Langevin dynamics simulations of the two-dimensional Su-Schrieffer-Heeger model

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We use Langevin sampling methods within the auxiliary-field quantum Monte Carlo algorithm to investigate the phases of the Su-Schrieffer-Heeger model on the square lattice at the O(4) symmetric point. Based on an explicit determination of the density of zeros of the fermion determinant, we argue that this method is efficient in the adiabatic limit. By analyzing dynamical and static quantities of the model, we demonstrate that a \((\pi, \pi)\) valence bond solid gives way to an antiferromagnetic phase with increasing phonon frequency.

I. INTRODUCTION

Phonons in systems of electrons or spins can generate many fascinating states of matter. Apart from superconductivity [1], this also includes phases that break lattice symmetries such as charge-density wave states (CDW) and various flavors of valence-bond solid (VBS) states [2]. In spin systems, the coupling to phonons can generate quantum phase transitions between antiferromagnetic (AFM) and VBS states [3]. Such interactions hence offer the possibility of investigating quantum phase transitions between various states of matter all characterized by a local order parameter. A particularly intriguing aspect is the possibility of realizing quantum phase transitions beyond the Landau-Ginzburg-Wilson paradigm in models relevant for materials.

The Debye frequency \(\omega_D\) is typically much smaller than the Fermi energy \(\epsilon_F\). This separation of energy scales underlies Migdal’s theorem [1, 4], which provides a small parameter, \(\hbar \omega_D / \epsilon_F\), to justify perturbative approaches to the electron-phonon problem. Fermion Monte Carlo simulations offer the possibility to take a step beyond perturbative approaches and thereby investigate competing instabilities [5]. In fact, it is known that the generic electron-phonon problem does not suffer from a negative sign problem, irrespective of the lattice geometry and band filling. In particular, for each space-time configuration of phonon fields, time-reversal symmetry ensures that the eigenvalues of the fermion determinant come in complex conjugate pairs [6]. This argument for the absence of a negative sign problem is valid only if the phonons are not integrated out, as done in Refs. [7–9]. As such, it should be a technically simple problem. However, this is not the case, since the key challenge is to find an adequate sampling scheme that deals with the separation of energy scales. Adopting a local updating scheme—as commonly used in Monte Carlo simulations of fermions—in which the phonon field is updated on a time scale set by the electron motion, leads to prohibitively long autocorrelation times [10]. Global updates of the phonon fields on the imaginary time scale of the inverse Debye temperature are highly desirable and have been achieved using, for example, self-learning methods [11].

In the one-dimensional case, there has been a number of simulations of the Su-Schrieffer-Heeger (SSH) model [2, 12]. The model exhibits many fascinating quantum phase transitions, including instances of deconfined quantum criticality in one dimension [13] between VBS and CDW states [14]. Simulations in two dimensions are still in their infancy. In Ref. [15], the authors show that the model sustains a VBS state. A parallel work to the results presented here shows that the model also supports an AFM phase [16].

The present work uses Langevin updates, as successfully applied before to the Holstein model [17]. Here, we will use an identical algorithm for the SSH model with Einstein phonons [18] on a square lattice at the O(4) symmetric point. In the very same way as the hybrid Monte-Carlo (HMC) approach discussed in Ref. [19], Langevin and HMC updates are global moves for which the acceptance rate is unity or can be made arbitrarily large. The key point for the success of Langevin and HMC approaches is the absence of singularities in the action. Since the action contains the logarithm of the fermion determinant, this requires that the latter does not vanish. In special cases where the action has no singularities, this class of updating schemes works very well. For a specific example, we refer to previous work on the one-dimensional Hubbard model with open boundary conditions [20].

For the electron-phonon problem in the adiabatic limit, the phonon fields are frozen in imaginary time. In this limiting case, the fermion determinant is strictly positive. A small phonon frequencies, we will show that the density of zeros of the fermion determinant is small so that
Langevin dynamics performs well. As the frequency of the phonons is increased, the density of zeros grows and the Langevin approach becomes unstable.

The main results and organization of the article are as follows. In Sec. [II] we define the SSH model considered. We will concentrate on a high-symmetry point with partial particle-hole symmetry that exhibits an $O(2N)$ symmetry for the general case of fermions with $N$ flavors. In Sec. [III] we discuss the numerical implementation, which makes use of a standard auxiliary-field quantum Monte Carlo (AFQMC) [21] formulation that allows us to use the ALF-2.0 package [20]. For the updating scheme, we have followed the work of Ref. [17] and implemented the Langevin updating scheme with Fourier acceleration. For $O(2N)$ symmetric problems, the fermion determinant for a single fermion flavor can be written in terms of the square of a Pfaffian [22]. The sign of the Pfaffian is not pinned to unity. Configurations at which the sign changes correspond to zeros of the fermion determinant. As such, the average sign of the Pfaffian provides a measure for the density of zeros. We will show that the average sign of the Pfaffian decreases with increasing phonon frequency, thus rendering Langevin simulations prohibitively hard in the high frequency limit. In Sec. [IV] we present our results for the adiabatic limit and nonzero phonon frequencies. Within our Langevin simulations, we observe two phases. A $(\pi, \pi)$ VBS phase that spontaneously breaks the $C_4$ symmetry of the lattice is observed at small phonon frequencies. At higher frequencies, the VBS state gives way to an AFM phase (see Fig 1). This Ising-like order parameter supports order at finite temperature. Since it changes sign under the partial particle-hole transformation, it indicates a spontaneous breaking of this symmetry.

In addition to the apparent global $SU(N)$ spin rotational symmetry, the model possesses an enlarged $O(2N)$ symmetry on a bipartite lattice. To prove this, we reformulate the Hamiltonian using Majorana fermions [19, 24]

$$\hat{P}_\sigma^{-1} \hat{c}^\dagger_{i,\sigma} \hat{P}_\sigma = \delta_{\sigma,\sigma'} \epsilon^{Q} Q_{i,\sigma,\sigma'} + (1 - \delta_{\sigma,\sigma'}) \hat{c}^\dagger_{i,\sigma}$$

where $Q = (\pi, \pi)$ for the square lattice. We can define a corresponding $Z_2$ order parameter, the fermion parity on site $i$ [24]

$$\hat{p}_i = \prod_{\sigma=1}^{N_\sigma} (1 - 2 \hat{n}_{i,\sigma}).$$

This Ising-like order parameter supports order at finite temperature. Since it changes sign under the partial particle-hole transformation, it indicates a spontaneous breaking of this symmetry.

II. MODEL AND SYMMETRIES

A. Hamiltonian

We consider an SSH model with optical phonons, defined by the Hamiltonian

$$\hat{H}_G = -t \sum_{(i,j)} \hat{K}_b + g \sum_{(i,j)} \hat{Q}_b \hat{K}_b + \sum_{b} \left[ \frac{\hat{P}_b}{2m} + \frac{k}{2} \hat{Q}_b^2 \right].$$

The operator $\hat{K}_b = \sum_{\sigma=1}^{N} (\hat{c}^\dagger_{i,\sigma} \hat{c}^\dagger_{j,\sigma} + h.c.)$ describes fermion hopping on a bond $b = (i,j)$ connecting two nearest-neighbor sites $i$, $j$ with hopping amplitude $t$. The operator $\hat{c}^\dagger_{i,\sigma}$ creates an electron centered at site $i$ and with $\sigma$-component of spin $\sigma$ that runs over $N$ flavors. We use anti-periodic boundary conditions $\hat{c}^\dagger_{i+L_{a_1},\sigma} = -\hat{c}^\dagger_{i,\sigma}$ in the direction of the primitive vector $a_1$ of the lattice and periodic boundary conditions $\hat{c}^\dagger_{i+L_{a_2},\sigma} = \hat{c}^\dagger_{i,\sigma}$ in the direction of $a_2$. The phonons are represented by harmonic oscillators that reside on the bonds. They are described by the momentum and position operators $\hat{P}_b$ and $\hat{Q}_b$ as well as the frequency $\omega_0 = \frac{\epsilon}{m}$. The hopping of the electrons is modulated by the phonon coordinate $\hat{Q}_b$ on the respective bond $b$ with coupling strength $g$.

B. Symmetries

The SSH model at half-filling and on a bipartite lattice, such as the square lattice considered here, is invariant under the partial particle-hole transformation

$$\hat{P}_\sigma^{-1} \hat{c}^\dagger_{i,\sigma} \hat{P}_\sigma = \delta_{\sigma,\sigma'} \epsilon^{Q} Q_{i,\sigma,\sigma'} + (1 - \delta_{\sigma,\sigma'}) \hat{c}^\dagger_{i,\sigma}$$

and the $O(2N)$ symmetry becomes obvious. Because of this symmetry, the model is free of a sign problem for odd values of $N$ [25]. For even $N$, time-reversal symmetry is sufficient to show the absence of a sign problem [6]. In the case of $N = 2$ considered here, the spin operators and the Anderson pseudospin operators [26] are the infinitesimal generators of the $SO(4)$ symmetry. They are defined by

$$\hat{S}_i = \frac{i}{2} \sum_{\sigma=1}^{N} \hat{c}^\dagger_{i,\sigma} \sigma_{\sigma,\sigma'} \hat{c}_{i,\sigma'} \quad \hat{\eta}_i = \hat{P}_3^{-1} \hat{S}_i \hat{P}_3$$

and where the vector $\sigma$ contains the three Pauli matrices. Both, the spin and the pseudospin components $(l, m, n)$ fulfill the Lie algebra of the $SU(2)$ group $[\hat{S}_i, \hat{S}_j, m] = i \hat{S}_{i,j} \sum_{n} \epsilon_{lmn} \hat{S}_{i,n}$ and commute among each other. Here, $\epsilon_{lmn}$ is the Levi-Civita symbol. The Lie algebra of the global $O(4)$ symmetry can be interpreted as $O(4) = SU(2) \times SU(2) \times Z_2$, where the additional $Z_2$ symmetry corresponds to the partial particle-hole symmetry [24]. Hence, an AFM phase is degenerate with a charge-density
wave (CDW) and an s-wave superconductor (SC). If the parity $\hat{\rho}_i$ orders and the particle-hole symmetry is spontaneously broken, either the spin or charge sector is explicitly chosen.

C. Limiting cases

In the adiabatic limit $\omega_0 \to 0$, imaginary-time fluctuations of the phonon fields are exponentially suppressed. The phonon displacements can be treated classically and the Hamiltonian can be written as

$$\hat{H} = \sum_b (-t + gq_b)K_b + \sum q_b^2. \quad (7)$$

Here, $\hat{Q}_b|q\rangle = q_b|q\rangle$. The Hamiltonian consists solely of a modulated hopping of the electrons and the potential energy of the phonon fields.

For $\omega_0 > 0$ we can integrate out the phonons to obtain an effective Hamiltonian for the electrons in the SSH model [24, 27]. This yields the action

$$S_{\text{eff}} = -\frac{g^2}{2\pi}\int_0^\beta d\tau d\tau' \int_0^\beta d\tau d\tau' \sum_b K_b(\tau)D(\tau - \tau')K_b(\tau') \quad (8)$$

with the local and retarded interaction

$$D(\tau) = \frac{\omega_0 e^{-\omega_0|\tau|} + e^{-\omega_0(\beta - |\tau|)}}{2 - e^{-\omega_0\beta}}. \quad (9)$$

By taking the antiadiabatic limit $\omega_0 \to \infty$ the interaction becomes instantaneous [24],

$$\lim_{\omega_0 \to \infty} D(\tau) = \delta(\tau). \quad (10)$$

The effective Hamiltonian of the SSH model in the antiadiabatic limit is given by

$$\hat{H}_{\text{eff}} = -t \sum_{i,j} \hat{K}_b - \frac{g^2}{2\pi} \sum_{i,j} \hat{K}_b^2. \quad (11)$$

For $N = 1$, this expression is equivalent to the Hamiltonian of the $t$-$V$ model if we identify the interaction strength with $g = \sqrt{kV}$. For two fermion flavors, $N = 2$, we can rewrite the interaction term as

$$-\frac{1}{4} \hat{K}_b^2 = \hat{S}_i \hat{S}_j + \eta_i \eta_j. \quad (12)$$

In this form, the O(4) symmetry of the system is obvious. In the high-frequency limit $\omega_0 \to \infty$, we expect a AFM/CDW/SC ground state.

III. METHODS

A. Langevin dynamics

Using the real-space formulation of the path integral for the phonon degrees of freedom with the eigenstates of the position operator $\hat{Q}_b|q\rangle = q_b|q\rangle$, the partition function of the model can be written as

$$Z = \int \prod_{b,\tau} dq_b,\tau e^{-S}, \quad (13)$$

$$S = S_0 + S_F = S_0 - N \ln \det [1 + B(\beta, 0)]$$

with

$$B(\tau_1, \tau_2) = \prod_{\tau = 2}^{\tau_1} \prod_b (e^{-\Delta \tau gq_b, \tau} K_b) e^{\Delta \tau} \sum_{l,l'} K_b \quad (14)$$

and $\hat{K}_b = \sum_{i,j,\sigma} \hat{c}_{i,\sigma}(\tau) K_b \hat{c}_{j,\sigma}^\dagger$. We have used the formula by Blankenbecler, Scalapino, and Sugar [21] to rewrite the trace over the fermionic degrees of freedom as a determinant. Furthermore, $\tau$ runs from $1 \cdots L_{\text{ Trot}}$ where the inverse temperature $\beta = L_{\text{Trot}} \Delta \tau$.

The phonon degrees of freedom have their own intrinsic imaginary-time dynamics governed by the action

$$S_0 = \Delta \tau \sum_{b,\tau} \left( \frac{1}{\omega_0^2} \left[ q_b,\tau - q_b,\tau' \right]^2 + q_b,\tau^2 \right). \quad (15)$$

Since a harmonic oscillator has only one free parameter, namely the frequency $\omega_0$, we set the force constant to $k = 2$.

To update the bosonic fields $q = \{q_b,\tau\}$ we use Langevin dynamics. The corresponding Langevin equation is a stochastic differential equation for the fields [17, 20],

$$\frac{dq(t)}{dt} = -Q \frac{\partial S(q(t))}{\partial q(t)} + \sqrt{2Q} \eta(t), \quad (16)$$

with an additional Langevin time $t_l$. The independent Gaussian random variables $\eta$ satisfy

$$\langle \eta_{b,\tau}(t) \rangle = 0, \quad \langle \eta_{b,\tau}(t) \eta_{b',\tau'}(t') \rangle = \delta_{b,b'} \delta_{\tau,\tau'} \delta(t - t'). \quad (17)$$

with $\delta$ being the Kronecker delta for the discrete indices and the Dirac delta function for the continuous $t_l$. The matrix $Q$ is an arbitrary positive-definite matrix. In order to use the Langevin equation in our AFQMC code we discretize the Langevin time $t_l$ with a finite time step $\delta t_l$. Using the Euler method, the discretized equation is given by [25]

$$q(t_l + \delta t_l) = q(t_l) - Q \frac{\partial S(q(t_l))}{\partial q(t_l)} \delta t_l + \sqrt{2Qt_l} \eta(t_l). \quad (18)$$

For the random variables $\eta$ we have to make the replacement $\delta(t_l - t'_l) \to \delta(t_l, t'_l)$. The systematic error introduced by discretizing the Langevin time is of linear order in $\delta t_l$ [17, 20]. By transforming the Langevin equation into the form of a Fokker-Planck equation one can show that the stationary probability distribution of finding the system in state $q$ is given by [25]

$$P(q) = \frac{e^{-S(q)}}{\int Dq e^{-S(q)}}. \quad (19)$$
A major aspect of Langevin dynamics are the forces, their computation, and characteristics. For the SSH model, using Eq. [13], the forces read

$$\frac{\partial S}{\partial q_{b, \tau}} = \Delta \rho k b_{b, \tau} + \frac{m}{\Delta \tau} (2q_{b, \tau} - q_{b, \tau+1} - q_{b, \tau-1}) \quad (20)$$

$$+ N \gamma \Delta \tau \{ K_0 (1 - G(b, \tau)) \}$$

with the Green function

$$G_{i,j}(b, \tau) = \frac{\text{Tr} \left[ \hat{U}^\gamma(b, \tau) \hat{\epsilon}_i^j \hat{U}^\gamma(b, \tau) \right]}{\text{Tr} \left[ \hat{U}(\beta, 0) \right]} \quad (21)$$

and the propagators

$$\hat{U}^\gamma(b', \tau) = \hat{U}(\beta, \tau) \prod_{b=b'}^{N_b} e^{-\Delta \tau g_{b, \tau} e^i K_{b, b}} \quad (22)$$

$$\hat{U}^\gamma(b', \tau) = \prod_{b=1}^{b'-1} e^{-\Delta \tau g_{b, \tau} e^i K_{b, b}} \sum_{b' = 1}^{N_b} e^{-\Delta \tau g_{b, \tau} e^i K_{b, b'}} \hat{U}(\tau - \Delta \tau, 0).$$

From Eq. [13] we see that the action has logarithmic divergences if the determinant vanishes. The O(2N) symmetry of the model only guarantees that the determinant is non-negative.

### B. Calculation of the Pfaffian

To consider possible divergences of the action we analyze the determinant that appears in the action [13]. First, we use the O(2N) symmetry of the model to express the determinant as a square of a trace over one of the two Majorana fermions:

$$Z^2 = \text{det} [1 + B(\beta, 0)] \quad (23)$$

$$Z_\gamma = \text{Tr} \left[ \prod_{b} \prod_{\tau} (e^{-\frac{1}{2} \Delta \tau g_{b, \tau} \gamma_i \gamma_j}) e^{\frac{1}{2} \Delta \tau \sum_b \gamma_i \gamma_j} \right].$$

Here and in the rest of this section, we drop the spin and Majorana kind indices since none of the quantities considered explicitly depend on them. One can show with a canonical transformation of the Majorana fermions on only one sublattice, $\gamma_i \rightarrow -\gamma_i$, that $Z_\gamma$ is real [22] and its square is non-negative.

The quantity $Z_\gamma$ can either be positive or negative in distinct regions of the configuration space. Since $Z_\gamma$ is an entire function, it necessarily has to vanish between these regions. Hence, the average sign of $Z_\gamma$ serves as an estimate of the number of zeros of the determinant. If the average sign is close to plus or minus unity, it is more improbable to cross a boundary between two regions in which $Z_\gamma$ has different signs. In contrast, for a vanishing average sign, there are more zeros.

To measure the sign of $Z_\gamma$ we reformulate it as a Pfaffian. First, we use an alternative Trotter decomposition and rewrite the exponentials as hyperbolic functions by using $(\gamma_i \gamma_j)^2 = -1$ to obtain

$$Z_\gamma = \text{Tr} \left[ \prod_{t} e^{y_t \gamma_i \gamma_j} \right] \quad (24)$$

$$= \prod_{t} \{ \cosh y_t \} \text{Tr} \left[ \prod_{t} (1 + i \gamma_i \gamma_j \tanh y_t) \right].$$

The tuple $t = (b, \tau)$ combines the bond index and the imaginary time slice into a new index that is ordered according to its position in the product $\prod_t$. To lighten the notation, we used $y_{b, \tau} = \frac{1}{2} \Delta \tau (t_b - gq_{b, \tau})$. Next, we introduce Grassmann variables $\xi_{i, j, \tau}$ on every site and imaginary time slice, where $i$ is on sublattice A and $j$ on sublattice B, and use the following formula for even $n$ [30]:

$$C_\pm = \prod_{t=1}^{n} \sqrt{\alpha(t)} = \int [d\xi] e^{\pm \sum_{i \neq j} \sqrt{\alpha(t)\alpha(t')} \xi_i \xi_j},$$

$$C_+ = (-i)^n, \quad C_- = 1.$$}

Here, $[d\xi] = d\xi_n \cdots d\xi_1$ is a time-ordered product. Finally, $Z_\gamma$ can be written as the Pfaffian over an antisymmetric matrix $A \in \mathbb{C}^{2N_b \times N_b}$ [30],

$$Z_\gamma = \prod_{t} \{ \cosh y_t \} \text{Tr} (1 - \text{Pf}(A)) \quad (27)$$

$$\text{Pf}(A) = \int [d\xi] e^{-\frac{i}{2} \xi^T A \xi} - \frac{1}{2} \xi^T A \xi =$$

$$- \sum_{i} \xi_i \xi_{i, t} + \sum_{i, (t < t')} m_{t'} \xi_{i, t} \xi_{i, t'} - \sum_{j, (t < t')} m_{t'} \xi_{j, t} \xi_{j, t'}. $$

where we defined $m_{t'} = \sqrt{\tanh (y_t) \tanh (y_{t'})}$. The vector $\xi$ contains all Grassmann variables.

For the numerical computation of the Pfaffian we used the software from Ref. [31]. Since the calculation of the Pfaffian is very expensive, we only considered small lattices and a small number of imaginary time slices. In Fig. 2 we plot the average sign of the Pfaffian as a function of coupling strength for the t-V model as well as for the SSH model as a function of phonon frequency.

The results for the t-V model illustrate a breakdown of Langevin dynamics due to severe divergences of the forces. Upon increasing the coupling strength, the average sign of the Pfaffian drops to zero and the measured observables deviated by up to a factor of $10^6$ from results obtained with a Metropolis-Hastings updating scheme. In the adiabatic limit of the SSH model, the average sign is close to unity and the simulations are stable. Increasing the phonon frequency leads to a decrease of the average sign and the updating tends to become unstable. In general, we found it easier to stabilize the simulations with our choice of boundary conditions (anti-periodic and periodic, a-p) as opposed to periodic boundary conditions in both directions (p-p).

To partially control the numerical instabilities we used an adaptive Langevin time step $\delta t$. At each Langevin
The variations of the Langevin time step have to be taken into account when measuring observables,

$$\langle \hat{O} \rangle = \frac{1}{N_m} \sum_{n=1}^{N_m} (\delta t)_n \left( \left\langle \hat{O} \right\rangle \right)_{\alpha}.$$  (29)

Here, $N_m$ is the total number of measurements and $\left\langle \hat{O} \right\rangle_{\alpha}$ denotes the value of the observable $\hat{O}$ for configuration $C_{\alpha}$ of the phonon fields.

### C. Fourier acceleration

Following Refs. [17][29] we used Fourier acceleration (FA) to decrease autocorrelations. The main idea of FA is to adapt the Langevin time step $\delta t_l$ according to the momentum of the phononic modes. Slow modes are multiplied with a larger step size than fast modes by using an adequate choice of the matrix $Q$ in the Langevin equation (33).

As a foundation for the choice of $Q$ we consider the non-interacting case ($g = 0$). We carry out a Fourier transformation of the force in imaginary time,

$$\tilde{F} \left[ \frac{dS}{dq_{b,k}} \right] = \left[ \delta(t) + \frac{2m}{\Delta \tau} \left( 1 - \cos \left( \frac{2\pi k}{\Delta \tau} \right) \right) \right] q_{b,k}.$$  (30)

with

$$\tilde{F} \left[ f(\tau) \right] = \tilde{f}(k_r) = \frac{1}{\Delta \tau} \sum_{r=1}^{L_r} e^{i \frac{2\pi}{\Delta \tau} k_r \tau} f(\tau).$$  (31)

The observable evaluated at time $t_1$ is given by $O(t_1)$ and $T_1$ is the maximal time at which measurements are taken. For uncorrelated measurements, the autocorrelation function drops to zero. The shorter the autocorrelation time, the faster the autocorrelation function should decay to zero. A decrease of autocorrelations by FA is clearly visible from Fig. 5(b).

Especially in the limit of small phonon frequencies $\omega_0$ the ratio is close to zero. We choose the factor $Q$ in Fourier space such that the prefactor of $\tilde{q}_{b,k}$ in Eq. (30) becomes independent of the momentum $k_r$,

$$\tilde{Q}(k_r) = \frac{\Delta \tau k_r + \frac{4m}{\Delta \tau}}{\Delta \tau k_r + \frac{4m}{\Delta \tau} \left( 2 - 2 \cos \left( \frac{2\pi k_r}{\tau} \right) \right)}.$$  (33)

To see the effect of FA on autocorrelation times, we measured the equal-time spin correlation function

$$S_S(q, \tau = 0) = \frac{1}{L^2} \sum_{i,j} e^{-iq(i-j)} \left( \left\langle \hat{S}_{i,z} \hat{S}_{j,z} \right\rangle - \left\langle \hat{S}_{i,z} \right\rangle \left\langle \hat{S}_{j,z} \right\rangle \right).$$  (35)

with FA [using Eq. (34) to update the fields] and without FA (by setting $Q = 1$). The spin correlation function at wave vector $q = (\pi, \pi)$ is shown in Fig. 3(a) as a function of the inverse Langevin time. The equilibration time is obviously reduced by FA and, as expected, the results of both methods agree at sufficiently long times.

We also consider the autocorrelation function [20]

$$C_S(t_1) = \sum_{t_0} \left( \left\langle O(t_1') - \left\langle \hat{O} \right\rangle \right\rangle O(t_1 + t_1) - \left\langle \hat{O} \right\rangle \right)^2.$$  (36)

The observable evaluated at time $t_1$ is given by $O(t_1)$ and $T_1$ is the maximal time at which measurements are taken. For uncorrelated measurements, the autocorrelation function drops to zero. The shorter the autocorrelation time, the faster the autocorrelation function should decay to zero. A decrease of autocorrelations by FA is clearly visible from Fig. 5(b).

### FIG. 2. (a) Average sign of the Pfaffian for the $t$-$V$ model as a function of $V/t$. Here, we consider a square lattice with a $\pi$-flux threading each plaquette. This model supports a Gross-Neveu transition at $V_c = 1.279(3)t$ [32]. We observe a strong decrease of the average sign of the Pfaffian already at high temperatures for increasing coupling strength. (b) Average sign of the Pfaffian for the SSH model with different boundary conditions at $\beta t = 5.0$, $\Delta \tau t = 0.1$, and $\delta t_l = 0.0005$.
IV. RESULTS

All simulations were carried out using the ALF package [20]. In our simulations, we set \( k = 2, t = 1, g = 1.5 \) and \( \Delta \tau = 0.1. \) We used a Langevin time step of \( \delta t_l = 0.01 \) in the adiabatic limit and \( \delta t_l = 0.0005 \) for nonzero phonon frequencies.

A. Adiabatic limit

With the aid of a mean-field approach we study the pattern of the fields \( q_b \) in the ground state. The nesting of the Fermi surface of the non-interacting model gives rise to a log divergence in the \( Q = (\pi, \pi) \) susceptibility at low temperatures. Hence, we expect an instability to a \( (\pi, \pi) \) VBS. In contrast to one dimension, where the ordering pattern is unique, in two dimensions there is a multitude of generalizations including staircase, columnar, staggered, and plaquette arrangements [34-35]. In our calculation, we use an enlarged \( 2 \times 2 \) unit cell and vary the bond variables independently according to the aforementioned symmetry (see Fig. 4(a)). In this way, we can resolve various patterns of \( (\pi, \pi) \) and \( (0, \pi) \) VBS orders. After minimization of the energy, the pattern we obtain is the \( (\pi, \pi) \) staggered VBS state illustrated in Fig. 4.

![Figure 4](image)

**FIG. 4.** (a) Unit cell used in the mean-field ansatz and (b) \( (\pi, \pi) \) VBS pattern suggested by our mean-field analysis. Strong bonds are colored while weak bonds are represented by black lines.

The phonons enhance the hopping amplitude on all bonds and effectively renormalize the bandwidth of the electronic band structure. Furthermore, they modulate the hopping in a \( (\pi, \pi) \) pattern (see Fig. 4(b)) that leads to a finite gap at the Fermi surface. Since the VBS ordering breaks the discrete \( C_4 \) symmetry of the lattice, the ordering can survive at finite temperatures.

In addition to the mean-field analysis, we used a classical Monte Carlo approach to study the adiabatic limit. In this way, we can observe the melting of VBS order as a function of the temperature \( T = \beta^{-1} \). The partition function simplifies to

\[
Z = \int \prod_b dq_b e^{-S},
\]

\[
S = \beta \sum_b \frac{k}{2} q_b^2 - N_s \ln \det \left[ 1 + e^{-\beta \sum_b (-t + gq_b) K_b} \right].
\]

The determinant is strictly positive since its argument is a symmetric matrix. Therefore, we can use Langevin dynamics without divergences in the forces to update the phonon fields via

\[
\frac{\partial S}{\partial q_b} = \beta q_b + \beta g N \text{Tr} \left\{ K_b (1 - G) \right\},
\]

\[
G_{i,j} = \frac{\text{Tr} \left[ e^{-\beta \sum_b (-t + gq_b)(K_b c_i^\dagger c_j + c_j^\dagger c_i)} \right]}{\text{Tr} \left[ e^{-\beta \sum_b (-t + gq_b) K_b} \right]}.
\]

To capture VBS order we measured the bond kinetic susceptibility

\[
\chi_K^{\delta,\delta'}(q) = \int_0^\beta d\tau \, S_K^{\delta,\delta'}(q,\tau)
\]

with the imaginary-time-displaced correlation function

\[
S_K^{\delta,\delta'}(q,\tau) = \langle \tilde{K}^{\delta'}(q,\tau) \tilde{K}^{\delta'}(-q) \rangle - \langle \tilde{K}^{\delta'}(q) \rangle \langle \tilde{K}^{\delta'}(-q) \rangle
\]

and

\[
\tilde{K}^{\delta}(q) = \frac{1}{\sqrt{N}} \sum_{i,\sigma} e^{i q \cdot i} \left( \hat{c}_{i,\sigma}^\dagger \hat{c}_{i+a_{\delta,\sigma}} + H.c. \right).
\]

Figure 5 shows the bond susceptibility as a function of temperature and system size at the ordering wave vector \( Q = (\pi, \pi) \).

![Figure 5](image)

**FIG. 5.** (a) Bond susceptibility as a function of temperature and system size. (b) Energy as a function of temperature for \( L = 12 \). Simulations were done at \( \delta t_l = 0.01 \) and starting from the mean-field configuration.

The simulations were started in the mean-field configuration to reduce warm-up times. At low temperatures, the susceptibility grows in accordance with a long-ranged \( (\pi, \pi) \) VBS state. On our largest lattice size \( (L = 12) \), we observe a sudden drop of the signal at \( T \approx 0.06 \) (see Fig. 5(a)). The energy \( \langle \hat{H} \rangle \) shows a kink at the same temperature [Fig. 5(b)]. Above this temperature, thermal fluctuations destroy the long-range order.
B. Finite phonon frequencies

1. Equal time and static quantities

To map out the phases as a function of phonon frequency we computed spin-spin correlations,

$$S_S(q, \tau) = \langle \hat{S}_z(q, \tau) \hat{S}_z(-q) \rangle - \langle \hat{S}_z(q, \tau) \rangle \langle \hat{S}_z(-q) \rangle,$$  

(41)

as well as the imaginary-time-displaced correlations of the bond kinetic energy defined in Eq. (39). Here,

$$\hat{S}_z(q) = \frac{1}{\sqrt{N}} \sum_i e^{i q \cdot \mathbf{r}_i} (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}).$$  

(42)

We also consider the bond-kinetic susceptibility of Eq. (38) and the equivalent form of the spin susceptibility, $\chi_S(q)$. As discussed in Sec. II, our Hamiltonian has an O(4) symmetry. Hence, the three components of the spin-spin correlations are degenerate with the charge-density wave (CDW) and s-wave superconducting (SC) correlations. As argued in Ref. 36, introducing an infinitesimally small positive (negative) Hubbard interaction will select the spin (CDW/SC) correlations. Here, we will discuss the results from the point of view of spin-spin correlations.

![Figure 6](image)

**FIG. 6.** (a) Size scans of the bond-kinetic susceptibility at $\beta t = 40$. (b) Temperature scans at $L = 12$ for the bond-kinetic structure factor $\chi_K(q = (\pi, \pi), \tau = 0)$. (c) Temperature scans of the bond-kinetic susceptibility for $L = 12$.

In Fig. 6 we present the dependence of the bond-kinetic susceptibility and structure factor on lattice size, temperature, and phonon frequency. As apparent, at the lowest frequency considered ($\omega_0 = 0.4$), $\chi_K(q = (\pi, \pi))$ grows as a function of size and inverse temperature, suggesting long-range $(\pi, \pi)$ VBS order as in the mean-field approximation. Note that cooling down our system to $\beta t = 40$ was not sufficient to achieve convergence of $\chi_K(q = (\pi, \pi))$ on an $L = 12$ lattice. As the phonon frequency grows, we observe a rapid drop in $\chi_K(q = (\pi, \pi))$ that indicates that the $(\pi, \pi)$ VBS state gives way to another phase.

![Figure 7](image)

**FIG. 7.** (a) Size scans of the spin susceptibility at $\beta t = 40$. (b) Temperature scans of the spin structure factor $S_S(q = (\pi, \pi), \tau = 0)$ for $L = 10$. (c) Temperature scans of the spin susceptibility for $L = 10$.

In Fig. 7(a), we show results for the spin degrees of freedom. At low temperatures, the size-dependence of the antiferromagnetic spin susceptibility shows a marked increase at large phonon frequencies. In Figs. 7(b) and (c), the temperature dependence at fixed lattice size shows that we are able to achieve convergence with respect to temperature. This allows us to compute the correlation ratio

$$R_{\chi, S} = 1 - \frac{\chi_S(q = (\pi, \pi) + \Delta q)}{\chi_S(q = (\pi, \pi))},$$  

(43)

where $|\Delta q| = 2\pi/L$. This renormalization group invariant quantity takes the value of unity (zero) in the ordered (disordered) phase. At $T = 0$ and for a continuous tran-
sition, it scales as

\[ R_{\chi,S} = f \left( \left[ \omega_0 - \omega_0^c \right] L^{1/\nu} \right) . \] (44)

In Fig. 8 we plot this quantity as a function of system size for the lowest temperature available (representative of the ground state). Although corrections to scaling, not included in Eq. (44), lead to a meandering of the crossing point, the results suggest a critical phonon frequency \( \omega_0^c \simeq 0.6 \) at which long ranged antiferromagnetic ordering sets in.

![Graph showing \( \chi_p(q = (0,0)) \) as a function of phonon frequency \( \omega_0 \).](image)

**FIG. 9.** Parity susceptibility as defined in Eq. (45) at \( \beta t = 10 \) as a function of phonon frequency \( \omega_0 \).

Being a modulation of the bond kinetic energy, the \((\pi, \pi)\) VBS state does not break the underlying \(O(4)\) symmetry of the lattice. However, it does break translation and rotational symmetries. On the other hand, the AFM phase breaks the \(O(4)\) symmetry. To document this symmetry breaking, we have computed the susceptibility of the parity operator,

\[ \chi_p(q) = \int_0^\beta d\tau \sum_\tau e^{i\mathbf{q} \cdot \mathbf{r}} \langle \hat{p}_r(\tau) \hat{p}_0 \rangle . \] (45)

Since \( \hat{p}_k \) is an Ising variable that changes sign under an \(O(4)\) transformation \( M \) with \( \text{det} M = -1 \), we expect \( \chi_p(q = 0) \) to diverge at a critical temperature corresponding to a 2D Ising transition. Being an 8-point correlation function, \( \chi_p(q) \) becomes very noisy at low temperatures and we are restricted to \( \beta t = 10 \). Our data as a function of system size and phonon frequency are plotted in Fig. 9. For \( \omega_0 = 2 \), \( \chi_p(q = 0) \) grows as a function of system size, suggesting that for this frequency the Ising temperature is below \( T = 0.1t \). On the other hand, for \( \omega_0 = 1 \) (still in the AFM phase) our temperature is certainly too high to capture the Ising transition. Based on these data, we conclude that the AFM phase breaks the \(O(4)\) symmetry down to \(SO(4)\) at a finite-temperature Ising transition occurring at \( T_c^I \). A natural conjecture is that \( T_c^I \) vanishes at \( \omega_0^c \).

We have used the ALF implementation [20] of the stochastic maximum entropy algorithm [32-35] to carry out the Wick rotation from imaginary to real time. The single-particle spectral function, \( A(k, \omega) \), is related to the imaginary-time Green function via

\[ \langle \hat{c}_{k,\sigma}(\tau) \hat{c}^\dagger_{k,\sigma}(0) \rangle = \frac{1}{\pi} \int d\omega \frac{e^{-\tau \omega}}{1 + e^{-\beta \omega}} A(k, \omega) . \] (46)

**FIG. 10.** Single-particle spectral function at (a) \( \omega_0 = 0.4 \), (b) \( \omega_0 = 1 \), (c) \( \omega_0 = 1.5 \), (d) \( \omega_0 = 2.0 \). Here, \( L = 12, \beta t = 40 \).

Figure 10(a) shows the single-particle spectral function at \( \beta t = 40 \) for \( L = 12 \). The coupling of the Einstein phonon mode to the electrons breaks the \( \hat{Q}_b \rightarrow -\hat{Q}_b \) symmetry. Consequently, \( \frac{1}{4N} \sum_b \langle \hat{Q}_b \rangle \) acquires a non-zero expectation value that renormalizes the bandwidth. At \( \omega_0 = 0.4 \), we measure \( \frac{1}{4N} \sum_b \langle \hat{Q}_b \rangle = -0.56510(7) \), so that the effective hopping matrix element at \( g = 1.5 \) becomes \( t_{\text{eff}} = 1.85 \). This explains the observed range of the band from \(-4t_{\text{eff}} \) at \( k = 0 \) to \( 4t_{\text{eff}} \) at \( k = (\pi, \pi) \). At this phonon frequency, the \((\pi, \pi)\) modulation of the hopping is at the origin of the gap that opens along the non-interacting Fermi surface \((k = (0, \pi) \text{ and } k = (\pi/2, \pi/2) \text{ in Fig. 10(a)})\). Both, the gap and the cosine band of width \( 8t_{\text{eff}} \) are features that can be accounted for at the mean-field level. However, the spectral function exhibits low-lying spectral weight that extends over the considered path in the Brillouin zone. In analogy with the one-dimensional case [39], we attribute this low-energy weight to polaron formation.

As the phonon frequency is enhanced to \( \omega_0 = 2 \) (see Fig. 10(b)-(d)), \( \frac{1}{4N} \sum_b \langle \hat{Q}_b \rangle \) remains almost constant and, consequently, the width of the cosine band does not change substantially. Upon inspection, we see that weight is transferred to the polaron. The origin of the gap at \( \omega_0 > \omega_0^c \) is to be found in antiferromagnetic ordering.

On a general basis, the \(O(4)\) symmetry of the model leads to the relation \( A(k, \omega) = A(k + Q, -\omega) \) with \( Q = (\pi, \pi) \). Hence, in the absence of symmetry breaking, the polaron band is nested and should show instabilities to antiferromagnetic order or to a \((\pi, \pi)\) VBS order.

Figure 11 shows the VBS dynamical structure factor \( S_K(q, \omega) \) at four different phonon frequencies. Using
the maximum entropy method, we compute the imaginary part of the VBS dynamical spin susceptibility, $\chi''(q, \omega)$, using

$$\text{Tr} S_K(q, \tau) = \frac{1}{\pi} \int d\omega \frac{e^{-\tau \omega}}{1-e^{-\beta \omega}} \text{Tr} \chi''(q, \omega). \quad (47)$$

The dynamical VBS structure factor then reads

$$S_K(q, \omega) = \frac{\text{Tr} \chi''(q, \omega)}{(1-e^{-\beta \omega})}. \quad (48)$$

Since the phonons couple to the bond kinetic energy, we expect $S_K(q, \omega)$ to reveal both the phonon dynamics and the particle-hole continuum. At $\omega_0 = 0.4$ (Fig. 11(a)), we see substantial very low-lying weight as well as high-energy features that reflect the particle-hole continuum. The low-lying excitation corresponds to the phonon mode, which is soft at $Q = (\pi, \pi)$ in accordance with our expectations. However, we cannot resolve the dispersion relation. In comparison to the bandwidth, the renormalized phonon modes are very slow and are at the origin of long autocorrelation times. As the frequency grows and in the antiferromagnetic phase (Fig. 11(b)-(c)), the phonon mode acquires a gap.

Finally, in Fig. 12 we show the dynamical spin structure factor, $S_S(q, \omega)$. Because phonons do not carry a spin, they are not visible in spin-flip scattering processes. The data in Fig. 12(a) show that $S_S(q, \omega)$ is dominated by the particle-hole continuum. Importantly, at low energies, and as we enter the antiferromagnetic phase (see Fig. 12(b)-(d)), spectral weight develops at $Q = (\pi, \pi)$ and reflects the onset of antiferromagnetic ordering.

V. DISCUSSION AND CONCLUSIONS

We have used a Langevin dynamics updating scheme with Fourier acceleration [17] in the framework of the auxiliary-field quantum Monte Carlo method to study the physics of the two-dimensional SSH model as a function of phonon frequency.

In contrast to Ref. [19], we computed forces exactly for a given field configuration. A comparison between stochastic and deterministic calculations of forces can be found in Ref. [40]. Although the CPU time per sweep is longer and scales as $L^5 \beta$, fluctuations, especially for time-displaced correlation functions, are smaller. One of the key difficulties encountered in Langevin dynamics are zeros of the determinant that lead to logarithmic singularities of the action. Using the $O(4)$ symmetry of the SSH model, the determinant can be written as the square of a Pfaffian. The average sign of the Pfaffian provides a measure for the density of zeros. We demonstrated that for small phonon frequencies the density of zeros is small so that Langevin simulations can be stabilized using an adaptive time step scheme. Nevertheless, simulations occasionally suffer from spikes in observables when the stochastic walk approaches a zero. Obviously, such configurations have very small weight and a hybrid molecular dynamics update may be more efficient. However, as shown in Ref. [19], this can lead to ergodicity issues that can be overcome by a complexification of the fields. For the Hubbard model, this is possible since the decoupling of the interaction can be done in various channels. In the case of phonons, we do not have such liberty. We believe that global Langevin updates are a good choice in the adiabatic limit where local moves fail. As the phonon frequency grows, Langevin dynamics becomes increasingly challenging but local updates, as discussed for example in Ref. [11], become increasingly attractive.

We have computed static and dynamical quantities to elucidate the physics of the SSH model at a fixed electron-phonon coupling as a function of the phonon frequency. The phase diagram is tied to the $O(4)$ symmetry of the model. In particular, the single-particle spectral function satisfies the condition $A(k, \omega) = A(k + Q, -\omega)$ with $Q = (\pi, \pi)$. Hence, any Fermi liquid state that does not break this symmetry will ultimately be unstable to orders that can open up a gap. This includes the $(\pi, \pi)$-VBS phase as well as antiferromagnetism. In the adiabatic limit, the problem simplifies since the phonons become classical. The ground state is a $(\pi, \pi)$ VBS phase. At nonzero phonon frequencies, we can integrate out the phonons in favor of a retarded interaction. At equal times, the latter...
reduces to $\frac{\eta^2}{4} \sum_{\langle\alpha,\beta\rangle} \hat{S}_i \hat{S}_j + \eta^2 \hat{n}_i^x \hat{n}_j^y - \eta^2 \hat{n}_i^y \hat{n}_j^x$. Note that for non-frustrating interactions, the sign of the transverse Anderson $\eta$-operators can be reversed via a canonical transformation, so as to yield Eq. (12). This interaction triggers AFM order that is degenerate with CDW and SC states. The $(\pi, \pi)$ VBS breaks lattice symmetries but not the O(4) symmetry. On the other hand, AFM or SC/CDW phases break the O(4) symmetry down to SU(2). This symmetry reduction occurs in two steps. At finite temperature, we expect an Ising transition corresponding to the spontaneous ordering of the parity operator. Even parity corresponds to the SC/CDW phase and odd parity to the AFM phase. At $T = 0$, the SU(2) spin (pseudospin) symmetry is spontaneously broken, leaving the SU(2) pseudospin (spin) symmetry unbroken. The single-particle spectral function supports the picture of a narrow polaronic band undergoing a transition from a $(\pi, \pi)$ VBS to AFM/CDW/SC. In the particle-hole channel, the dynamical VBS correlation function reveals the phonon dynamics as a function of decreasing phonon frequency, including a softening at $(\pi, \pi)$. On the other hand, as $\omega_0$ grows, we observe enhanced spectral weight at low energies and at $Q = (\pi, \pi)$ in the spin channel.

FIG. 13. A vortex of the $C_4$ symmetry breaking VBS state with a featureless core.

Generically the O(4) symmetry will be broken down to SU(2) by, for example, adding a next-nearest-neighbor hopping. In this case, we expect that the phase diagram will be dominated by an SC phase. This conjecture is based on the fact that the Cooper instability is insensitive to the shape of the Fermi surface. The stability of the VBS phase as a function of an O(4) symmetry breaking interaction such as a chemical potential or a next-nearest-neighbor hopping is certainly an interesting topic for future investigations.

The nature of the transition remains elusive. We cannot understand it in terms of a deconfined quantum critical point (DQCP) [42, 43]. To see this, we can adopt the Dirac fermion understanding of DQCP put forward in Refs. [44, 45] in terms of five anti-commuting AFM and VBS mass terms of an 8-component Dirac metal. The algebra of the mass terms guarantees that the vortex core of the VBS order carries a spin-1/2 excitation. In this framework, the VBS order has momentum $(0, \pi)$ and $(\pi, 0)$. In contrast, the $(\pi, \pi)$ VBS observed here does not correspond to a Dirac mass term. This point of view is substantiated by noticing that a $C_4$ vortex of the $(\pi, \pi)$ VBS can be trivial, as shown in Fig. 13.

During the preparation of this manuscript, we became aware of the work of Ref. [16]. Our results are in agreement with their findings.

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