Influence of electron-phonon interaction on soliton mediated spin-charge conversion effects in two-component polymer model

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Abstract

By mapping a Hubbard-like model describing a two-component polymer in the presence of strong enough electron-phonon interactions (κ) onto the system of two coupled nonlinear Schrödinger equations with $U(2)$ symmetry group, some nontrivial correlations between topological solitons mediated charge Q and spin S degrees of freedom are obtained. Namely, in addition to a charge fractionalization and reentrant like behavior of both $Q(\kappa)$ and $S(\kappa)$, the model also predicts a decrease of soliton velocity with κ as well as spin-charge conversion effects which manifest themselves through an explicit $S(Q,\Omega)$ dependence (with Ω being a mixing angle between spin-up and spin-down electron amplitudes). A possibility to observe the predicted effects in low-dimensional systems with charge and spin soliton carriers is discussed.

Keywords: Conducting polymers; Electron-phonon interactions; Solitons; Charge fractionalization; Spin-charge conversion effects

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INTRODUCTION

In an attempt to better understand the underlying transport mechanisms in conducting polymers, based on the Su-Schrieffer-Heeger (SSH) model and its modifications [1–8], some extensive numerical simulations have been carried out in recent years (see, e.g., [9–11] and further references therein). In particular, Förner et al. [9] confirmed that, at the self-consistent field level, the soliton velocity decreases with the inclusion of electron-electron interactions into the conventional SSH calculations. At the same time, recently performed thorough analysis by Ma and Schollwöck [11] on the relationship between electron-electron interactions and charged soliton transport in conjugated polymers under the influence of an external time-dependent electric field revealed that the dependence of the stationary velocity of a charged soliton on the on-site Coulomb interactions U and the nearest-neighbor interactions V is due to the extent of delocalization of the charged soliton defect.

Besides, some novel phenomena have been observed or predicted to occur in nodal antiferromagnetic insulators (with spin-charge-separated solitons, which are similar to that in the quasi one-dimensional conductor polyacetylene) and other low-dimensional physical systems with nontrivial topology, including charge and spin fractionalization phenomena, doping mediated boson-fermion mutations of mobile half skyrmion quasiparticles, etc [12–19].

On the other hand, recent experimental and theoretical results on charge-spin exchange effects in quasi-1D organic charge transfer salts have re-kindled the interest to their unusual transport properties [20] which in many respects resemble the behavior of conducting polymers.

In this paper we consider the influence of electron-phonon interactions on soliton mediated spin-charge correlation effects within a tight-binding approximation of the SSH-based extended Hubbard Hamiltonian describing a two-component polymer. First, we show that treating electron correlations on the ground state only allows to map the microscopic model onto the system of two coupled nonlinear Schrödinger equations (NLSE) with $U(2)$ symmetry group (which is known to describe many different phenomena, including "dark" solitons in self-focusing media [21], two-component Bose gas with repulsion [22], etc). Next, we obtain exact topological soliton solutions (kinks) of NLSE corresponding to non-trivial boundary conditions. And finally, we discuss the charge Q and spin S properties of the obtained solutions. In particular, we shall demonstrate that in addition to a reentrant like dependence of

both Q and S on electron-phonon coupling parameter κ and decrease of soliton velocity with κ, the model also predicts a charge fractionalization as well as some interesting spin-charge exchange (conversion) effects.

THE MODEL

Let us consider a modified Hubbard model (based on the SSH Hamiltonian) describing a two-component polymer (with two magnetic sublattices, A and B) in the presence of strong enough electron-phonon interactions. The effective Hamiltonian of the system under consideration can be cast into the following form (Cf. [22]):

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_{ph} + \mathcal{H}_{e-ph} \tag{1}$$

where

$$\mathcal{H}_e = -t_0 \sum_{n\sigma} \left(c^{+A}_{n\sigma} c^{B}_{n+1\sigma} + c^{+B}_{n\sigma} c^{A}_{n+1\sigma} + h.c. \right) + \frac{U}{2} \sum_{a=A,B} \sum_{n\sigma} n^{a}_{n\sigma} n^{a}_{n-\sigma} \tag{2}$$

$$\mathcal{H}_{ph} = \frac{M}{2} \sum_{n} \dot{R}^2_n + \frac{\alpha}{2} \sum_{n} (R_{n+1} - R_n)^2 \tag{3}$$

and

$$\mathcal{H}_{e-ph} = I \sum_{n\sigma} (u_{n+1} - u_n) \left(c^{+A}_{n\sigma} c^{B}_{n+1\sigma} + c^{+B}_{n\sigma} c^{A}_{n+1\sigma} + h.c. \right) \tag{4}$$

Here, $c^{+}_{n\sigma}(c_{n\sigma})$ is the creation (annihilation) operator of π-electron with spin σ in a Wannier state of the n-th atom, t_0 is the hopping integral between nearest neighbors, U is the repulsive interaction between electrons of the same atom, M is the mass of a monomer, α is the elastic constant, $R_n = R_{n0} + u_n$ is the position of the n-th atom (with u_n being the deviation from its equilibrium position R_{n0}), $n^{A}_{n\sigma} = c^{+A}_{n\sigma} c^{A}_{n\sigma}$ is the number operator, and I is the amplitude of electron-phonon interactions.

The Heisenberg equations of motion for $c^{A}_{n\sigma}(t)$ read:

$$i\hbar \dot{c}^{A}_{i\sigma} = \left[c^{A}_{i\sigma}, \mathcal{H} \right] = U c^{A}_{i\sigma} n^{A}_{i-\sigma} + \left[t_0 + I(u_i - u_{i+1}) \right] c^{B}_{i+1\sigma} + \left[t_0 + I(u_{i-1} - u_i) \right] c^{B}_{i-1\sigma} \tag{5}$$

By introducing properly defined ground state $|0>$ for the problem at hand, we can map the above operator equations onto their c-number counterparts on wave function amplitudes $\phi_{i\sigma} =< 0|c_{i\sigma}|0 >$ (assuming a standard products decoupling procedure [22]) which obey the conventional Hamilton equations of motion:

$$i\hbar \dot{\phi}^{A,B}_{j\sigma} = U \phi^{A,B}_{j\sigma} |\phi^{A,B}_{j-\sigma}|^2 + \left[t_0 + I(u_j - u_{j+1}) \right] \phi^{B,A}_{j+1\sigma} + \left[t_0 + I(u_{j-1} - u_j) \right] \phi^{B,A}_{j-1\sigma} \tag{6}$$

As usual, these equations should be completed by the lattice vibrations:

$$M\ddot{R}_j = \alpha(R_{j+1} - 2R_j + R_{j-1}) + I\sum_\sigma[\phi^{*A}_{j\sigma}(\phi^A_{j+1\sigma} - \phi^A_{j-1\sigma}) + \phi^{*B}_{j\sigma}(\phi^B_{j+1\sigma} - \phi^B_{j-1\sigma}) + c.c.] \quad (7)$$

Let us consider a continuous approximation of the initial discrete model (1) when the lattice parameter $a \to 0$. In this approximation we have:

$$\begin{aligned} R_{j\pm1} &\to u(x,t) \pm a u_x(x,t) + \frac{a^2}{2}u_{xx}(x,t) + ..., \\ \phi_{j\pm1\sigma} &\to \phi_\sigma(x,t) \pm a\phi_{\sigma x}(x,t) + \frac{a^2}{2}\phi_{\sigma xx}(x,t) + ... \end{aligned} \quad (8)$$

In such a way, the equations of motion (6) and (7) become:

$$i\hbar\dot{\phi}^{A,B}_\sigma = U\phi^{A,B}_\sigma|\phi^{A,B}_{-\sigma}|^2 + 2\left(t_0 - Iau_x\right)\phi^{B,A}_\sigma + \frac{a^2}{2}\phi^{B,A}_{\sigma xx} \quad (9)$$

and

$$M\ddot{u} = \alpha a^2 u_{xx} + 2Ia\sum_\sigma \frac{\partial}{\partial x}\left(|\phi^A_\sigma|^2 + |\phi^B_\sigma|^2\right) \quad (10)$$

To emphasize the role of the electron-phonon interaction in the charge transfer mechanism, we neglect the Coulomb repulsion of electrons (assuming $U \ll t_0$), taking electron correlations on the level of the ground state only. In particular, for the antiferromagnetic ground state, this leads to the constraint $\phi^B_{-\sigma} = \phi^A_\sigma \equiv \phi_\sigma$. Furthermore, keeping in mind only wave-like solutions for both electron amplitudes $\phi_\sigma(z)$ and displacement field $u(z)$ with $z = x - vt$, the first integral of Eq.(10) reads:

$$u_z + 2Iad\sum_\sigma V(\phi_\sigma) = C \quad (11)$$

where $V(\phi_\sigma) = |\phi_\sigma|^2 + |\phi_{-\sigma}|^2$, $d^{-1} \equiv \alpha a^2 - Mv^2$, C is the integration constant (see below), and $\sigma = (\uparrow, \downarrow)$.

In view of this result, Eq.(9) produces the Hartree-Fock (HF) type system with the self-consistent potential:

$$i\hbar\dot{\phi}_\sigma + a^2T\phi''_{-\sigma} + \left[2T - 4I^2a^2d\sum_\sigma V(\phi_\sigma)\right]\phi_{-\sigma} = 0 \quad (12)$$

where $T = CIa - t_0 > 0$.

Finally, introducing the spin mixture amplitudes $\Phi_\pm(x,t) = \phi_\uparrow \pm \phi_\downarrow$, we obtain the system of two coupled nonlinear equations:

$$\begin{aligned} i\hbar\dot{\Phi}_+ \; + \; a^2T\Phi''_+ - 2\left[-T + I^2a^2dV(\Phi_\pm)\right]\Phi_+ = 0 \\ i\hbar\dot{\Phi}_- \; - \; a^2T\Phi''_- + 2\left[-T + I^2a^2dV(\Phi_\pm)\right]\Phi_- = 0 \end{aligned} \quad (13)$$

with $V(\Phi_\pm) = |\Phi_+|^2 + |\Phi_-|^2$ which can be readily cast into the canonical form of the U(2) NLSE model [21–23]:

$$\begin{aligned} i\psi_{1\tilde{t}} + \psi_{1\tilde{x}\tilde{x}} - 2(|\psi_1|^2 + |\psi_2|^2 - \rho^2)\psi_1 &= 0 \\ i\psi_{2\tilde{t}} + \psi_{2\tilde{x}\tilde{x}} - 2(|\psi_1|^2 + |\psi_2|^2 - \rho^2)\psi_2 &= 0 \end{aligned} \tag{14}$$

with $\psi_1 \equiv \Phi_+$, $\psi_2 \equiv \Phi_-^*$, $\kappa = I^2a^2d/T$, and $\rho^2 = \frac{2}{\kappa}$. Hereafter, $\tilde{x} = \sqrt{\frac{\kappa}{2a^2}}x$ and $\tilde{t} = \left(\frac{T\kappa}{2\hbar}\right)t$ stand for dimensionless space-time variables.

By introducing a two-component vector $\psi(x,t) = \binom{\psi_1}{\psi_2}$, we can rewrite the system (14) in the compact form

$$i\psi_t + \psi_{xx} - 2[(\bar{\psi}\psi) - \rho^2]\psi = 0 \tag{15}$$

with an explicit U(2) inner product $(\bar{\psi}\psi) \equiv |\psi_1|^2 + |\psi_2|^2$. It can be easily verified that Eq.(15) is generated by the Hamiltonian $H = \bar{\psi}_x\psi_x + (\bar{\psi}\psi - \rho^2)^2$. Thus, any transformations $\psi' = \mathcal{R}\psi$ of the vector ψ which conserve the inner product $(\bar{\psi}'\psi') = (\bar{\psi}\psi)$ are the symmetry transformations of the system because they will also conserve the Hamiltonian H and will not change Eq.(15). In our particular case, U(2) symmetry describes intrinsic degrees of freedom with a possibility of mixing between spin-up and spin-down electron amplitudes.

To study the evolution of the system from the antiferromagnetic ground state, it is natural to consider the non-vanishing (that is constant at both limits) boundary conditions

$$\lim_{x\to\pm\infty}\psi(x,t) = \psi_\pm, \qquad \lim_{x\to\pm\infty}\psi_x(x,t) = 0 \tag{16}$$

leading to $(\bar{\psi_+}\psi_+) = (\bar{\psi_-}\psi_-) = \rho^2$.

RESULTS AND DISCUSSION

Turning to the analysis of the above-obtained $U(2)$ NLSE system describing transport properties of the original Hubbard model, notice first of all that it is electron-phonon interaction I which is actually responsible for nonlinear character of the dynamics. Indeed, as it can be easily verified, the system (16) possesses the kink (topological or "dark" soliton) type solution [21–23]:

$$\psi(x,t) = \psi_+ \left(\frac{\lambda - i\nu \tanh \nu z}{\lambda - i\nu} \right) \tag{17}$$

where $z = \tilde{x} - 2\lambda\tilde{t}$ with $\nu z \equiv \gamma(x - vt)$. The dimensionless spectral parameters λ and ν obey the boundary conditions imposed constraint $\lambda^2 + \nu^2 = \rho^2$ and are related to the decaying length γ and kink velocity v as follows, $\nu = \gamma a$ and $\lambda = v/v_0$ (with $v_0 = 2aT/\hbar$ being some characteristic velocity).

Before we proceed any further, let us briefly discuss the ground state properties of the system (16) whose energy is given by $E = \int_{-\infty}^{+\infty} dx[\bar{\psi}_x \psi_x + (\bar{\psi}\psi - \rho^2)^2]$. It can be shown [24] that a trivial "vacuum" solution with $\psi_v = 0$ is unstable under the assumed boundary conditions. Instead, a stable ground-state solution of this model (which has a zero energy) is given by "condensate" amplitudes (with a constant density ρ which is related to the electron-phonon coupling constant κ within our model as $\rho = \sqrt{\frac{2}{\kappa}}$): $\psi_{1c} = \frac{1}{\sqrt{2}}\rho e^{i\theta_1}$ and $\psi_{2c} = \frac{1}{\sqrt{2}}\rho e^{i\theta_2}$ (where $\theta_{1,2}$ are constant phases). In turn, using the method of Ref. [24], it can be also demonstrated that the above-introduced kink solution is a stable excitation (based on the "condensate" background) for all velocities and has the energy $E_K = \frac{2}{3}(1 + \frac{2}{\kappa})\nu^3$. Besides, it is worthwhile to mention that the $U(2)$ NLSE model with non-vanishing boundary conditions is an integrable system [25] which is another confirmation of the soliton stability.

Let us return now to the initial physical model of this paper and discuss the above-obtained exact results in terms of electron amplitudes. Performing step by step a series of transforms, from Eq.(17) we obtain finally:

$$\phi_\uparrow(z) = \phi_{+\uparrow} \left(1 - \frac{\nu^2 e^{-\nu z}}{\rho^2 \cosh \nu z} \right) + i\phi_{+\downarrow} \left(\frac{\lambda \nu e^{-\nu z}}{\rho^2 \cosh \nu z} \right) \tag{18}$$

and

$$\phi_\downarrow(z) = \phi_{+\downarrow} \left(1 - \frac{\nu^2 e^{-\nu z}}{\rho^2 \cosh \nu z} \right) + i\phi_{+\uparrow} \left(\frac{\lambda \nu e^{-\nu z}}{\rho^2 \cosh \nu z} \right) \tag{19}$$

for spin-up and spin-down kink-type state amplitudes, respectively.

In turn, the above amplitudes contribute to the formation of kink-mediated charge-density-wave (CDW)

$$n(z) = |\phi_\uparrow|^2 + |\phi_\downarrow|^2 = n_0 \left(\frac{\lambda^2 + \nu^2 \tanh^2 \nu z}{\rho^2} \right) \tag{20}$$

and spin-density-wave (SDW)

$$\mu(z) = |\phi_\uparrow|^2 - |\phi_\downarrow|^2 \;=\; \mu_0 \left(\frac{\lambda^2 + \nu^2 \tanh^2 \nu z}{\rho^2} - \frac{2\lambda^2 \nu^2 e^{-2\nu z}}{\rho^4 \cosh^2 \nu z} \right) + \; 2\lambda\nu\mu_1 e^{-\nu z} \left(\frac{\lambda^2 \cosh \nu z + \nu^2 \sinh \nu z}{\rho^4 \cosh^2 \nu z} \right) \sin\Omega \tag{21}$$

local profiles, where

$$\begin{aligned} n_0 \;&=\; \lim_{z\to+\infty} n(z) = |\phi_{+\uparrow}|^2 + |\phi_{+\downarrow}|^2 \\ \mu_0 \;&=\; \lim_{z\to+\infty} \mu(z) = |\phi_{+\uparrow}|^2 - |\phi_{+\downarrow}|^2 \\ \mu_1 \;&=\; 2|\phi_{+\uparrow}||\phi_{+\downarrow}| = \sqrt{n_0^2 - \mu_0^2} \end{aligned} \tag{22}$$

and $\Omega = \arg\phi_{+\uparrow} - \arg\phi_{+\downarrow}$ is the mixing angle.

The evolution of the local profiles of kink mediated CDW and SDW with electron-phonon constant κ (for $\lambda = 1$ and $\Omega = 0$) is shown in Fig.1 and Fig.2, respectively (recall that $\nu = \sqrt{\rho^2 - \lambda^2}$ with $\rho^2 = \frac{2}{\kappa}$).

Furthermore, based on the above local densities, $n(z)$ and $\mu(z)$, it is natural to introduce the kink-carrying net topological charge

$$Q = Q_0 \int_{-\infty}^{+\infty} dz \left[\frac{n(z) - n_0}{n_0} \right] = -\frac{2\nu}{\rho^2} Q_0 \tag{23}$$

and spin

$$S = \int_{-\infty}^{+\infty} dz \left[\frac{\mu(z)}{\mu_0} \right] = \frac{2\nu(\lambda^2 - \nu^2)}{\rho^4} + \frac{4\lambda\nu^2}{\rho^4} f(p,\Omega) \tag{24}$$

Here, $f(p,\Omega) = \sqrt{(1-p^2)/p^2}\sin\Omega$ with $p = \mu_0/n_0 = (|\phi_{+\uparrow}|^2 - |\phi_{+\downarrow}|^2)/(|\phi_{+\uparrow}|^2 + |\phi_{+\downarrow}|^2)$ being an effective spin polarization.

The analysis of the above expressions reveals that both charge Q and spin S depend on electron-phonon constant κ, namely

$$q(\kappa) \equiv \frac{Q(\kappa)}{Q_0} = -\sqrt{2\kappa - \lambda^2\kappa^2} \tag{25}$$

and

$$S(\kappa) = (\lambda^2\kappa - 1)\sqrt{2\kappa - \lambda^2\kappa^2} - \lambda\kappa(\lambda^2\kappa - 2) f(p,\Omega) \tag{26}$$

The dependence of $q = Q/Q_0$ on κ for different values of kink velocity $\lambda = v/v_0$ is shown in Fig.3. Notice its reentrant behavior with minima corresponding to fractional charge values.

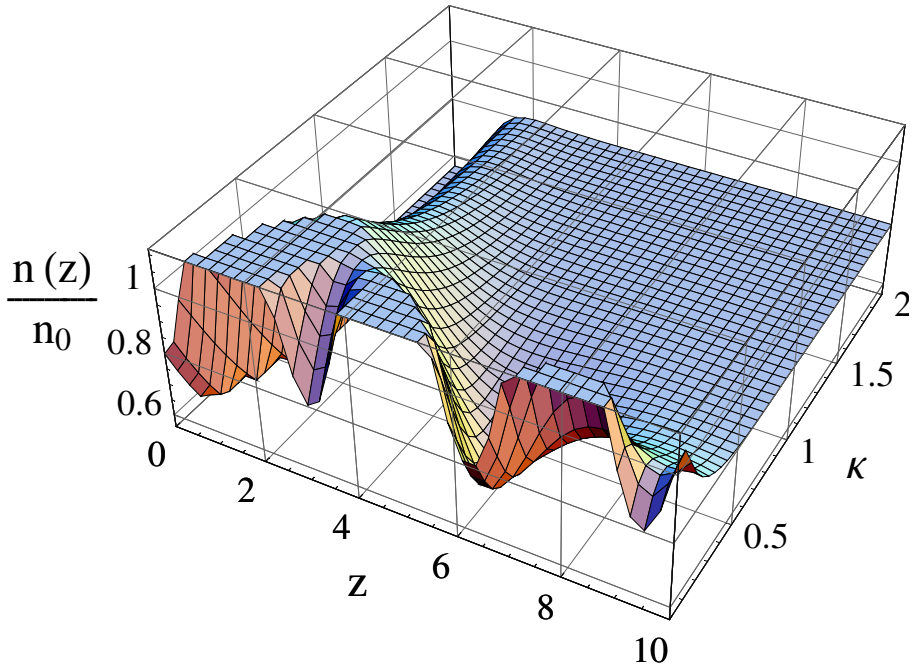

FIG. 1: The dependence of the local profile of kink mediated CDW on electron-phonon constant κ for $\lambda = 1$.

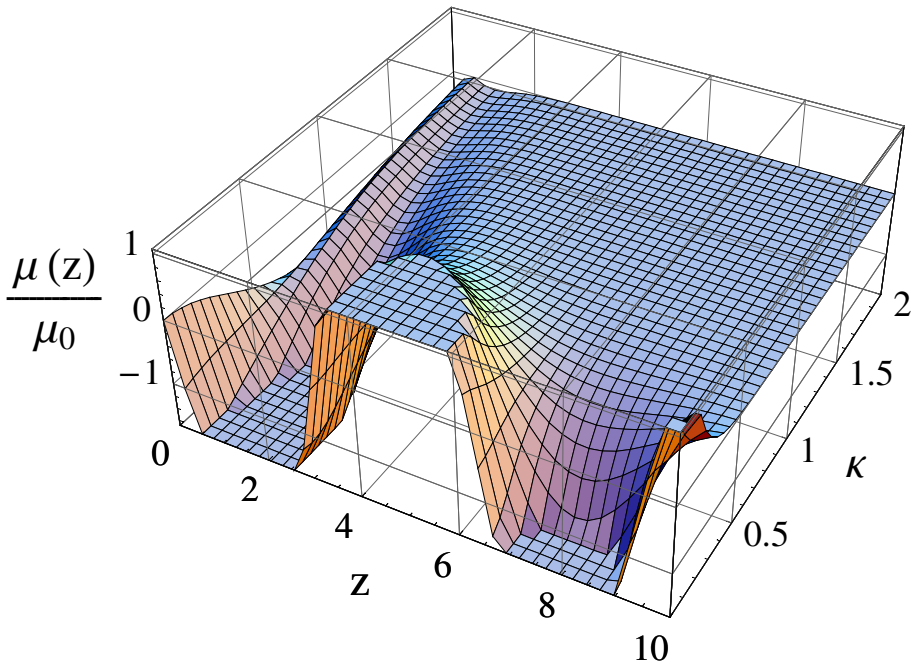

FIG. 2: The dependence of the local profile of kink mediated SDW on electron-phonon constant κ for $\lambda = 1$ and $\Omega = 0$.

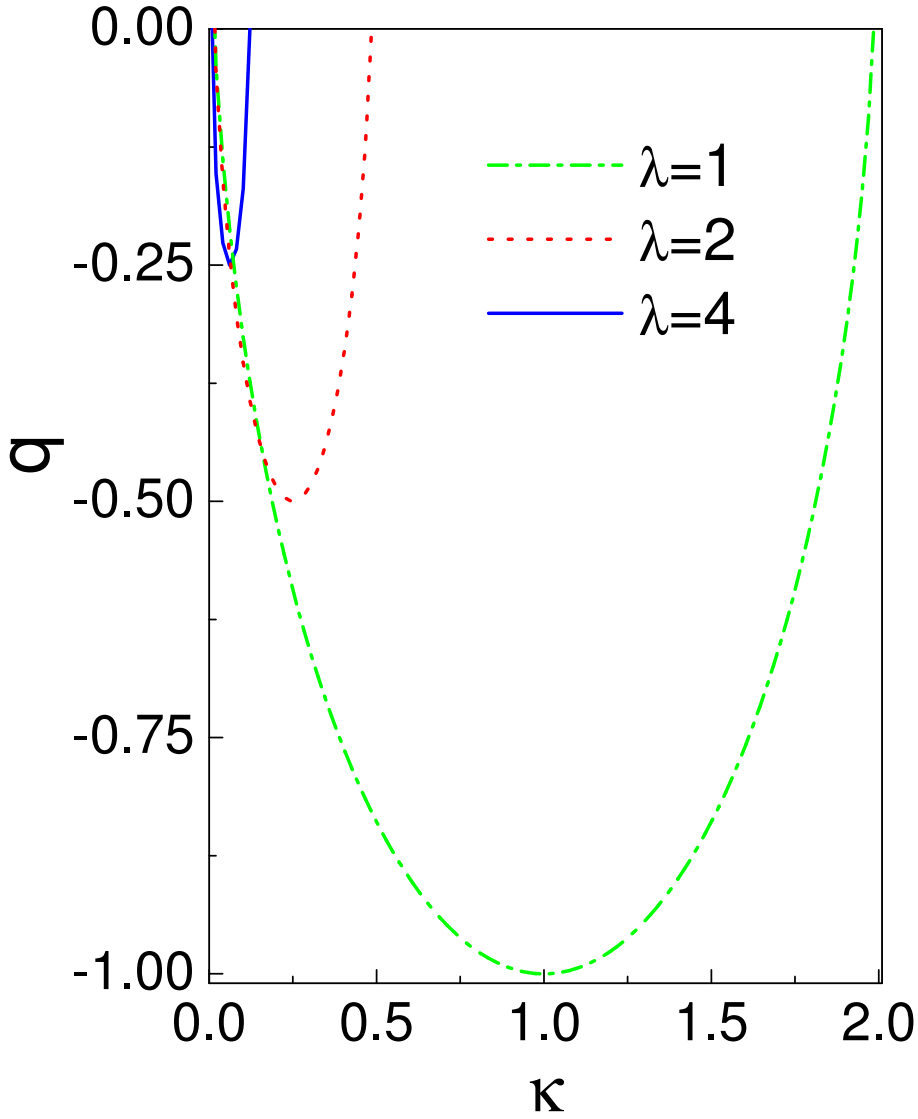

FIG. 3: The dependence of topological charge q on electron-phonon constant κ for different values of kink velocity λ.

In turn, Fig.4 depicts evolution of the effective spin S with κ for different values of λ with polarization $p = 0.5$ and mixing angle $\Omega = \frac{\pi}{2}$.

Moreover, by combining Eqs.(25) and (26) and treating the mixing angle Ω as a random variable, we observe that kink mediated charge q and spin S degrees of freedom are actually interdependent. More precisely, spin can be presented as a function of charge:

$$S(q, \Omega) = S_{av}(q) + S_{fl}(q) \sin \Omega \tag{27}$$

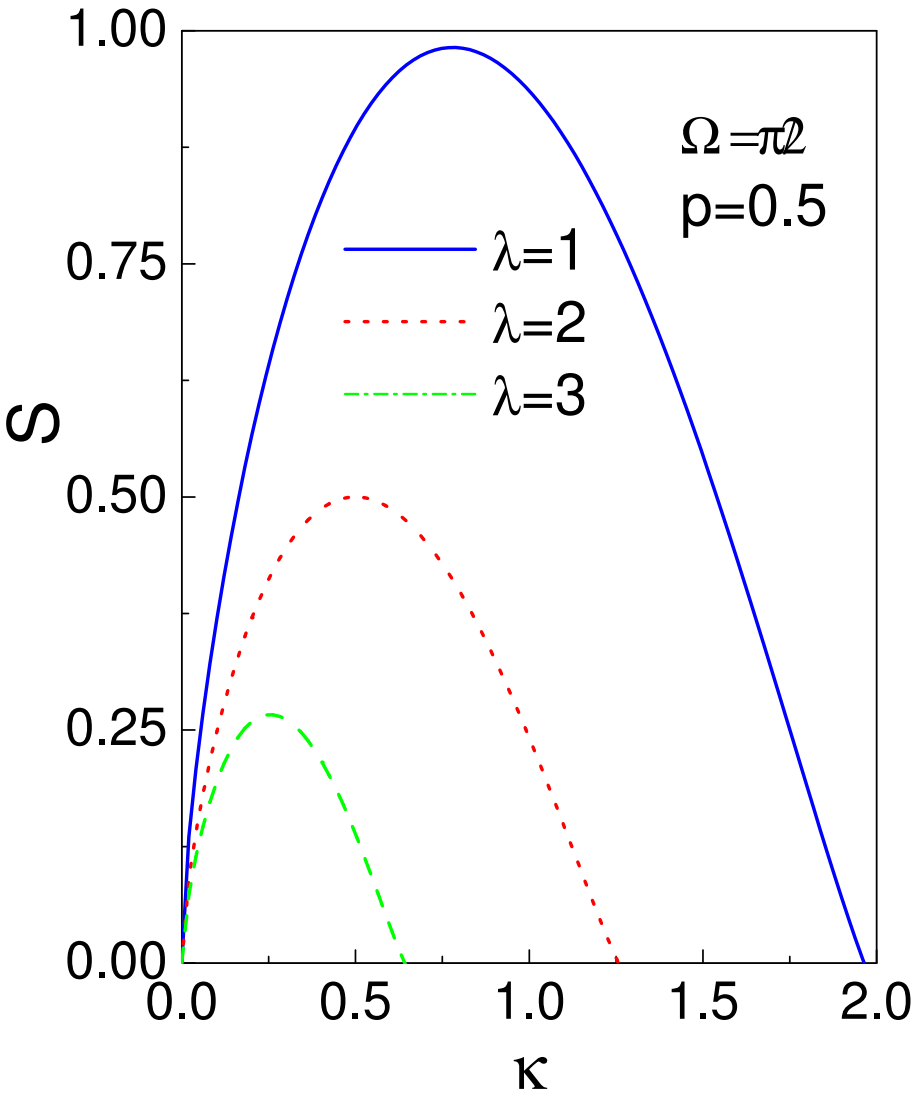

FIG. 4: The dependence of topological spin S on electron-phonon constant κ for different values of kink velocity λ (for $\Omega = \frac{\pi}{2}$ and $p = 0.5$).

where

$$S_{av}(q) \equiv < S >= \int_0^{2\pi} S(q,\Omega) d\Omega = q\left(\frac{\Pi^2}{1-\sqrt{1-\Pi^2}} - 1\right) \tag{28}$$

and

$$S_{fl}(q) \equiv \sqrt{< S^2 > - < S >^2} = q\Pi \left[\frac{\sqrt{2\left(1-\sqrt{1-\Pi^2}\right) - \Pi^2}}{1-\sqrt{1-\Pi^2}}\right] f\left(p, \frac{\pi}{2}\right) \tag{29}$$

stand for an average and fluctuation contributions to $S(q)$ dependence, respectively. Here, $\Pi \equiv q\lambda$.

Notice that the average contribution $< S >$ as a function of kink charge q (shown in Fig.5

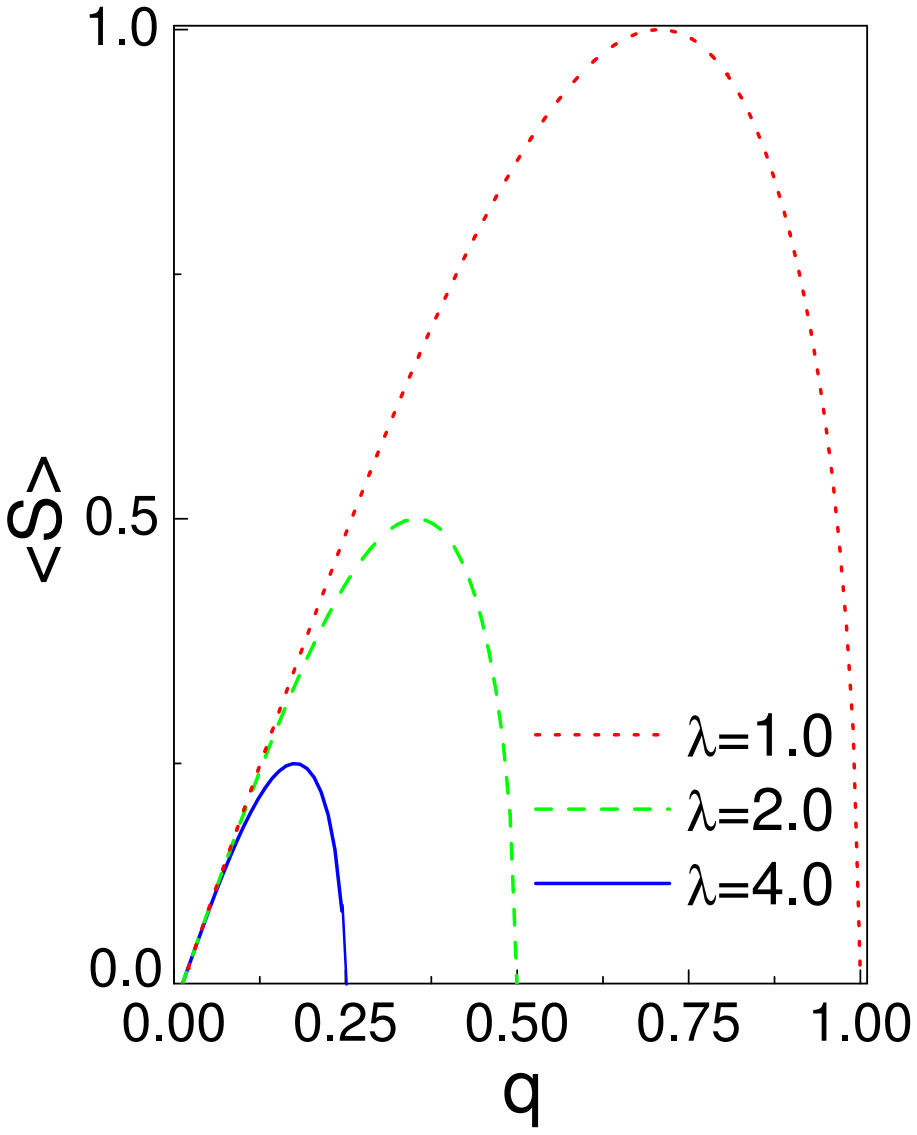

FIG. 5: The dependence of average kink spin $< S >$ on kink charge q for different values of kink velocity λ.

for different values of the kink velocity λ) exhibits some nontrivial behavior with a spinless state ($< S >= 0$) corresponding to fractional values of the effective charge ($q = \frac{1}{4}$ and $\frac{1}{2}$). At the same time, it is important to point out that the fluctuation contribution S_{fl} strongly depends on effective polarization p and completely disappears for totally polarized carriers (that is $S_{fl}(p = 1) = 0$).

As for the soliton charge Q, due to its independence from the mixing angle, there are no charge fluctuations (since $Q_{av} \equiv < Q >= Q$, $< Q^2 >= Q^2$, and $Q_{fl} \equiv \sqrt{< Q^2 > - < Q >^2} = 0$).

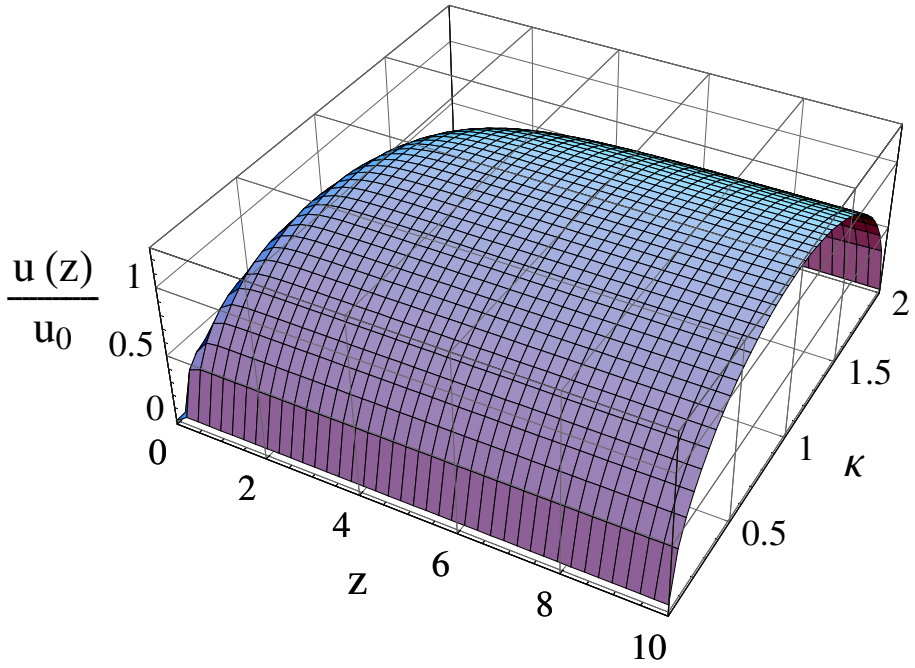

FIG. 6: The dependence of the local profile of kink mediated displacement field on electron-phonon constant κ (for $\lambda = 1$ and $\Omega = 0$).

Besides, in view of Eq.(11), kink electron amplitudes (18) and (19) also participate in formation of angle-dependent kink-mediated lattice displacement field

$$u(z) = u_\infty \tanh \nu z \cos \Omega \tag{30}$$

where $u_\infty = C\nu/\rho^2$ with $C = 2Iad$ being the integration constant introduced earlier in Eq.(11). Notice that the above displacement field u is created by the same electron-phonon interaction I (recall that $\nu = \sqrt{\rho^2 - \lambda^2}$ with $\rho^2 = \frac{2}{\kappa}$ and $\kappa \propto I^2$) which is responsible for nonlinear electron transport behavior within this model. The evolution of the local profile of kink mediated displacement field $u(z)$ with κ (for $\lambda = 1$ and $\Omega = 0$) is shown in Fig.6.

Notice also that (contrary to the soliton charge Q) the averaged over the mixing angle Ω displacement field has a zero mean value $u_{av}(z) \equiv < u >= 0$ with a possibility of lattice fluctuations $u_{fl}(z) \equiv \sqrt{< u^2 > - < u >^2} = \frac{1}{2} u_\infty \tanh \nu z$. Furthermore, by rewriting Eq.(21) in the form of Eq.(27), that is $\mu(z) = \mu_{av}(z) + \mu_{fl}(z) \sin \Omega$, we arrive at the following scaling relation between kink mediated CDW, SDW and displacement field:

$$\left[\frac{\mu(z)-\mu_{av}(z)}{\mu_{fl}(z)}\right]^2+\left[\frac{u(z)}{u_{fl}(z)}\right]^2=\left[\frac{n(z)}{n_{av}(z)}\right]^2 \tag{31}$$

Let us estimate now the main parameters of the model using some typical experimental values. Notice in this respect that in the adiabatic approximation ($\alpha a^2 \gg Mv^2$) we have $d^{-1} \simeq \alpha a^2$ resulting in $\kappa \simeq I^2/\alpha T$ for the electron-phonon coupling constant with κ dependent transition amplitude $T = CIa - t_0 \simeq (2I^2\rho^2/\alpha) - t_0 \simeq 2\rho^2 T\kappa - t_0$. Given $\rho^2 = 2/\kappa$, this leads to the following modification of the bare amplitude t_0 in our model: $T \simeq t_0/(2\kappa\rho^2 - 1) \simeq t_0/3$. Recall that in the limit of weak electron-phonon coupling [26], $T \simeq t_0$, $\kappa \simeq I^2/\alpha t_0$ and $v_0 \simeq 2at_0/\hbar$. Moreover, assuming [8] $t_0 = 2.5eV$, $I = 4eV/\text{Å}$, $a = 1.2\text{Å}$, and $\alpha = 20eV/\text{Å}^2$ for hopping integral, electron-phonon, lattice and power constants, we obtain $\kappa = I^2/\alpha T \simeq 0.5$ and $v_0 = 2aT\hbar \simeq 10^4 m/s$ for estimates of the electron-phonon coupling constant and characteristic kink velocity within our model, respectively. Hence, like electron-electron correlations [11], electron-phonon interactions also result in decreasing of the soliton velocity $v = \lambda v_0$, making it even harder to observe soliton motion in conjugated polymers [3, 8]. Notice that the maximum value of the dimensionless electron-phonon parameter $\kappa_m = 2$ (allowed by the model considered here) corresponds to $I_m = \sqrt{2\alpha t_0/3} \simeq 6eV/\text{Å}$. This value is quite typical for many realistic low-dimensional conducting materials, providing thus an optimistic possibility for experimental verification of the predicted here interesting charge-spin conversion effects.

And finally, some discussion is in order regarding the relationship between the classical SSH model and its two-component vector generalization considered here. First of all, the ground state of our vector model is quite different from the classical case of the so-called degenerate ground-state (DGS) polymers considered in the original SSH model. The latter is known [1] to support topological soliton excitations (given by either neutral spin-$\frac{1}{2}$ or charged spinless states) in the form of a domain wall separating the two DGS structures. Recall that the continuum version of the original SSH model [26] is mapped onto a Dirac type Hamiltonian which preserves the electron-hole symmetry of the original discrete SSH model, leading thus to a "relativistic" energy spectrum and very distinctive ground state (with mutually exclusive CDW and SDW configurations). At the same time, a continuum limit of the vector model presented here results in a Schrödinger Hamiltonian with "non-relativistic" spectrum which does not *explicitly* preserve the electron-hole symmetry of the original discrete model. Instead, the resulting system (14) possesses a new degree of freedom

(given by a mixing angle Ω) which triggers the interference effects between spin-up ($\phi_{+\uparrow}$) and spin-down ($\phi_{+\downarrow}$) electron amplitudes.

Turning to the influence of the HF approximation on the soliton type structure of the resulting continuum system (14), it is instructive to observe that, within continuum approximation, a topological nature of soliton excitation is a result of assumed non-vanishing "condensate" type boundary conditions (with $\rho^2 \propto \kappa^{-1} \neq 0$) imposed on the solution of Eq.(14) rather than a direct consequence of the HF approximation itself. Indeed, it can be easily verified (see [21–23] for discussion) that for substantially depleted "condensate" (when $\rho^2 \propto \kappa^{-1} \to 0$), kink solution (also known as a "dark" soliton) becomes unstable prompting the system (14) to choose a more stable conventional (non-topological) soliton solution of the localized type (also known as a "bright" soliton). Thus, based on the results of the present investigation, we can conclude that (i) a stronger electron-phonon interaction should result in a stronger localization of the soliton excitation, and (ii) a long-range order of the SDW within the HF approximation is a consequence of a rather weak electron-phonon coupling constant κ leading to strong "condensate" effects of the topological soliton (with $\rho^2 \propto \kappa^{-1} \neq 0$).

In conclusion, within a tight-binding approximation, the influence of electron-phonon interactions on soliton-like excitations in two-component extended Hubbard model was studied. By mapping the original model onto the system of two coupled nonlinear Schrödinger equations with $U(2)$ symmetry group, some interesting correlations between soliton mediated charge Q and spin S degrees of freedom were obtained.

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