gives rise to a contribution of the same order as  $\langle K \rangle_{\rm MF}$  in the quarter-filled case when the on-site interaction *U* is of the order of the bandwidth. In Eqs. (3.23) and (3.24),  $j_{\mu}^{\nu}$  and *K* can be expressed as  $[\phi_k = (\phi_{k\uparrow}, \phi_{k\downarrow})^t, \nu = x, y]$ 

$$j_0^{\nu}(\tilde{q}=0) = \frac{1}{\sqrt{N}} \sum_k \phi_k^{\dagger} \sigma_{\nu} \phi_k, \qquad (3.26)$$

$$j_{x}^{\nu}(\tilde{q}=0) = \frac{1}{\sqrt{N}} \sum_{k} (2t \sin k \phi_{k}^{\dagger} \sigma_{\nu} \phi_{k})$$
$$-2it_{d} \cos k \phi_{k}^{\dagger} \sigma_{\nu} \phi_{k+2Q_{0}}), \qquad (3.27)$$

$$K = \frac{1}{N} \sum_{k} (-2t \cos k \phi_{k}^{\dagger} \phi_{k} - 2it_{d} \sin k \phi_{k}^{\dagger} \phi_{k+2Q_{0}}).$$
(3.28)

#### **IV. SPIN-WAVE VELOCITY**

In this section, we evaluate the spin-wave velocity at zero temperature (T=0). We take t=1 and calculate the velocity normalized to its value at  $V=V_2=0$  and  $t_d=0$ .



FIG. 1. Phase diagram in the V-V<sub>2</sub> plane for U=4 and  $t_d=0$  (Ref. 8). The three different regions correspond to (I) pure  $2k_F$  SDW, (II) coexisting  $2k_F$  SDW and  $4k_F$  CDW, (III) coexisting  $2k_F$  SDW. The dash-dotted curves denote the corresponding boundaries for  $t_d=0.1$ .

The phase diagram of the present model as a function of V and  $V_2$  is shown in Fig. 1 for U=4 and  $t_d=0$  (solid curve).<sup>8</sup> For small V and  $V_2$ , there is a pure  $2k_F$  SDW state (region I). A large V induces a phase with both a  $2k_F$  SDW and  $4k_F$ CDW (region II), while in the presence of a large  $V_2$  there is coexistence between a  $2k_F$  SDW, a  $2k_F$  CDW and a  $4k_F$ SDW (region III). The dashed curve denotes the boundary at which a first-order transition occurs between regions II and III. The dash-dotted curve shows the phase diagram for  $t_d$ = 0.1. The sliding modes are gapped in all three regions. However, the charge fluctuations become gapless at the transition between I and II. We discuss below the spin-wave velocity [Eq. (3.25)] as a function of V and  $V_2$  for both  $t_d$ = 0 and  $t_d \neq 0$ .

# A. U dependence $(V=V_2=0 \text{ and } t_d=0)$

The spin stiffness  $\rho$  and the susceptibility  $\chi$  are shown in Fig. 2(a) as a function of U for  $V=V_2=0$  and  $t_d=0$ . Both  $\rho$  and  $\chi$  are almost constant for small U and decrease monotonically for large U. The inset shows the corresponding U dependence for  $\langle K \rangle_{\rm MF}$  and  $\Pi_{j_x^x j_x^x}$  which determine  $\rho$  [Eq. (3.24)]. A behavior similar to the incommensurate case is



FIG. 2. (a) U dependence of  $\rho$  and  $\chi$  for  $V=V_2=0$  and  $t_d=0$ . The inset shows the U dependence of  $\langle K \rangle_{\rm MF}$  and  $\prod_{j_{x'x}^{x}}$  (b) U dependence of v (solid curve) and  $v[1-2\chi U]^{1/2}$  (dashed curve). The open circles denote the exact result for the one-dimensional Hubbard model (Ref. 21).



FIG. 3. *V* dependence of the spin-wave velocity velocity *v*, susceptibility  $\chi$ , and spin stiffness  $\rho$  for U=4,  $t_d=0$ , and  $V_2=0$ .  $v^0$  (=1.286),  $\chi^0$  (=0.103), and  $\rho^0$  (=0.171) are the values for  $V=V_2=0$ . There is a small jump at the critical value  $V_c=0.34$ , which is shown by the arrow. The inset shows the *V* dependence of the order parameters  $S_1$  (2 $k_F$  SDW) and  $D_2$  (4 $k_F$  CDW).

seen for  $U \leq 2$ :  $\prod_{j_{\chi}^{\chi_{j_{\chi}}}}$  is vanishingly small, and  $\chi$ ,  $\rho$ , and  $\langle K \rangle_{\rm MF}$  are almost constant with respect to U. The limiting values for small U are given by  $\chi = 1/(2\sqrt{2}\pi) \approx 0.113$ ,  $\langle K \rangle_{\rm MF} = -2\sqrt{2}/\pi \approx -0.90$ , and  $v = \sqrt{2}$ . The variation of these quantities for  $U \geq 2$  comes from the effect of commensurability at quarter-filling.

In Fig. 2(b) (solid curve), we show the spin-wave velocity v [Eq. (3.25)], which is almost independent of U although slightly suppressed at large U. Here we note that we have neglected the coupling to long-wavelength spin fluctuations. In the Hubbard model  $(V=V_2=0)$ , the spin-wave velocity  $v = (\rho/\chi)^{1/2}$  becomes  $(\rho/\chi)^{1/2} [1-2\chi U]^{1/2}$  when this coupling is taken into account within the RPA.<sup>27</sup> One obtains 1  $-2\chi U = 1 - UN(0)$  in the weak-coupling limit where  $N(0) = 1/\sqrt{2}\pi$  at quarter-filling. In Fig. 2(b), we show v and  $v[1-2\chi U]^{1/2}$  (dashed curve). The open circles denote the exact result for the one-dimensional Hubbard model.<sup>21</sup> For  $U \leq 2$ , the RPA result turns out to be a good approximation, while the difference becomes noticeable at larger U. Nevertheless we use  $v = (\rho/\chi)^{1/2}$  as a first step to examine the spin-wave velocity as the function of V and  $V_2$ . The present calculation is performed by choosing U=4, which leads to  $v \simeq 1.29$  for  $V = V_2 = 0$  and  $t_d = 0$ .

# **B.** *V* dependence $(V_2=0 \text{ and } t_d=0)$

Now we consider the V dependence of the spin-wave velocity for  $V_2=0$ ,  $t_d=0$ , and U/t=4. Contrary to the weakcoupling limit that can be studied analytically as the incommensurate case,<sup>25</sup> this intermediate-coupling regime requires numerical calculation. Figure 3 shows the V dependence of v,  $\chi$ , and  $\rho$  (all quantities are normalized to their value at  $V=V_2=0$  and  $t_d=0$ ). The arrow indicates the critical value  $V_c=0.34$  separating regions I ( $S_1 \neq 0$ ) and II ( $S_1, D_2 \neq 0$ ). In region II ( $V > V_c$ ), both  $\rho$  and  $\chi$  decrease for decreasing V. The stronger decrease of  $\rho$  results in a decrease of the spinwave velocity. For large V, both the spin stiffness and the



FIG. 4.  $V_2$  dependence of v,  $\chi$ , and  $\rho$  for U=4,  $t_d=0$ , and V=0. There is a cusp at the critical value  $V_{2c}=1.32$  corresponding to the transition from state I to state III. The inset shows the  $V_2$  dependence of the order parameters  $S_1$ ,  $D_1$  ( $2k_F$  CDW), and  $S_2$  ( $4k_F$  SDW).

spin-wave velocity vanish. It seems that the decrease of v in region II mainly comes from the reduction of kinetic energy due to the formation of the  $4k_{\rm F}$  CDW. Note that the spin-wave velocity is discontinuous at the critical value  $V=V_c$ . The small jump at  $V_c$  originates in the discontinuity of  $S_1$  and  $D_2$  (see inset of Fig. 3), which is found only for  $t_d=0.^6$ 

# C. $V_2$ dependence $(t_d=0)$

In this section, we analyze the  $V_2$  dependence of the spinwave velocity for U=4,  $t_d=0$  and different values of V. Figure 4 shows  $v/v^0$ ,  $\chi/\chi^0$ , and  $\rho/\rho^0$  in the case V=0 (the inset shows  $S_1$ ,  $D_1$ , and  $S_2$  as a function of  $V_2$ ). There is a transition between regions I and III at the critical value  $V_{2c}$ .  $v/v^0$ ,  $\chi/\chi^0$  and  $\rho/\rho^0$  are constant for  $V_2 < V_{2c}$  and decrease for  $V_2 > V_{2c}$  (note that v actually slightly increases at large  $V_2$ ). However, all these quantities remain finite in the limit of large  $V_2$ . This is to be contrasted to the large-V limit (region II) where the spin-wave velocity vanishes (Fig. 3). Such a behavior can be understood as follows. For  $V_2 \rightarrow \infty$ (region III), the spin- and charge-density waves in the ground state are of the type  $(\uparrow,\downarrow,0,0)$  and (1,1,0,0), respectively. Our numerical calculation shows that this behavior already shows up for  $V_2/t \approx 4$ . In this limit  $(V_2/t \approx 4)$ , the onedimensional chain divides into independent two-site clusters. For this problem, one can find the exact expression of the spin-wave velocity (Appendix B):

$$v/v^{0} = \left(\frac{\rho}{\chi}\right)^{1/2} / v^{0} = (t - t_{d})/v^{0}.$$
 (4.1)

For U=4,  $v^0=1.286$ , so that  $v/v^0=0.777$ . For  $V_2/t=4$  and 13, the numerical calculation gives  $v/v^0=0.763$  and 0.776, respectively, in excellent agreement with the analytical result of the two-site problem.

Now we consider the  $V_2$  dependence of  $\chi/\chi^0$ ,  $\rho/\rho^0$  and  $v/v^0$  for V=0, 1, 2, and 3. For V=1, there is first a transition from region II to region I, and then a transition from I to III. For V=2 or 3, there is a single transition occuring be-



FIG. 5. (a)  $V_2$  dependence of  $\chi$  for V=0 (Fig. 4), 1, 2, and 3. There is a jump due to the first-order transition between II and III indicated by the dashed curve in Fig. 1. The inset shows the  $V_2$ dependence of  $\rho$ . (b)  $V_2$  dependence of v for V=0 (Fig. 4), 1, 2, and 3. For V=1, there is a small jump at  $V_2=0.66$ , which corresponds to the transition between II and I. This discontinuity can also be seen in Fig. 3.

tween II and III. The ratios  $\chi/\chi^0$  and  $\rho/\rho^0$  (inset) exhibit a similar behavior [Fig. 5(a)]. They are constant in region I, and increase (decrease) in II (III) when  $V_2$  increases. Figure 5(b) shows the spin-wave velocity  $v/v^0$ , which turns out to be mainly determined by  $\rho/\rho^0$ . Except in region I and for large values of  $V_2$ , v varies strongly as a function of  $V_2$ .

Here we comment on the fact that v remains finite at large  $V_2$ . Within the mean-field treatment, which is expected to be valid for a moderate coupling between chains, both  $\chi$  and  $\rho$  remain finite at large  $V_2$ . On the other hand, for one-dimensional systems it is known from bosonization that  $\chi$  vanishes at large  $V_2$  due to the formation of a spin gap.<sup>34</sup> Thus, we expect our mean-field analysis in region III of Fig. 1 to break down when the interchain coupling becomes sufficiently small.

### **D.** Effect of dimerization

Finally, we consider the effect of dimerization on the spin-wave velocity v. Figure 6(a) shows the V dependence for U=4,  $V_2=0$  and  $t_d=0$  (solid curve), 0.1 (dotted curve), 0.3 (dashed curve) and 0.5 (dash-dotted curve). The effect of dimerization is large in region I, but rather small in region II. A finite  $t_d$  increases the band gap. This induces a suppression of  $\prod_{j=1}^{x_{j=1}} a$  and  $\rho$ , and leads ultimately to a reduction of the



FIG. 6. (a) V dependence of v for U=4,  $V_2=0$ , and  $t_d=0$ , 0.1, 0.3, and 0.5. (b)  $V_2$  dependence of v for U=4, V=0, and  $t_d=0$ , 0.1, 0.3, and 0.5.

spin-wave velocity. We note that the reduction of  $S_1$  and  $D_2$  in region II by the dimerization has little effect on v, since the dependence of  $S_1$  and  $D_2$  on dimerization is very small for  $V \leq 4$ .

Figure 6(b) shows the  $V_2$  dependence of v for U=4, V=0, and  $t_d=0$  (solid curve), 0.1 (dotted curve), 0.3 (dashed curve), and 0.5 (dash-dotted curve). The effect of dimerization is noticeable in both regions I and III. The limiting behavior for large  $V_2$  is given by Eq. (4.1). In that limit, the SDW exists for  $U>2(t-t_d)$  and the spin-wave velocity v depends only on t and  $t_d$ .

#### **V. CONCLUSION**

In conclusion, the nearest- and next-nearest-neighbor interactions strongly affects the spin-wave velocity in the intermediate-coupling regime  $U \sim 4t$ . Our main results are as follows. (i) In the pure SDW state (region I), the spin-wave velocity v is independent of the nearest (V) and next-nearest ( $V_2$ ) interaction (Fig. 3). (ii) For coexisting  $2k_F$  SDW and  $4k_F$  CDW (region II), v decreases (increases) as a function of  $V(V_2)$  [Figs. 3 and 5(b)]. It is slightly discontinuous at the transition between I and II and vanishes (as well as the spin stiffness) at large V (Fig. 3). (iii) For coexisting  $2k_F$ SDW,  $2k_F$  CDW, and  $4k_F$  SDW (region III), v is suppressed by  $V_2$ . It tends to a finite value at large  $V_2$  [Figs. 4 and 5(b)]. (iv) The dimerization decreases the spin-wave velocity [Figs. 6(a) and 6(b)].

As discussed in Sec. III B, our approach is limited to the weak- to intermediate-coupling regime and should hold when  $U, V, V_2 \leq 4t$ . In the half-filled Hubbard model, a strong-coupling is known to reduce the spin-wave velocity from v = O(t) to v = O(J) (with  $J = 4t^2/U \ll t$ ). We also expect a decrease of the spin-wave velocity in the more general case we have studied when  $U, V, V_2$  become larger than 4t. Therefore, our main conclusion (a reduction of the spin-wave velocity by the interactions  $V, V_2$ ) is likely to be strengthened by strong coupling effects. The Stoner factor  $(1 - 2\chi U)^{1/2}$ , which arises from the coupling to long-wavelength spin fluctuations, was not considered in our analysis. It leads to a decrease of v when the on-site interaction U increases. Whether the Stoner factor depends on the interactions V and  $V_2$  remains an open question.

In the compounds that have been studied experimentally,<sup>4,5</sup> the Bechgaard salts  $(TMTSF)_2PF_6$  and  $(TMTSF)_2AsF_6$  and the Fabre salt  $(TMTTF)_2Br$ , the electron-electron interaction is expected to be in the intermediate coupling regime  $(U \sim 4t)$ . Furthermore, estimates by Mila<sup>36</sup> and quantum-chemistry calculations<sup>37</sup> have revealed the finite-range part of the Coulomb potential, the first-neighbor interaction V being equal or even larger than U/2. We therefore think that our conclusions are relevant to the Bechgaard-Fabre salts studied in Refs. 4 and 5.

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#### **APPENDIX A: DERIVATION OF EQ. (3.22)**

We rewrite Eq. (3.19) as

$$\mathcal{S}_{\text{eff}} = \frac{1}{2} \int d\xi \, d\tau \{ \chi(\partial_{\tau} \mathbf{n})^2 + \rho(\partial_{\xi} \mathbf{n})^2 \} - \frac{1}{2} \sum_{\tilde{q}} \{ (\langle K \rangle_{\text{MF}} + \prod_{j_x^z j_x^z}) |A_x^z(\tilde{q})|^2 + \prod_{j_0^z j_0^z} |A_0^z(\tilde{q})|^2 \},$$
(A1)

where  $\rho$  and  $\chi$  are given by

$$\rho = -\frac{1}{4} (\langle K \rangle_{\rm MF} + \Pi_{j_x^{x_j x}}) = -\frac{1}{4} (\langle K \rangle_{\rm MF} + \Pi_{j_x^{y_j y}}), \quad (A2)$$

and

$$\chi = \langle S_{\nu} S_{\nu} \rangle_{\rm MF} = \frac{1}{4} \Pi_{j_0^{\nu} j_0^{\nu}}, \quad \nu = x, y.$$
 (A3)

To show that the second term of Eq. (A1) vanishes, we use the invariance of the action under the gauge transformation  $A^{z}_{\mu}(\xi,\tau) \rightarrow A^{z}_{\mu}(\xi,\tau) + \frac{1}{2}\partial_{\mu}\Lambda(\xi,\tau)(\mu = \xi \text{ or } \tau).^{33}$  This transformation corresponds to a rotation of  $\mathbf{n}_{\text{MF}} = \hat{\mathbf{z}}$  around the  $\hat{\mathbf{z}}$ axis and does not change the state of the system. The invariance of the action in this gauge transformation implies

$$-\frac{1}{2}\sum_{\tilde{q}}\left\{\left(\langle K\rangle_{\rm MF}+\Pi_{j_x^z j_x^z}\right)\left[\frac{1}{4}q_x^2|\Lambda(\tilde{q})|^2-iA_x^z(\tilde{q})q_x\Lambda\right.\\\left.\left(-\tilde{q}\right)\right]+\Pi_{j_0^z j_0^z}\left[\frac{1}{4}\Omega^2|\Lambda(\tilde{q})|^2+iA_0^z(\tilde{q})\Omega\Lambda(-\tilde{q})\right]\right\}=0.$$
(A4)

Since Eq. (A4) should be valid for an arbitrary function  $\Lambda$ , we deduce

$$\langle K \rangle_{\rm MF} + \prod_{j_x^z j_x^z} = 0, \qquad (A5)$$

$$\Pi_{j_0^z j_0^z} = 0, \tag{A6}$$

which lead to the vanishing of the second line of Eq. (A1).

Equations (A5) and (A6) can also be obtained from the U(1) electromagnetic field gauge invariance. Noting that  $\Pi_{j^z_{\mu}j^z_{\mu}} = \Pi_{j^0_{\mu}j^0_{\mu}}$ , Eqs. (A5) and (A6) can be rewritten as

$$\langle K \rangle_{\rm MF} + \prod_{j^0,j^0} = 0, \qquad (A7)$$

$$\Pi_{j_0^0 j_0^0} = 0. \tag{A8}$$

We recognize here the components of the polarization tensor for the usual U(1) electromagnetic gauge field. Equations (A7) and (A8) follow from (electromagnetic) gauge invariance.<sup>35</sup>

# APPENDIX B: LIMITING CASE OF LARGE V2

When  $V_2 \rightarrow \infty$ , the mean-field solution in region III corresponds to that of a half-filled two-site system given by

$$H = -(t - t_{\rm d}) \sum_{\sigma} (C^{\dagger}_{1\sigma}C_{2\sigma} + \text{H.c.})$$
$$+ U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) + V \sum_{\sigma,\sigma'} n_{1\sigma}n_{2\sigma'}, \quad (B1)$$

where  $n_{1\sigma}$   $(n_{2\sigma}) = C_{1\sigma}^{\dagger} C_{1\sigma}$   $(C_{2\sigma}^{\dagger} C_{2\sigma})$  and  $C_{1\sigma}^{\dagger}$   $(C_{2\sigma}^{\dagger})$  denote the creation operators of an electron at site 1 (2) with spin  $\sigma$ . The mean-field equations are given by

$$\sum_{\sigma} \langle C_{1\sigma}^{\dagger} C_{1\sigma} \rangle = \sum_{\sigma} \langle C_{2\sigma}^{\dagger} C_{2\sigma} \rangle = 1, \qquad (B2)$$

$$\sum_{\sigma} \langle C_{1\sigma}^{\dagger} C_{1\sigma} \rangle \operatorname{sgn}(\sigma) = \Delta, \qquad (B3)$$

$$\sum_{\sigma} \langle C_{2\sigma}^{\dagger} C_{2\sigma} \rangle_{\text{sgn}}(\sigma) = -\Delta, \qquad (B4)$$

where the average  $\langle \rangle$  is performed with the mean-field Hamiltonian

$$\begin{split} H_{\rm MF} &= -\left(t - t_{\rm d}\right) \sum_{\sigma} \left(C_{1\sigma}^{\dagger}C_{2\sigma} + {\rm H.c.}\right) \\ &+ \sum_{\sigma} \left[ \left(\frac{U}{2} + V - {\rm sgn}(\sigma) \frac{U}{2}\Delta\right) C_{1\sigma}^{\dagger}C_{1\sigma} \right. \\ &+ \left(\frac{U}{2} + V + {\rm sgn}(\sigma) \frac{U}{2}\Delta\right) C_{2\sigma}^{\dagger}C_{2\sigma} \right] \\ &- \frac{U}{2} - V + \frac{U}{2}\Delta^2. \end{split} \tag{B5}$$

From Eqs. (B2), (B3), (B4), and (B5), the self-consistency equation for  $\Delta$  is expressed as

$$1 = \frac{U/2}{\sqrt{[(U/2)\Delta]^2 + (t - t_d)^2}},$$
 (B6)

where  $\mu = U/2 + V$  at half-filling. The solution of Eq. (B6) is obtained as

$$\Delta = \pm \sqrt{1 - \left(\frac{2(t - t_{\rm d})}{U}\right)^2},\tag{B7}$$

for  $U/(t-t_d) > 2$ . By using Eq. (B7), we compute the uniform transverse spin susceptibility  $(\chi')$  and the spin stiffness  $(\rho')$ :

$$\chi' \equiv \frac{1}{2} \sum_{n,n'=1,2} \left[ \frac{1}{4} \langle j_0^x(n) j_0^x(n') \rangle |_{i\Omega=0} \right] = \frac{1}{2U} - \frac{2(t-t_d)^2}{U^3},$$
(B8)

$$\rho' = -\frac{1}{4} \left( \langle K' \rangle + \Pi'_{j_x^x j_x^x} \right) = (t - t_d)^2 \left( \frac{1}{2U} - \frac{2(t - t_d)^2}{U^3} \right),$$
(B9)

where the kinetic energy per site  $(\langle K' \rangle)$  and the spin currentcurrent correlation function  $(\Pi'_{i^x i^x})$  are given by

$$\langle K' \rangle \equiv \frac{1}{2} \left\langle -(t-t_{\rm d}) \sum_{\sigma} (C^{\dagger}_{1\sigma}C_{2\sigma} + \text{H.c.}) \right\rangle = -\frac{2(t-t_{\rm d})^2}{U},$$
(B10)

$$\Pi' j_{x}^{x} j_{x}^{x} \equiv \frac{1}{2} \sum_{n,n'=1,2} \langle j_{x}^{x}(n) j_{x}^{x}(n') \rangle |_{i\Omega=0} = \frac{8(t-t_{d})^{4}}{U^{3}},$$
(B11)

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with

$$j_{x}^{x}(n) = -\frac{i(t-t_{d})}{2} \sum_{\sigma} (C_{1,\sigma}^{\dagger}C_{2,-\sigma} - C_{2,\sigma}^{\dagger}C_{1,-\sigma}).$$
(B13)

By noting that  $\chi = \chi'/2$  and  $\rho = \rho'/2$ , we obtain the spinwave velocity of the one-dimensional system [Eq. (2.1)] in the limit  $V_2 \rightarrow \infty$  as

$$v = \left(\frac{\rho}{\chi}\right)^{1/2} = t - t_d \,. \tag{B14}$$

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