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GROUND STATES, OPTICAL ABSORPTION, AND PHONONS

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ABSTRACT

Using the Lanczos method for exact diagonalization on systems up to 14 sites, combined with a novel "phase randomization" technique for extracting more information from these small systems, we investigate several aspects of the one-dimensional Peierls-Hubbard Hamiltonian, in the context of *trans*-polyacetylene: (1) the dependence of the ground state dimerization on the strength of the electron-electron interactions, including the effects of "off diagonal" Coulomb terms generally ignored in the Hubbard model; (2) the phonon vibrational frequencies and dispersion relations, and (3) the optical absorption properties, including the spectrum of absorptions as a function of photon energy. These three different observables provide considerable insight into the effects of electron-electron interactions on the properties of real materials and thus into the nature of strongly correlated electron systems.

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INTRODUCTION

The nature of electron-electron interactions in "Strongly Correlated Electron Systems" has recently emerged as a subject of intense interest and debate. Much of the recent discussion has been stimulated by experimental work on exciting novel materials, including high-temperature superconducting copper oxides, "heavy-fermion" systems, organic synthetic metals, and halogen-bridged transition-metal chains. Unlike conventional metals, for which standard single-electron (band) theories describe quantitatively the electronic structures and excitations, these new materials are currently thought to have properties dominated by many-body effects arising from strong electron-electron interactions. To describe these materials it is essential to have tractable models that capture the essence of both electron-phonon (e-p) and electron-electron (e-e) interactions and that represent faithfully their synergetic, or competing, effects.

In contrast to the relative simplicity of independent-electron theories, models describing strongly correlated electrons are in general difficult to treat adequately. In their full complexity, many-electron problems involving N electronic orbitals – each of which can be empty, singly occupied with an electron of either spin, or doubly occupied – require the solution of Hamiltonian matrices of size roughly 4^N by 4^N . For a given problem, symmetries and selection rules (total spin, mirror plane or electron-hole symmetry, etc.) can be used to reduce the size of the matrix, but its growth with N will still be exponential. Often one attempts to avoid this difficulty by use of approximations involving *effective* single-particle methods – such as Hartree-Fock or Fermi liquid theory – which assume that the full problem can be treated in terms of self-consistent (or renormalized) nearly independent quasi-particle states. In Hartree-Fock, for example, one assumes that the full many-body wavefunction can be written as a single Slater determinant of one-particle wave functions. Accordingly, the problem for an N orbital system involves only an N by N matrix, albeit typically with self-consistency constraints on the parameters occurring in the Hamiltonian. Unfortunately, for strongly correlated systems such mean-field approaches can break down entirely. Worse still, when the physical systems involve electronic motion in reduced dimensions – as is the case in many of the experimentally interesting materials – the strong quantum fluctuation effects can dominate the physics, making this breakdown both more likely and more catastrophic.

Thus in studies of strongly correlated electron systems one is trapped between the Scylla of exponential growth of the number of states in any exact many-body basis and the Charybdis of the failure of mean-field theories to capture adequately the effects of interactions. In the present article we focus on one technique – the Lanczos method^{1,2} – which, at least in the case we treat here, appears (to continue the metaphor) to allow us to sail the narrow channel between these two hazards. In contrast to Quantum Monte Carlo methods, which circumvent the exponential growth of states by statistical techniques and importance sampling, the Lanczos

approach attacks this problem head-on by diagonalizing the full Hamiltonian. In view of the limited system size for which such an approach can be applied, it is important that we also use novel "phase randomization" techniques^{3,4} to investigate several aspects of the one-dimensional Peierls-Hubbard Hamiltonian, which has been widely used to model quasi-one-dimensional materials, including conducting polymers. For definiteness, we shall treat the model in the context of *trans*-polyacetylene (*trans*-(CH)_x). For this system, we shall study (1) the dependence of the ground state dimerization on the strength of the electron-electron interactions, including the effects of "off-diagonal" Coulomb terms generally ignored in the Hubbard model; (2) the phonon vibrational frequencies and dispersion relations, and (3) the optical absorption properties, including the spectrum of absorptions as a function of photon energy. These three different observables provide considerable insight into the effects of electron-electron interactions on the properties of real materials and thus into the nature of strongly correlated electron systems.

A GENERAL ONE-DIMENSIONAL "PEIERLS-HUBBARD" MODEL

Over the past several years the Peierls-Hubbard Hamiltonian⁵ has emerged as an important model in which to analyze the competing (or synergetic) effects of electron-phonon (e-p) and electron-electron (e-e) interactions in a variety of quasi-one-dimensional systems, including charge transfer salts, halogen-bridged metallic chains, and conducting polymers. In the context appropriate to describe *trans*-(CH)_x, the Hamiltonian, containing *all* electron-electron interactions involving up to nearest neighbor^{6,7,8}, takes the form

$$H = \sum_{\ell} (-t_0 + \alpha \delta_{\ell}) B_{\ell, \ell+1} + \frac{1}{2} K \sum_{\ell} (\delta_{\ell} - a)^2 + \frac{1}{2M} \sum_{\ell} p_{\ell}^2 + U \sum_{\ell} n_{\ell\uparrow} n_{\ell\downarrow} + V \sum_{\ell} n_{\ell} n_{\ell+1} \\ + X \sum_{\ell} B_{\ell, \ell+1} (n_{\ell} + n_{\ell+1}) + W \sum_{\ell} (B_{\ell, \ell+1} \quad , \quad (1)$$

We consider H defined on a ring of N sites and note that (1) $c_{\ell\sigma}^{\dagger}(c_{\ell\sigma})$ creates (annihilates) an electron in the Wannier orbital at site ℓ ; (2) $n_{\ell\sigma} = c_{\ell\sigma}^{\dagger} c_{\ell\sigma}$, $n_{\ell} = n_{\ell\uparrow} + n_{\ell\downarrow}$; (3) $B_{\ell, \ell+1} = \sum_{\sigma} (c_{\ell\sigma}^{\dagger} c_{\ell+1, \sigma} + c_{\ell+1, \sigma}^{\dagger} c_{\ell, \sigma})$ is the "bond-charge" operator; (4) t_0 is the hopping integral for the uniform (CH) chain; (5) α is the electron-phonon coupling describing the modification of the hopping between adjacent sites due to the distortion of the underlying discrete chain; (6) δ_{ℓ} is the relative displacement between the (CH) units at sites ℓ and $\ell+1$; (7) K represents the cost of distorting the "lattice" of (CH)_x moieties; and (8) p_{ℓ} is the momentum of the (CH) unit at site ℓ and mass M . The distortion δ_{ℓ} is determined by minimizing the total energy, with a defined to be the value needed in order that the ground state distortion have no constant piece. The value of a is important only in the calculation of the phonon modes.

In the limit $U = V = X = W = 0$, eqn. (1) reduces to the familiar Su-Schrieffer-Heeger (SSH) model⁹ of *trans*-(CH)_x. For definiteness we use the conventional SSH-polyacetylene parameters $\alpha = 4.1\text{eV/\AA}$, $K = 21\text{eV/\AA}^2$, and $t_0 = 2.5\text{eV}$. The Coulomb repulsions among electrons are parameterized with U , V , X , and W . U represents the on-site Coulomb repulsion, and V the nearest-neighbor repulsion. These terms are familiar from the conventional extended Hubbard model. In addition, however, the general Peierls-Hubbard model in eqn. (1) contains "off-diagonal" terms: that is, interactions that can not be expressed in terms of on-site electron density operators alone. The X term involves "mixed" on-site and "bond-charge" effects, and W is the pure "bond-charge/bond-charge" repulsion. The presence of such terms follows directly from the original many-body Hamiltonian, including Coulomb interactions; the explicit derivations are available in the literature^{8,9,10,11}. U , V , and all the longer-ranged *diagonal* terms will always contain contributions dependent only on the range of the electron-electron potential, whereas W and X are suppressed by the atomic orbital overlap. Since one of our primary

interests in the present study is the influence of *non-perturbative* e-e interactions, we shall focus on the intermediate-coupling regime by considering $U = 4t_0$, which is the full single-particle bandwidth. When the off-diagonal terms are not *a priori* negligible, the issue is the extent to which they produce results qualitatively different from those predicted in their absence. To answer this question correctly, one must adopt a method that gives correct results in this parameter regime; hence we shall focus on (numerically) exact many-body methods known to be reliable in the intermediate-coupling regime. Nonetheless we shall see that examining various limiting cases gives useful insight into the exact results.

For studies of the phonon dispersion relation, we need to evaluate the dynamical matrix

$$D_{\ell,\ell'} = \langle -\text{Tr } y_\ell^q(\tau) y_{\ell'}^q(0) \rangle = \partial^2 E / \partial y_\ell y_{\ell'} . \quad (2)$$

Phonon eigenmodes y_ℓ^q and eigenfrequencies ω_q^2 are found from $D_{\ell,\ell'} y_\ell^q = M \omega_q^2 y_\ell^q$. The Greens function formalism is useful to calculate the formulas for the infrared absorption, but the formula derived from it for the phonon modes involves a sum over excited states. Thus the numerical second derivative of the total energy is most useful for the determination of the modes. To reduce the number of diagonalizations we have used one discrete and one analytic derivative, i.e., we approximate $D_{\ell,\ell'}$ as

$$D_{\ell,\ell'} \simeq \left(\frac{\partial E}{\partial y_\ell} [y_{\ell'}^0 + dy_{\ell'}] - \frac{\partial E}{\partial y_{\ell'}} [y_\ell^0] \right) / dy_{\ell'} \quad (2')$$

where $\frac{\partial E}{\partial y_\ell} = -\alpha(B_{\ell,\ell+1} - B_{\ell-1,\ell}) - K(\delta_\ell - \delta_{\ell-1})$. Note $\partial E / \partial y_\ell [y_\ell^0] = 0$.

For studies of the optical transitions, we shall need the current operator

$$j_{\ell,\ell+1} = i(t_0 - \alpha\delta_\ell) \sum_\sigma (c_{\ell+1}^\dagger - c_{\ell\sigma}^\dagger c_{\ell\sigma} - c_{\ell\sigma}^\dagger c_{\ell+1\sigma}) . \quad (3)$$

The Fourier transform of $j_{\ell,\ell+1}$ is $J_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-iq(\ell+1/2)} j_{\ell,\ell+1}$. The optical - absorption coefficient $\alpha(\omega)$ is given by

$$\alpha(\omega) = \frac{1}{\omega} \sum_m | \langle m | J_q | 0 \rangle |^2 \delta(\omega - (E_m - E_0)) . \quad (4)$$

Due to the pathologies — including violation of the f-sum rule and difficulties both with physical interpretation of the geometry¹² and with phase-randomization — that arise when we attempt to define $\alpha(\omega)$ on a closed N-site ring for $q = 0$, we will study the smallest allowed nonzero momentum value, $q = 2\pi/N$.

THE LANCZOS METHOD

Our very large-scale diagonalization studies are made feasible by the Lanczos method^{1,2}, which in essence involves expressing the Hamiltonian in a cleverly chosen basis. One starts generating the basis set by normalizing some trial wavefunction, which we typically express in terms of real space occupations. We have usually chosen to start from a random wavefunction, subject only to the constraint that $S_z = 0$, where S_z is the z-component of the total spin. Since the Hamiltonian contains no (net) spin flip operators, this constraint is preserved throughout the calculations. Choosing a random starting wave function does not cost much extra computing time in most cases and, importantly, it statistically prevents one from picking a wavefunction with the wrong symmetry.

The Lanczos procedure is to generate the matrix elements of the Hamiltonian in a basis that is built up from this trial state. The basis is incremented one wavevector at a time by operating on the last basis state with the Hamiltonian and then orthonormalizing the product to all previous basis states. Notice that by construction $\langle j|H|i \rangle$ is tridiagonal^{13,14}. Within this basis, that linear combination of states with the lowest expected energy forms the estimate of the ground state. The basis will probably not be complete: we generally will truncate it when we have run out of computer memory, when the estimate of the ground-state energy stops dropping, or when the residual of a new state, after orthogonalizing to other components, is negligible.

When calculating the phonon modes, if we are interested only in the LO ($q = 0$ longitudinal optical or "soft") mode of the uniform ground state, we need only to evaluate $E[\delta]$ at three different δ near the equilibrium geometry $\delta = \delta_0$, as $y_n^{LO} = [(-1)^n \delta / 2]$ is an eigenmode. This is a minimal additional time demand. In fact, the necessary information is generated when searching for the ground state, so this information is obtained "at no cost" if advance planning is done. If we are interested in all modes, or a defect, then the calculation is more complicated, especially since we must expand around an equilibrium (optimized) geometry. This requirement is important, for if the geometry is not optimized, spurious imaginary eigenfrequencies will be found. We have stored the equilibrium eigenstate and used it as the initial electronic wavefunction for each of the stepped geometries to avoid "artifacts" of other phonon modes. Further, we have Fourier transformed and used as basis states the y_l^j for zero electron-phonon coupling, again in order to "guide" the calculation toward the correct eigenstates; this approach is useful, since wavefunctions from exact diagonalizations are not as reliable as energies.

Importantly, the calculations of optical absorption spectra — and hence also gaps, conductivities, and susceptibilities — are easily carried out by generating H in a suitable basis. For the optical absorption, we first calculate the ground state, $|\psi_0 \rangle$ using the technique described above. We then generate a new basis, using $J_q|\psi_0 \rangle$ as the first state and obtaining subsequent states by the application of H . Once the basis has been generated, the problem of calculating $\alpha(\omega)$ reduces to finding the spectral weight of this first state for the tridiagonal Hamiltonian. In essence, this amounts to determining the spectrum by measuring the moments of H^n and using the cumulant expansion.

Given the size of the diagonalizations, the calculations are remarkably fast. To sweep a parameter range — say, a dozen different values of the dimerization — takes about twenty minutes on a CRAY supercomputer for a 12-site system. Though we do not report those measurements here, we have run up to 14-site lattices and could run 15-site chains on a CRAY 2 without incorporation of additional symmetries.

Phase Randomization

For (small) finite clusters with any given boundary conditions, the lattice-size dependence in numerical calculations is great. This is very familiar in the band theory limit (weak e-e interactions), in which the density of states for a finite-size lattice is a series of delta-function spikes at the k values allowed by the boundary conditions. Since the low-energy physics of the system depends on the states near the Fermi energy, this physics is highly dependent on whether such a spike lies on or near the Fermi surface or not.

A slightly different perspective on this strong finite size dependence provides an important hint as to how to improve the situation. In an infinitely deep but finitely wide square well potential, the quantum energy levels are discrete, with spacing in energy determined by the width of the well. To use a well of a given width to mimic a wider well, with more closely spaced energy levels, we could "play" with the walls to randomize the phase every time the electron "interacts" with the wall. In the currently relevant case of a one-dimensional system (which we will (somewhat sloppily) refer to as a "chain") the quantum phase of an electron traveling on the chain is well preserved if the chain is short. For ring boundary conditions, an

electron, traveling around the ring, still "remembers" its phase after completing a full circuit. For open-ended chains, an electron, bouncing off the ends, builds up waves in the bulk. Thus, just as in the case of the energy levels in a square well, the quantum nature of these charge carriers leads to the marked sensitivity on size and boundaries.

Although there has been some limited earlier work on using modified boundary conditions in the context of the Hubbard model^{3,4}, there is as yet no provably accurate prescription for randomizing the phase effectively for arbitrary U and V . The most obvious scheme is to change the complex phase of one of the hoppings on a closed ring^{3,4}. Physically, this corresponds to putting a magnetic flux through the ring and changes the locations of the momentum-space states. For $U = V = X = W = 0$, one can show that this approach ("complex-phase-averaging") is just using Bloch's theorem to construct larger units from smaller units by averaging over many different boundary conditions on the smaller units¹⁴, and, if properly carried out, is *exact*. However, for the half-filled band systems we are currently considering, in the strongly correlated ($U \rightarrow \infty$) limit, the effect of the flux is eliminated to lowest order and the bond-phase scheme becomes ineffective.

In the absence of any provable prescription, one must rely on the following intuitive "rules" for choosing a randomization scheme. First, whatever change is made to randomize the phase must, of course, randomize the phase effectively. Second, the change in the system must be negligible as the lattice size is increased to infinity. Finally, the behavior for small lattice sizes must be illustrative of the infinite-size limit. Put another way, one must study results on various lattice sizes and still make some sort of extrapolation to the infinite chain. Our choice for phase randomization is to multiply one of the hoppings by a real number x in the range $-1 \leq x \leq 1$. One can argue¹⁴ that this effectively randomizes the electronic phase in the strong-coupling limit. Note that this approach clearly incorporates not only cases of the periodic ($x = 1$) and antiperiodic ($x = -1$) rings but also the case of the open chain ($x = 0$). Thus it is in accord with our comments about "filling in" the k -values in the Brillouin zone. As we shall see in the ensuing section, this "scaled-hopping" phase randomization technique produces results in good agreement with expectations based on both strong- and weak-coupling perturbation theory arguments.

RESULTS FOR GROUND STATES IN 1-D CORRELATED BANDS

Effects Of The Hubbard U

It is well known that the Hubbard U counterintuitively initially increases dimerization for weak electron-phonon coupling. In Fig. 1 we show the dimerization as a function of U for various lattice sizes with the boundary condition averaged over several complex phases ("complex-phase-averaged"). This figure illustrates the convergence of the Lanczos technique with system size along with the effects of periodic, anti-periodic, and chain versus complex-phase-averaged boundary conditions. The chain restricted to be uniformly dimerized is most easily extrapolated to the infinite case. However, note that complex-phase-averaging yields a behavior for 10 sites that is comparable to the infinite case, whereas the single boundary condition results yield this behavior only after extrapolation. Fig. 1 will also prove instructive in our later discussion of the phonon modes.

Effects Of Off-Diagonal Electron-Electron Interactions

We have studied how off-diagonal Coulomb interactions - the X and W terms in eqn. (1) affect the ground state of the half-filled band⁶. Before we present the results from the exact diagonalizations, it is instructive to look at two limiting cases: strong coupling perturbation theory and the dimer.

Fig. 1. (a) (left): Self-consistent dimerization (δ) as a function of Hubbard U for several N with $48/N$ different phase boundary conditions summed ($50/N$ for 10 sites; solid lines) compared to the extrapolation to 48 sites from the chain constrained to have uniform dimerization (dashed line). Note the counter-intuitive *increase* of δ with U can be seen on systems as small as 8-sites.
 (b) (right): The complex-phase-averaged result on 10 sites (solid) is compared with the 10-site chain (dotted) and 10-site ring with periodic and anti-periodic boundary conditions (dashed), where finite-size effects obscure the enhancement.

Strong coupling perturbation theory — In the limit that $U \rightarrow \infty$, double occupancy of any site is energetically not allowed. The resulting spin-Peierls Hamiltonian^{5b,15} is

$$H_{eff} = \frac{K}{2} \sum_i \delta_i^2 + N \cdot V + \sum_i \left(\frac{t_{i,X}^2}{U-V} - W \right) (4\vec{S}_i \cdot \vec{S}_{i+1} - 1) \quad (5)$$

where $t_{i,X} = ((t_0 - 2X - \alpha\delta_i))$. The first effect of W , then, is to *suppress* antiferromagnetism. Further, to lowest order in δ_i , the spin coupling is proportional to

$$t_{i,X}^2 - W(U-V) \simeq t_0'^2 - 2\alpha't_0'\delta_i + O(\delta_i^2),$$

where $t_0' \equiv \sqrt{(t_0 - 2X)^2 - W(U-V)}$ and $\alpha' = \alpha(t_0 - 2X)/t_0'$. For given t_0 and X , since the effective t_0' decreases with W , the effective electron-phonon coupling $\pi\lambda' \equiv 2\alpha'^2/Kt_0'$ increases with W , due both to the increase in α' and the decrease in t_0' . This leads to the initially surprising conclusion that, for large U , the dimerization should initially *increase* with W , the bond-charge repulsion.

When W reaches a critical value $W_c \simeq (t_0 - 2X)^2/(U-V)$, the spin coupling becomes *ferromagnetic*. The spins will then tend to align, forming a ferromagnetic SDW with $4\vec{S}_i \cdot \vec{S}_{i+1} \simeq 1$. The minimum energy configuration has $\delta_i = 0$, and the ground state is an undimerized ferromagnetic SDW. The resulting phase diagram is shown in Fig. 2a.

Analytic results for a dimer — The “dimer” — two electrons on two sites — provides surprisingly accurate insight into many aspects of the behavior of larger systems. For comparison with the numerical results, we use periodic boundary conditions, so that $c_j^\dagger = c_1^\dagger$ and similarly for all other operators. The Hamiltonian in (1) then assumes the explicit form

$$H_d = -2t_0 B_{1,2} + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) + 2Vn_1n_2 + 2X B_{1,2}(n_1 + n_2) + 2W(B_{1,2})^2 \quad (6)$$

Since there is no possibility of bond alternation with only one bond, no explicit electron-phonon coupling appears. Further, one *always* has $n_1 + n_2 \equiv 2$; thus just as in the case of the $U \rightarrow \infty$ limit, the X term simply renormalizes the hopping to $t \equiv t_0 - 2X$.

Simple counting shows that there are six possible states for two electrons on two sites. As basis states we choose

$$\begin{aligned} |1, 1\rangle &\equiv c_{1\uparrow}^\dagger c_{1\uparrow}^\dagger |0\rangle, \quad |1, -1\rangle \equiv c_{2\downarrow}^\dagger c_{1\downarrow}^\dagger |0\rangle, \quad |1, 0\rangle \equiv \frac{1}{\sqrt{2}}(c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger + c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger) |0\rangle, \\ |0, 0\rangle &\equiv \frac{1}{\sqrt{2}}(c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger - c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger) |0\rangle, \\ |S\rangle &\equiv \frac{1}{\sqrt{2}}(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger) |0\rangle, \quad |A\rangle \equiv \frac{1}{\sqrt{2}}(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger - c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger) |0\rangle. \end{aligned}$$

As the notation suggests, the first three states are, respectively, the $S_z = +1, -1$, and 0 components of the spin triplet state and, by the spin symmetry of H , must all have the same energy. The state $|0, 0\rangle$ is a spin-singlet made entirely from singly-occupied states, while $|S\rangle$ and $|A\rangle$ are, respectively, spin-singlets made from symmetric and antisymmetric combinations of the two states involving double occupancy. Trivial algebra leads to the following results: (1) the triplet states are degenerate eigenstates of H_d , with eigenvalue $E_T = 2V$; (2) the state $|A\rangle$ is also an eigenstate, with eigenvalue U ; and (3) the states $|0\rangle$ and $|S\rangle$ are coupled, with the two eigenvalues $E_{\pm} = 8W + U/2 + V \pm \Delta/2$ where $\Delta = ((U - 2V)^2 + (8t_0 - 16X)^2)^{1/2}$. The ground state "phase diagram" for the dimer follows immediately by comparing these eigenenergies. For $U \equiv U = 4t$ (intermediate coupling), this diagram as a function of W/t and V/t is shown in Fig. 2b. For small values of W , the state E_- is always the ground state. This state, which in the absence of e-e interactions is just the $k = 0$ band state, corresponds to the "dimerized/BOW" phase and indeed, in the larger systems shows non-zero values of the dimerization. In the region bounded by AB and BC, the triplet state is the ground state; this corresponds to the ferromagnetic SDW phase found in larger systems. Finally, in the region bounded by BC and BD, the ground state is the state $|A\rangle$; this corresponds to the CDW phase in larger systems.

Fig. 2. The phase diagram as a function of V/t and W/t for intermediate coupling $U = 4t = 4t_0 - 8X$ (a) from strong-coupling perturbation theory and (b) for the half-filled dimer.

Exact diagonalization results — We focus on the phase diagram as a function of W and V at fixed $U = U_0$ in the region of intermediate e-e coupling anticipated to apply to many novel materials. Surprisingly, even for intermediate coupling the primary effect of X is merely to renormalize t_0 . The details of results including the X term in this calculation are reported elsewhere⁸.

Fig. 3 shows the phase diagram for an 8-site ring; comparison with 4-, 6-, and 10-site results, as well as the analytic strong coupling and dimer predictions, suggests this diagram reflects the infinite-ring behavior. The phase boundaries in Fig. 3 in general reflect a “first order transition” in the dimerization order parameter, δ_0 : that is, there is a sudden qualitative change in the nature of the ground state, and δ_0 drops almost immediately from a finite value to zero. However, for short segment of the BOW/CDW boundary near $W = 0$ — the range is roughly $0 < W < 0.1$ — the transition becomes second order. Except for this short segment, the dimerized phase has non-zero dimerization on its boundary.

Fig. 3: The phase diagram as a function of V/t_0 and W/t_0 for intermediate coupling $U = 4t_0 = 10\text{eV}$, and $X = 0$. Phase boundaries are plotted for a 8-site ring. The ground-state changes discontinuously across solid lines, smoothly across the dotted line.

In Figs. 4 and 5 we show the optimal dimerization δ_0 versus W when $U_0 = 4t_0 (= 10\text{eV})$, $V = 0$ and $V = 3\text{eV}$, respectively. Note the distinction between “Jahn-Teller” ($4N$) and “non-Jahn-Teller” ($4N + 2$) systems persists even away from the band theory limit. These figures also suggest that systems with $N \geq 8$ are near the converged large N behavior. Incidentally, the dotted regions of the 4-site ring results reflect the dimerization observed in the BOW phase. However, the actual ground state of the 4-site system at values of W in these dotted regions is a different, small-ring phase, which does not appear in the larger rings. Thus the solid line for the 4-site system, which shows the dimerization going to zero at relatively small values of W , although strictly correct, is essentially an artifact of the small system size. The dotted line, which explicitly ignores this small-ring phase and plots the dimerization assuming the BOW state remains the ground state until the transition to a ferromagnetic SDW, shows more clearly the true finite size effects on W_c and δ_0 vs. W .

The dimerized/BOW phase persists for a substantial range of Coulomb repulsion, both diagonal and off-diagonal. Indeed, dimerization increases monotonically with W before dropping rapidly to zero in a “first order phase transition” at $W = W_c$ in agreement with the strong coupling arguments above. In particular, as shown in Fig. 4, even for $V = 0$, W does

Fig. 4 (left): Dimerization as a function of W/t_0 for $U = 4t_0 = 10\text{eV}$ and $V, X = 0$ for 4-, 6-, 8-, and 10-site rings. For the 4-site ring, the dotted line gives results for the lowest energy dimerized state even though for this small ring the ground state is not dimerized for intermediate values ($0.10 < W/t_0 < 0.225$) of W/t_0 .

Fig. 5 (right): Dimerization as a function of W/t_0 for $U = 4t_0 = 10\text{eV}$, $V = 3\text{eV}$, and $X = 0$ for 4-, 6-, 8-, and 10-site rings. The 4-site ring is not dimerized for intermediate values ($0.16 < W/t_0 < 0.29$) of W/t_0 .

not destroy dimerization until $W_c = 0.6\text{eV} \approx 0.25t_0$. For $0 < V < U_0/2$, the dimerized phase persists until still larger values of W , and again W increases dimerization (slightly) until the BOW/FM SDW boundary is reached (Fig. 5). Note the increase in W_c relative to the $V = 0$ case, as expected from the strong coupling arguments. The existence of real materials with $W > W_c$ remains an open question; it is conceivable that the recently observed organic ferromagnetic materials may be modeled using parameters in this range. However, for $(\text{CH})_x$ and the other conjugated polymers, the experimentally observed dimerization requires, within the model Hamiltonian, $W < W_c$. Importantly, one still finds dimerization for strong, internally consistent Coulomb interactions; the assumption of weak e-e interactions is *not* required. This is fortunate, for in the case of $(\text{CH})_x$, such an assumption appears inconsistent with both observed spin density ratios¹⁶ and optical absorption involving neutral and charged solitons^{5f}.

Increasing W , of course, must suppress bond-charge correlations. The average bond charge, $\langle B \rangle = \frac{1}{N} \sum B_{l,l+1}$, does not fall off as dramatically as the correlation and indeed, for small W , the bond charge stays remarkably flat. As we have seen earlier, the alternating bond charge, which is related to the dimerization by $\langle B' \rangle = \frac{1}{N} \sum (-)^l B_{l,l+1} = K\delta/\alpha$, increases with W . Although W does suppress bond-charge correlations, the effects on average and alternating bond charge are quite different, and, in particular, small values W enhance the dimerization.

Although the off-diagonal terms produce only minor quantitative effects on dimerization, for other observables they can have important qualitative consequences. The mixed bond-site term X breaks charge conjugation/particle-hole symmetry; its inclusion in models of $(\text{CH})_x$ may thus help explain the puzzling "intensity anomaly" in polaron/bipolaron optical absorption¹⁷ experiments and also the ratio of neutral ($S^0 - S^0$) to charged ($S^+ - S^-$) soliton pairs in the decay channels of electron-hole pairs in photo-excitation of *trans*-($\text{CH})_x$ ^{5f}. In both these cases, the X term may well be more important than the straightforward next-nearest neighbor hopping term, t_2 ; within a tight-binding model, $t_2 \propto e^{-\alpha a} t_0$. Further, when X terms are included in H , the hopping in effect acquires a band-filling dependence; this may

be quite significant in applying Hubbard-like models to situations other than the half-filled band. In particular, Hirsch¹⁸ has recently argued that such an X term, corresponding to density-dependent hopping, could lead to superconductivity in bands with only a few holes. Nonetheless, despite this intriguing speculation, in the ensuing sections we set $X = W = 0$ and study how the conventional extended Hubbard interactions alter the expectations based on simple non-interacting electron models.

RESULTS FOR PHONONS IN 1-D CORRELATED BANDS

The correct parameters to model systems such as polyacetylene are a matter of much debate¹⁹. By calculating the phonon vibrational frequencies we gain additional insight into the possible parameter values. In the case of phonon vibrational frequencies, since we must expand about a minimum, it is unclear how to formulate a "phase randomization" technique, such as discussed for the optical absorption below, to determine full dispersion relations, especially for non-uniform ground states. Thus we can obtain only limited information about the full dispersion curve. Fig. 6 shows for periodic boundary conditions the dispersion relation for the 10 site half-filled band at several U . It appears that there are no surprises in its shape as U is increased. For the LO mode frequency of the uniform ground state complex-phase-averaging can be used to advantage though. Fig. 7 shows the LO mode frequency as a function of U and system size. Note that this mode tracks the dimerization, as can be seen by comparing Figs. 7 and 1. We have obtained dispersion and infrared absorption information for solitons, but do not report it here as, in its present crude form, it is rather unenlightening.

Fig. 6 (left). The dispersion relation for the 10 site half-filled band with periodic boundary conditions at several U . The dispersion relation for zero electron-phonon coupling is also shown (dashed line).

Fig. 7 (right). LO mode frequency as a function of Hubbard U for several N with $48/N$ different phase boundary conditions summed ($50/N$ for 10 sites). Note it tracks the dimerization shown in Fig. 1. The complex-phase-averaged result on 10 sites is compared in the inset with the 10-site ring with periodic and anti-periodic boundary conditions (dashed).

RESULTS FOR OPTICAL ABSORPTION IN 1-D CORRELATED BANDS

The optical spectra of many novel solid-state materials provide crucial insights into both the relative strengths of electron-phonon (e-p) and electron-electron (e-e) interactions and the nature of the charge carriers. The case of the dominant e-p interactions has been widely studied in applications to quasi-one-dimensional conducting polymers. The classic example is the application of the Su-Schrieffer-Heeger (SSH) model⁹ to *trans*-(CH)_x. Here, the optical absorption spectrum of the ideally dimerized ground state exhibits a square-root singularity — characteristic of one-dimensional independent-electron systems — at the edge of the optical gap. Further, the nonlinear excitations — “kink” solitons, polarons, and bipolarons — produce clear signatures in the form of midgap absorptions with well-defined relative intensities (see, e.g.,¹⁷ for a summary of these features). Conversely, motivated by potential applications to certain classes of charge-transfer salts²⁰, the case of dominant e-e interactions has also been studied extensively, both within the Hartree-Fock approximation²¹ and using various strong-coupling approaches^{21,22,23,24} or diagonalization of small systems¹². In this strongly correlated electron coupling limit, the spectra — at least for weakly dimerized systems — are typically shifted to higher frequencies and do not exhibit the characteristic square-root singularity at the onset of absorption. Similarly, the characteristic midgap absorptions associated with the localized nonlinear excitations are also shifted substantially — and, in some cases, essentially removed²⁵ — from their positions in the e-e interaction case.

To begin our discussion we recall the analytic forms for the optical absorption spectra that are available in a wide range of limiting cases. In the absence of electronic correlations, the Peierls-Hubbard model reduces to the SSH model. Here a number of analytic results are available, particularly if one works in the continuum limit, an approximation valid if, as is the case for *trans*-(CH)_x, the optical gap is small compared to the bandwidth and the excitations (e.g., solitons and polarons) extend over many lattice spacings. The uniform dimerization of the lattice caused by the e-p coupling opens up a gap between the valence and conduction bands, while defects in the uniform distortion appear as localized states in the gap. For the purely dimerized case¹⁷,

$$\alpha(\omega) \propto 1 / \omega^2 \sqrt{\omega^2 - \Delta^2} \quad , \quad (7)$$

where Δ is the gap energy. There is a characteristic square-root singularity at the gap edge due to the divergence in the density of states for transitions from the top of the valence band to the bottom of the conduction band. For the lattice model, the primary qualitative difference is that the absorption is cut off at the bandwidth $4t_0$ with another square-root singularity. Provided Δ is much less than $4t_0$, this difference is small, however, since it occurs at high energy, where all absorptions are attenuated by the $1/\omega^2$ factor due both to vanishing matrix elements and large energy denominators. For a soliton, transitions between the midgap state and one of the two bands give rise to a contribution of the form¹⁷

$$\alpha_s(\omega) \propto (\omega^2 - (\Delta/2)^2)^{-1/2} \times \text{sech}^2 \frac{\pi}{\Delta} (\omega^2 - (\Delta/2)^2)^{1/2} \quad , \quad (8)$$

while somewhat bleaching the interband spectrum. This midgap absorption has the same singular structure due, again, to the divergent density-of-states at the gap edge.

In the limit of large U (compared to t_0), the optical absorption is expected to be quite different. Since no two electrons, independent of spin, may occupy the same site, at half-filling, the sites are all “jammed”: each has exactly one electron and none of the electrons may move. Indeed, in this limit one may prove to leading order in t_0/U the equivalence of the system to a completely filled (and therefore inert) band of *spinless* fermions²⁶. If, on the other hand, one electron is removed, then the resultant hole moves as a free particle against this packed background with the same energy $\epsilon_k = -2t_0 \cos(k)$ as an electron moving in an otherwise empty band. Meanwhile, although adding an extra electron to the half-filled lattice costs the large

energy U , once that energy has been paid, the double occupancy also moves as a free particle, with energy $U + \epsilon_k$. Starting with the fully filled background, then, the optical excitations create double occupancies and holes in pairs at a total energy $U + 2\epsilon_k$ relative to the ground state; hence the range of the absorption should be from $U - 4t_0 < \omega < U + 4t_0$. Longer-range Coulomb repulsions produce an attractive interaction between the double occupancy and the hole – the standard excitonic binding mechanism – and thus skew the absorption spectrum toward lower energies. If the system is dimerized, the Brillouin zone is halved, giving rise to $\pm \sqrt{\epsilon_k^2 + (\Delta/2)^2}$ bands for the hole and $U \pm \sqrt{\epsilon_k^2 + (\Delta/2)^2}$ bands for the double occupancy. The gap which opens up in the bands opens a companion gap around the line $\omega = U$ in the optical absorption. These arguments show us where allowable transitions may occur. More detailed calculations^{22,23,24}, which incorporate information about the density of states and transition matrix elements, are needed to determine the shape of the spectra.

We can obtain further insight by considering a different “solvable” situation. In the limit of large dimerization – which, for purposes of illustration, we assume to be fixed, i.e. not self-consistently determined as a function of U – the hopping integral on the long bonds vanishes exponentially. For the model Hamiltonian in eqn. (1), this overlap vanishes completely for dimerization δ_0 satisfying $t_0 - \alpha\delta_0 = 0$. In this “decoupled dimer” limit, the chain may be thought of as being composed of independent, two-site systems, each having two electrons with an enhanced hopping parameter $t' = t_0 + \alpha\delta$. Further, each two-site cell has only one optical transition, at energy $\omega = U/2 + \sqrt{(U/2)^2 + (2t')^2}$, which, in strong coupling, is the absorption $\omega = U$ described above.

Armed with these analytic results for the limiting cases of strong and weak coupling and the “decoupled dimers”, we investigate the optical absorption using exact diagonalizations. We have measured the optical gap as a function of Coulomb terms U and V and lattice distortion δ . Our computed values for the gap for U and δ agree with Soos and Ramesesha²⁷ on both chains and rings to stated precision. (Actually, Soos and Ramesesha simply measure the gap to the lowest excited state of the correct symmetry while we measure the lowest-energy absorption. For doubly-even rings, there exists a low-lying state for which the matrix element for excitation from the ground state is zero. Hence, for these rings these two definitions of the gap are not equivalent and produce different results.) We find that the increase of the gap due to dimerization is greatest for intermediate couplings $U \approx 4t_0 \approx 10\text{eV}$. All the same, even for intermediate couplings, the gap is already dominated by the contribution from e-e interactions rather than by that from the lattice distortion. While V lowers the gap for the finite chains, the extrapolated result is remarkably flat in strong coupling. To understand this result we recall our earlier remark that the effect of longer range Coulomb interactions — e.g. the Hubbard V term — is to provide an attraction between the double occupancy (charge e^-) and the hole (charge e^+) created in the optically excited state²³. This attraction lowers the expectation value of the energy of that state and hence skews the absorption spectrum to lower energy. The current operator has odd parity, however, and thus a weak attraction will not be sufficient to bind the excitonic components (the double occupancy and the hole) in the optically excited state. In particular, if the lowest-energy component of the state is unbound, the double occupancy and the hole will be delocalized and the ability of the electrostatic attraction between them to decrease the gap energy will vanish with chain length. Thus we conclude that the gap will decrease with V as $N \rightarrow \infty$ only when the off-site Coulomb force is strong enough to bind the exciton.

The most difficult aspect in measuring spectra is the sparseness of the spectral peaks for finite-size systems. Clearly, there will only be a limited number of transitions for a finite-size system. One might imagine that, since the number of states in the system grows exponentially with the number, N , of spatial sites, the finite sampling of the infinite-ring spectrum presents no great difficulties. In fact, however, the number of significant transitions typically grows only linearly with N . In the limit of weak electronic correlations, for example, the electrons are essentially noninteracting and the optical transitions can be described in terms of the

N different single-particle energy levels. Meanwhile, when the Hubbard U is very large, the electrons essentially become noninteracting, spinless fermions, whose transitions, again, are characterized by N different energies. Further, even in intermediate coupling ($U = 10\text{eV}$) and on fairly large ($N = 12$) rings, one gets only four absorption peaks for periodic boundary conditions for the dimerized lattice. Clearly all this depends on the symmetry of the lattice distortion as well as on the strength of the electronic interactions. In highly asymmetrical cases the non-randomized spectra may have reasonable numbers of peaks. However, in these asymmetric cases it is typically difficult to distill the essential physics from the spectra. In sum, we find that for any fixed set of boundary conditions the optical spectra are sampled in a (disappointingly!) sparse manner over the entire range of electronic correlations: said another way, finite-size effects appear in a decidedly quantum fashion in the absorption spectra.

We have already indicated that "phase randomization techniques" can help us resolve this problem and further given some qualitative arguments about what to expect. In Fig. 8 we show plots of phase-randomized spectrum - using the "bond phase/ magnetic flux" method^{3,4} discussed above - for two values of U in the weak coupling regime: $U = 1\text{eV}$ and $U = 4\text{eV}$, with the bandwidth taken to be $4t_0 = 10\text{eV}$. Note that in the Fig. 8 we have already "smoothed" the δ -function spikes by replacing them by Lorentzians of width 0.5eV to produce a continuous spectrum. While the $U = 1\text{eV}$ curve (the lower, smoother one) is reasonable, the $U = 4\text{eV}$ curve is starting to show signs of fairly sparse structure, despite the Lorentzian smoothing. This indicates the breakdown, anticipated in our earlier discussion, of the "magnetic flux/bond phase" randomization scheme.

Fig. 9. The optical absorption spectra calculated using the "bond phase/ magnetic flux" phase randomization method for $U = 1\text{eV}$ (lower smoother curve) and for $U = 4\text{eV}$ (upper, more jagged curve) for the case in which the full band width $4t_0 = 10\text{eV}$. Note the "sparseness" of the spectrum in the latter case.

To transcend the limitations of this "bond phase/magnetic flux" approach, we have adopted the "scaled hopping" procedure discussed in the previous section and have randomized the phase by averaging the different spectra that are found by varying the magnitude of the "boundary" hopping - i.e., between sites 1 and N - from $-(t_0 - \alpha\delta_N)$ to $+(t_0 - \alpha\delta_N)$ in ten equal steps. Again we smooth the spectrum by replacing the δ -function spikes by Lorentzians of width 0.5eV .

In Fig. 9, we show the phase-randomized spectra produced by this technique for electrons on a 12 site ring in the strongly interacting case with $U = 30\text{eV}$ for both a uniform lattice ($\delta = 0$),

solid line) and for a strongly distorted lattice ($\delta = 0.14\text{\AA}$, dashed line). The gross features of the spectra are predicted by strong-coupling calculations^{22,24}. The numerical spectra, however, show substantially more interesting detail. The optical absorption, which to first order in the hopping is rounded, symmetric, and extends from $U - 4t_0$ to $U + 4t_0$, is shifted to higher energies in higher order. It is still centered about $\omega = U$ and so becomes skewed for finite U . In particular, the absorption has a fairly sharp onset at the gap while at high energies $\alpha(\omega)$ vanishes with a finite slope. In the presence of a strong dimerization, the gap is enhanced slightly and a strong absorption appears at $U/2 + \sqrt{(U/2)^2 + (2t')^2} = 31.2\text{eV}$, as predicted by the decoupled-dimer argument. The peak due to the dimerization is decidedly asymmetric, with, again, a sharp onset on the low-energy side. The undimerized absorption is noticeably depleted on the high-energy side of the absorption peak, corresponding to the gap which opens up in the strong-coupling absorption²⁴ due to the gaps in the single-particle bands. There may be a companion depletion on the low-energy side, but it appears to disappear with increasing ring size.

Fig. 9 The phase randomized optical spectra obtained using the "scaled-hopping" approach described in the text for 12-site rings at strong coupling ($U = 30\text{eV}$). The solid and dashed lines are for the uniform and dimerized ($\delta = 0.14\text{\AA}$) lattices, respectively.

For intermediate coupling $U = 4t_0 = 10\text{eV}$, Fig. 10 shows phase-randomized spectra for a uniform lattice ($\delta = 0$, solid line) and for a strongly distorted lattice ($\delta = 0.14\text{\AA}$, dashed line) of 12 sites. The scale of $\alpha(\omega)$, of course, is greater than in the case of stronger coupling shown in Fig. 9, as one would predict from the f-sum rule^{12,28,29}.

The results in Fig. 10 are truly hybrids of the weak- and strong-coupling absorptions. The undimerized spectrum might be thought of as strong-coupling absorption²² — as in Fig. 9 — which has been strongly skewed to the low-energy side, as we would expect from the small value of U . A more natural picture, however, might be to associate the gap-edge peak with the square-root singularity from the diverging density-of-states, as in the noninteracting case, in spite of the fairly substantial value of U . Despite this interpretation, we should stress that, as a comparison of the two curves in Fig. 10 demonstrates, the gap is due mostly to e-e interactions. The dimerization raises the gap somewhat — more here, in any case, than for the $U = 30\text{eV}$ case shown in Fig. 9 — but its principal effect is to give rise to a "decoupled-dimer" peak, characteristic of strong coupling. If we were to plot spectra for strongly distorted lattices over a wide range of U , all on the same plot, we would observe two envelopes. One envelope would

Fig. 10 The phase randomized optical spectra obtained using the “scaled-hopping” approach described in the text for 12-site rings at intermediate coupling ($U = 10\text{eV}$). The solid and dashed lines are for the uniform and dimerized ($\delta = 0.14\text{\AA}$), lattices, respectively.

trace out the decoupled-dimer peak, pronounced at large U and swallowed up at small U by the weak-coupling absorption. Conversely, the other envelope, corresponding to the density-of-states peak, would dominate at small U , but then disappear under the decoupled-dimer peak at higher energies. In intermediate coupling, both structures are comparable. Notice, finally, that, apart from a slight, familiar depletion on the high-energy side of the peak, in Fig. 10 the decoupled-dimer peak appears not to bleach the undimerized spectrum but simply to increase the integrated weight of the spectrum. This is related by the f-sum rule^{12,28,29} to the increase in the magnitude of the delocalization energy as the dimerization gap is opened up.

We have also investigated the effect of a nearest-neighbor V on the absorption spectrum. At half-filling, the effect in strong coupling of V on the *ground state* is almost exactly to reduce the effective value of U to $U - V$. For optical spectra, V only qualitatively reduces the effective value of U . As noted earlier, V is somewhat ineffectual in reducing the gap energy until it is strong enough to bind the optically excited exciton. On the other hand, the centroid of the spectrum, which we define as $\int \omega^2 \alpha(\omega) / \int \omega \alpha(\omega)$, is quite nearly equal to $U - V$. Hence, V skews the absorption toward lower energies, much as for a reduced U . Turning on V is also like a reduced U in that V suppresses the decoupled-dimer peak.

Finally, Fig. 11 shows the absorption of a neutral and of a charged *soliton* on a 11-site ring. Phase randomization has not been used to produce these spectra in part because the reduced symmetry of the problem gives richer structure but mainly because we have been unable to find a scheme which effectively randomizes electronic phases while locking the “midgap” state at midgap. As a consequence, the figure is not extremely illuminating. It does serve to show, as discussed in a number of articles, that the effect of an intermediate $U = 4t_0 = 10\text{eV}$ is to shift the charged midgap absorption (dashed line) to lower energy while shifting the neutral soliton (solid line) to higher ω , where it blends into the intergap absorption.

CONCLUSIONS AND OPEN ISSUES

We believe that our results establish that the combination of Lanczos exact diagonalizations with phase randomization techniques can be used to obtain insight into many properties of strongly interacting electron systems from studies of (even small) finite-size systems. First,

Fig. 11 The optical spectra for 11-site rings at intermediate coupling ($U = 10\text{eV}$, $\delta = 0.14\text{\AA}$). The solid and dashed lines are for the neutral and charged solitons, respectively.

the effect of electron-electron interactions remains “counterintuitive”, even in the presence of X and W terms. The dimerized/BOW phase “persists” for a substantial range of Coulomb repulsion, both diagonal and off-diagonal. Indeed, dimerization increases monotonically with W before dropping rapidly to zero in a “first order phase transition” at $W = W_c$, in agreement with the strong coupling arguments above. In particular, as shown in Fig. 4, even for $V = 0$, W does not destroy dimerization until $W_c = 0.6\text{eV} \approx 0.25t_0$. For $0 < V < U_0/2$, the dimerized phase persists until still larger values of W , and again W increases dimerization (slightly) until the BOW/FM SDW boundary is reached (Fig. 5).

In studying the effects of strong electron correlations on the phonon vibrational frequencies, we encounter a number of more challenging problems. Since we must expand about an optimal geometrical configuration, it is not clear how to formulate the “phase randomization” techniques to determine full dispersion relations, especially for non-uniform ground states. Accordingly, we have found that the small system sizes have limited the amount of useful information about defect modes; in particular, we have been so far unsuccessful in extracting information which could be usefully extrapolated to the infinite case about localized phonon modes in the presence of defects, and thus we have not been able to obtain useful results concerning infrared absorption. However, the dispersion relation of the $2k_F$ phonon appears to show no surprises as U changes, the amount of softening just tracking the degree of dimerization. We are able to reliably extract the LO mode frequency for the case of uniform dimerization, which is important for determining parameters.

In the case of optical absorption spectra, since electron phases interfere quantum mechanically over the entire extent of small rings or chains, small systems are strongly discrete and have very sparse spectra. Phase randomization is essential to produce high-resolution spectra from exact diagonalizations on these small (up to 12-site) rings. Simple results from limits of strong and weak electronic correlations and of large lattice distortions help us to understand results in the difficult intermediate-coupling regime. In the limit of infinite U , half-filled rings show wide, rounded absorption spectra centered about $\omega = U$. As U is decreased or V is turned on, this structure is skewed toward lower energies. In the limit of vanishing U , the skewed absorption turns into a peak at the gap edge as a square-root divergence develops in the density-of-states. For infinite U , dimerization introduces a strong peak, corresponding to the limit of decoupled two-site dimers, in the middle of the absorption. Dimerization opens

up gaps in the single-particle bands and so should also open up gaps in the optical absorption around the decoupled-dimer peak. In finite U , the decoupled-dimer peak is suppressed and the gaps in the absorption are somewhat washed out, particularly on the low-energy side of the peak. In weak coupling, there are neutral- and charged-soliton absorptions at midgap. For finite U , the neutral-soliton absorption is shifted to higher energies while the charged-soliton midgap peak moves to lower ω .

Clearly much work remains. In particular, we have begun to perform these diagonalizations in momentum space to gain full control of electronic phase randomization. Our analyses of solitons and other localized defects are very preliminary, and one could indeed argue that since both our phase randomization technique and these intrinsic defects can be viewed as $1/V$ effects, it may prove very difficult to extract more reliable information about solitons than is already available. However, we hope to be able to incorporate our knowledge of important physical features — *e.g.*, midgap states — of one-dimensional electron-phonon models to a greater extent in calculating high-resolution spectra in the presence of difficult excitations, such as solitons and polarons.

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