Peierls-Hubbard Finite Systems: A General Method

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We extend a continued matrix method, developed earlier. to solve finite size Peierls-Hubbard Hamiltonians. In particular, ire solve tlie dimer case, compare witli existing results, aiid discuss tlie advantages of tlie method presented: it can be generalized, in a straightforward aiid systematic fashion, to larger systems; tlie method is amenable to tlic introduction of small "fields", necessary to breali symmetries in finite systems, therefore enabling us to probe tlie stability of tlic various ordered states; furthermore it allows tlie computation of observables in a simple aiid economic fashion; and tlie several approximations available for infinite systeins can be tested and compared as function of tlie system's size.

I. Introduction

Peierls-Hubbard Hamiltonians (PHH) consider tlie interplay of electron- electron aiid electron- lattice interactions, of relevance in a Iarge variety of problems iii both condensed matter and molecular pliysics, e.g., charge transfer, metal-insulator transitions, valente fluctuations. bond order and so on. As examples we mention: numerical[1-4], variational[5] and mean field[6] approaches to one and two dimensional PHH, all within the adiabatic approximation[7]; and a non-adiabatic effective medium approach[8]. Also perturbative methods have been utilized, as in refs [9, 10] to deal witli organic ion-radical compounds and probe their inicroscopic parameters via optical lineshape calculations. General solutions for finite PHH are desirable not only to study energy transport aiid lineshapes of molecular clusters, they also provide guidelines to probe tlie validity of existing approximations for infinite systeins, as tlie system size is increased. We developed a Green's Function Matrix Continued Fraction Method for exciton-phonon interacting systems[11-14], aiid apply it here to PHH (see also refs. [15-17] for related methods).

II. Peierls-Hubbard Hamiltonian

A cluster witli N sites, N electrons and $N_{\mathbf{m}}$ lattice modes is modeled with tlie Hamiltonian

$$\mathbf{H} = \mathbf{H_{el}} + \mathbf{H_{ph}} + \mathbf{H_{ep}}, \tag{1}$$

with

$$\mathbf{H_{el}} = \sum T_{ij}\, c_i^\dagger c_j + \sum U_{ijkl}\, c_i^\dagger c_j^\dagger c_k c_l,$$

$$\mathbf{H_{ph}} = \sum \omega_\alpha b_\alpha^\dagger b_\alpha,$$

$$\mathbf{H_{ep}} = \sum \mathcal{M}_\alpha^{ij}\, c_i^\dagger c_j (b_\alpha^\dagger + b_\alpha),$$

where $\mathbf{H_{el}}$ is tlie electroiiic, $\mathbf{H_{ph}}$ tlie lattice, and $\mathbf{H_{ep}}$ tlie electron-lattice contribution to H, respectively; i a site (and spin) index ($\mathrm{i} \leq N$), a a lattice mode index ($\alpha \leq N_m$). Tlie T's and U's are transfer and Coulomb repulsion terms respectively. Tlie ω's are tlie several latticc modes (in tlie harmonic approximation) and tlie $\mathcal{M}$'s tlie (linear) electron-lattice interaction strength. Tlie operator c (b) destroys an electron (phonon) at site i, spin σ (mode a). Since tlie total number of electrons N is a constant of the motion, tlie Hamiltonian can be reduced to a similar Hamiltonian $\mathbf{H_r}$ with renormalized ($\mathbf{T}, U$, w, $\mathcal{M}$)'s witli $N_m - 1$ modes plus a decoupled displaced oscillator (mode B. frequency Ω and strength λ), namely as:

$$\mathbf{H} = \mathbf{H_r} + \Omega B^\dagger B + \lambda(B^\dagger + B). \tag{2}$$

Now aiid throughout, our H will stand for tlie reduced $\mathbf{H_r}$; solutions of tlie full Hamiltonian (1) are necessary, for exainple, to compute the actual optical lineshapes[18].

Here we present tlie zero temperature, one mode ($N_m - 1 = 1$) case. For the general case approximations have been developed[12-14,19]. Tlie exact solution is obtained in several steps. as sketched below (see details in [11,12]):

i) Solve for $\mathbf{H_{el}}$ and obtain a basis set $|\phi_j\rangle$, $j \leq N_s$, with N_s tlie number of electronic states, in general greater than N.

ii) Calculate the electron plionon interacting matrix M witli components

$$\mathbf{M}_{ij} = \langle \phi_i | \sum_{kl} \mathcal{M}_{kl} c_k^\dagger c_l \, | \phi_j \rangle$$

iii) Define tlie (retarded) Green's Function Matrix $\mathbf{G}(z)$ witli components

$$\mathbf{G}_{ij}(z) = -i\int_0^\infty dt e^{izt}\,\langle\langle\ |\phi_i(t)\rangle\langle\phi_j(0)|\ \rangle\rangle, \quad (3)$$

witli $\mathrm{Im}z = 0^+$, $((\ldots))$ denotes average over both tlie electron and phonon vacuum and tlie time evolutioii of $|\phi_i(t)\rangle$ is givtn by $\mathbf{H_T}$. If tlie full solution is needed, G must be replaced by $\mathcal{G}$, a Poissonian convolution of G witli tlie displaced decoupled oscillator[20], given by

$$\mathcal{G}(z) = e^{-g}\sum_{l=0}^{\infty}\frac{g^l\ \mathbf{G}[z-(g-l)\Omega]}{l\,!}, \quad (4)$$

witli $g = (\lambda/\Omega)^2$, see equation (2).

iv) Defini tlie pure electronic Green's Function $\mathbf{G_0}(z)$, as in iii) but with tlie time evolution of $|\phi(t)\rangle$ given by $\mathbf{H_{el}}$.

v) Define an auxiliary function $\mathbf{D}(z)$ satisfying a Dyson Type equation, see for example[11-14]

$$\mathbf{D}(z) = \mathbf{G_0}(z) + \mathbf{G_0}(z)\mathbf{H_{ep}}\mathbf{D}(z). \quad (5)$$

$\mathbf{D}(z)$ lias matrix components, $\langle n|\,\mathbf{D}(z)\,|m\rangle$, on tlie electronic Hilbert space (i,$j \leq$ N,) and on tlie harmonic oscillator Hilbert space $(|n\rangle, |m\rangle; \mathrm{n}, m = 1, 2, \ldots)$. Tlirougliout this paper, we keep matrix notation for tlie electronic part and display explicitly tlie oscillator's coinponents.

Finally, tlie solution is $\mathbf{G}(z) = \langle 0|\,\mathbf{D}(z)\,|0\rangle$, with tlie recursion relations (see again, refs. [11-14])

$$\langle m|\,\mathbf{D}(z)\,|n\rangle = \mathbf{G_0}(z)\delta_{mn} + \mathbf{G_0}(z)\mathbf{M}\,\langle m|\,\Theta(z)\,|n\rangle\,, \quad (6)$$

where

$$\Theta(z) = b^\dagger\mathbf{D}(z+\omega) + b\mathbf{D}(z-\omega).$$

The diagonal part can be solved via a continued matrix algoriihm as

$$\langle n|\,\mathbf{D}(z)\,|n\rangle^{-1} = \mathbf{G_0^{-1}}(z) - \theta_n(z), \quad (7)$$

with

$$\theta_n(z) = \mathbf{M}\,\frac{n+1}{\mathbf{G_0^{-1}}(z-\omega) - \theta_{n+1}(z-\omega)}\,\mathbf{M},$$

and n > 0. Nom, for N_m inodes with frequency w, and interaction matrix $\mathbf{M}_\alpha$, with $1 \leq a \leq N_m$, a sound approximation[13,14,19] was found to be

$$\theta_n(z) = \sum_{\alpha=1}^{N_m}\mathbf{M}_\alpha\,\frac{n+1}{\mathbf{G_0^{-1}}(z-\omega_\alpha) - \theta_{n+1}(z-\omega_\alpha)}\,\mathbf{M}_\alpha.$$

The inforination contained in $\mathbf{G}(z)$ is extracted via expectation values and susceptibilities probing our system witli small external fields. Any given operator A may be decomposed a.s A = $\mathbf{A}_e\mathbf{A}_p$ where A, is tlie electroiiic, and $\mathbf{A}_p$ tlie lattice part of A, respectively. Let's define tlie spectral density of sucli opcrator as

$$\mathbf{S_A}(z) = -\frac{Im}{\pi}\sum_n \mathrm{Trace}\,\mathbf{A}_e\,\langle 0|\,\mathbf{D}(z)\,|n\rangle\,\langle n|\,\mathbf{A}_p\,|0\rangle\,. \quad (8)$$

If a small external static field $\mathcal{H}$ is introduced, by adding to H tlie incremental $\mathrm{AH} = -0.5\mathcal{H}\,\mathbf{B}$, with 13 tlie conjugate operator to H, and witli $n(z)$ tlie spectral density of tlie identity operator (tlie density of states DOS), then tlie expectation value $((\mathbf{A}(z)))$ aiid tlie susceptibility $\chi_{\mathbf{B}}(z)$ can be cast. respectively as

$$\begin{aligned}\langle\langle\ \mathbf{A}(z)\ \rangle\rangle &= \frac{\mathbf{S_A}(z)}{n(z)}\\ \chi_{\mathbf{B}}(z) &= \lim_{\mathcal{H}\to 0}\frac{\langle\langle\ \mathbf{B}(z)\ \rangle\rangle}{\mathcal{H}}\end{aligned} \quad (9)$$

To solve for $\mathbf{G}(z)$ is equivalent to find the normalized eigenvectors and eigenvalues $|\psi_\mu\rangle, \varepsilon_\mu$ of H, respectively. This equivalence may be displayed as

$$\langle\langle\ \mathbf{A}(\varepsilon_\mu)\ \rangle\rangle = \langle\psi_\mu|\,\mathbf{A}\,|\psi_\mu\rangle\,.$$

III. Tlie Dimer Case

Consider a tivo site, two electron system (N = 2, tlie smallest finite size counterpart to tlie lialf filled band case), witli diagonal electron-lattice interaction $\mathcal{M}_{ii} = S^{1/2}$ and off-diagonal electron-lattice interaction $\mathcal{M}_{12} = \kappa$. Periodic boundary conditions require us to take botli sites and modes to be identical, a restriction to be lifted without further complications, if we want to study for example, a lieteronuclear diatomic molecule. From tlie two normal modes (frequency w), conveniently written as

$$b_\pm = \sqrt{1/2}\,(b_1 \pm b_2),$$

tlie symmetric mode (+) is decouplecl when reducing tlie Hamiltonian, as in equation (2), witli B = b_+. Also tlie only relevant Coulomb term is tlie intrasite repulsion U (all others' eliminated via tlie constant of the motion N into effectives T and U). Also we introduce a staggered "electric" and "magnetic" field; h_q and $\boldsymbol{h_{,,}}$ respectively, in order to study cliarge and spin transfer states, precursor states for charge and spin density waves in infinite systems. These fields are essential in finite systems, as symmetry breaking devices.

Then, tlie reduced Hamiltonian H is

$$\mathrm{H} = \mathbf{H_{el}} + \mathrm{H}', \quad (10)$$

with

$$\mathbf{H_{el}} = -0.5(h_q Q + h_\sigma m_\sigma) - T\mathcal{B} + U\sum_\sigma n_{i\uparrow}n_{i\downarrow}, \quad (11)$$

and

$$\mathbf{H}' = \omega b_-^\dagger b_- + [\sqrt{S/2}Q + \kappa\mathcal{B}](b_-^\dagger + b_-), \qquad (12)$$

with

$$\begin{aligned} \mathcal{B} &= \sum_\sigma (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}), \\ Q &= \sum_\sigma (n_{1\sigma} - n_{2\sigma}), \\ m_\sigma &= \sum_\sigma \sigma(n_{1\sigma} - n_{2\sigma}), \end{aligned}$$

wliicli represeiit the boiid strength, cliarge transfer aiid spin transfer operators, respectively. Tlie electronic basis set is $|\phi_i\rangle$, i = 1 − 4, with

$$|\phi_{1,2}\rangle = \sqrt{1/2}(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger \pm c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger)\,(0)\,,$$

and

$$|\phi_{3,4}\rangle = \sqrt{1/2}\,(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger \pm c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger)\,|0\rangle\,,$$

where $|0\rangle$ is the electronic vacuuin. The two remaining triplet states have no inatrix elenients in the relevant Hilbert space. Then, the electronic Green's function $\mathbf{G_0}$ is given by

$$\mathbf{G_0^{-1}}(z) = \begin{pmatrix} z & h_\sigma & 0 & 0 \\ h_\sigma & z & 0 & 2T \\ 0 & 0 & z-U & h_q \\ 0 & 2T & h_q & z-U \end{pmatrix}. \qquad (13)$$

Let us define tlie following auxiliary inatrix

$$\mathbf{\Gamma}(a,b,c) = \begin{pmatrix} 0 & a & 0 & 0 \\ a & 0 & 0 & b \\ 0 & 0 & 0 & c \\ 0 & b & c & 0 \end{pmatrix}. \qquad (14)$$

Then, in tlie electronic basis, the bond strength, charge transfer and spin transfer operators defined above are represented by

$$\mathbf{A}_\mathcal{B} = \mathbf{\Gamma}(0,2,0), \quad \mathbf{A}_Q = \mathbf{\Gamma}(0,0,2), \quad \mathbf{A}_\sigma = \mathbf{\Gamma}(2,0,0),$$

respectively, and the interacting matrix M is given by $\mathrm{M} = \sqrt{2S}\mathbf{A}_Q + \kappa\mathbf{A}_\mathcal{B}$.

IV. Results

The dimer, for tlie diagonal case (ti = O), has been solved in the adiabatic limit[21] and via direct diagonalization[22−25] (ref. [26] considers tlie off - diagonal phonon). In all tliese cases no spin susceptibility was calculated, so tlie relevant basis set required only tlie tliree singlet states $|\phi_i\rangle$, i = 2, 3, 4. We iieed to increment tlie basis set in order to iiiclude tlie triplet state with tlie z spin coinponent equal to zero (i=1); thus we notice the first advantage of tlie method presented here: with a single stroke we incorporate both cliarge (witli or without lattice deformatioii) and spiii symmetry breaking devices, introducing tlie "small" fields. Our formalism allow us to classify in a natural fasliion any state, say with energy ε_0, as being eitlier a spin traiisfer (STS)or a cliarge transfer (QTS) state. We do tliis by computing both tlie spin and cliarge transfer susceptibilities, at equal strength fields. Tlie STS is probed with tlie condition

$$\rho = \left|\frac{\chi_\sigma(\varepsilon_0)}{\chi_Q(\varepsilon_0)}\right| > 1. \qquad (15)$$

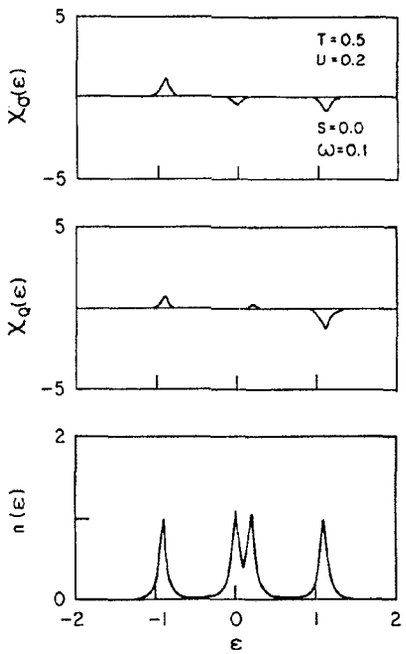

Figure 1: $n(\varepsilon)\chi_Q(\varepsilon) and \chi_\sigma(\varepsilon)$, for tlie parameter set T = 0.5, $U = 0.2$, $S = 0.0$ and $\omega = 0.1$.

Conversely tlie QTS is probed requiring p < 1. The lattice deformation is quantified witli tlie bond strength ratio

$$\xi = \left|\frac{\langle\langle\ \mathcal{B}(\varepsilon_0)\ \rangle\rangle}{\langle\langle\ \mathcal{B}_0(\varepsilon_0)\ \rangle\rangle}\right|, \qquad (16)$$

wliere the subscript 0 in $\mathcal{B}$ means the expectation value is evaluated at tlie null value for the lattice parameters (S = κ = w = O). The sign of ρ, if no absolute value was taken merely defines the parity of tlie state. For a given set of parameters (T,U,S,κ,w) the character of

the system is defined according to tlie character of tlie ground state. Any given state shows as a siinple pole of the DOS r (E). For computational and display purposes we use a finite energy imaginary part 6, therefore poles will be displayed as local maxima. A qualitative classification for tlie STS or QTS character of tlie system[21,23,24], for tlie diagonal case ($\kappa = 0$ and hereafter restrict to this case) is: tlie former occurs in the small S/T, large U/T regions of parameter space and the latter (possibly accompanied by a lattice distortion) for large S/T, small U/T or small ω/T. Tlierefore U (Coulomb correlations) and S (electron lattice interactions) compete to define tlie STS or QTS character of the system. Particular cases are (for infinite systems) the insulating antiferromagnet ($U \gg T, S \ll U$) and the Peierls Instability ("band limit" with $\mathbf{S,T} \gg$ U). We plot the DOS and both susceptibilities, as function of energy with an energy imaginary part $\delta = 0.05$ and fields $h_Q = h, = 10^{-7}$ in dimensionless units. In Figures 1 and 2 we consider the pure electronic case (i.e. $\mathbf{S} = 0$) for two sets of values for T and U. In botli cases tlie system has a STS character, the transition to QTS only to occur exactly at $U = 0$ refs. [21, 23, 24]. As S is increased (say for fixed U) tliere is a smooth crossover to QTS ,in agreement with[23–25]. In Figures 3 and 4, for tlie same values of T and U, but with $\mathbf{S} = 0.5$, a clear QTS regime is displayed. Notice that excited states in both cases are STS, the effect more pronounced for the case $U >$ T. Furthermore Figures 5 and 6 with $\mathbf{S} = 1.0$ show the same trends as is tlie previous set of Figures, also highlighting the vast number of excited statrs and their symmetries (parity) on both their spin and charge attributes (given by tlie sign of the susceptibilities at the poles).The boundary between STS and QTS can be calculated in parameter space. Let us remark that our spectral densities are, due to tlie finite size of our system, of the type

$$\mathbf{S_A}(z) = \sum_{\mu=0}^{\infty} n(\varepsilon_\mu) \langle \psi_\mu | \mathbf{A} | \psi_\mu \rangle \ \delta(z - \varepsilon_\mu),$$

where tlie μ i:; the eigenvalue index and ψ_μ the normalized eigenvector as defined at the end of section II. Therefore the spectral densities will be very sensitive to the actual value of the energy's imaginary part 6, both on the computed values for tlie poles (eigenvalues) and for tlie residues (expectation values) as well. Thus, caution must be exercised as a "small" δ is chosen. Fortunately, this numerical inconvenience is easily surmounted with a fast analytic continuation algorithm as in ref. [27]. In fact, only in order to determine tlie ground state energy such caution should apply, all otlier observables are ratios of spectral densities, the latter found to be weakly dependent on the smallness of δ. Notice that all matrix elements of $\mathbf{G}(z)$ are determined in one stroke and that the diverse observables are obtained as the imaginary part of linear combinations of the $\mathbf{G}(z)$'s matrix eleinents.

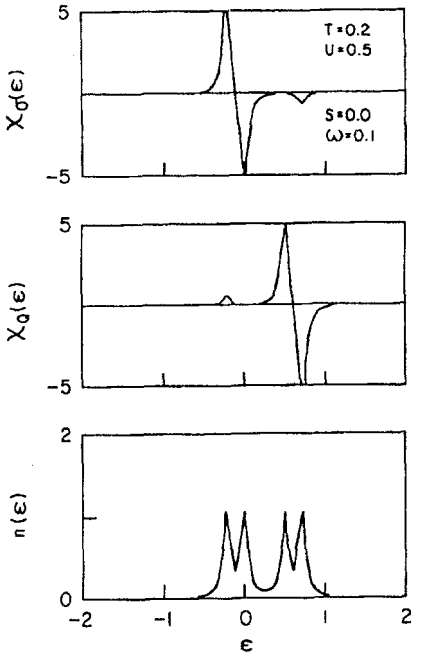

Figure 2: $n(\varepsilon), \chi_Q(\varepsilon) and \chi_\sigma(\varepsilon)$, for tlie parameter set $\mathrm{T} = 0.2, U = 0.5, S = 0.0$ and $\omega = 0.1.$,

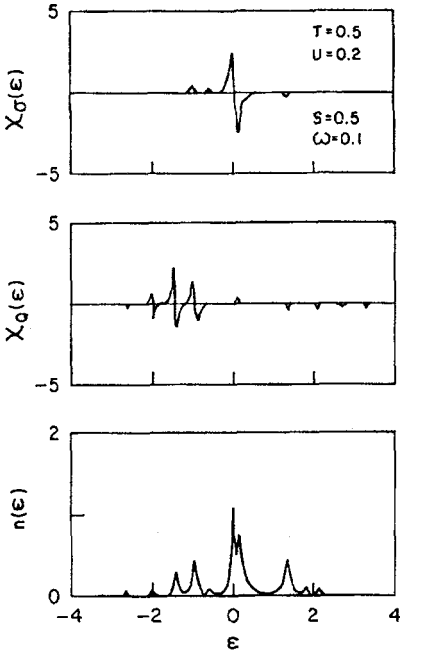

Figure 3: $n(\varepsilon), \chi_Q(\varepsilon), \chi_\sigma(\varepsilon)$ (see text), for the parameter set $\mathrm{T} = 0.5, U = 0.2, S = 0.5$ and $w = 0.1$.

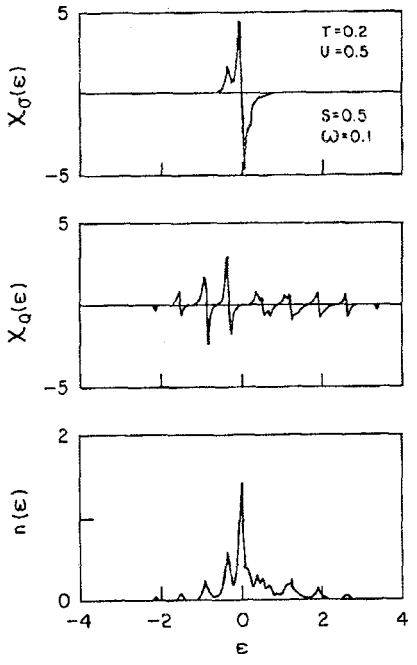

Figure 4: $n(\varepsilon), \chi_Q(\varepsilon) and \chi_\sigma(\varepsilon)$, for tlie parameter set T = $0.2, U = 0.5, S = 0.5$ and $w = 0.1$.

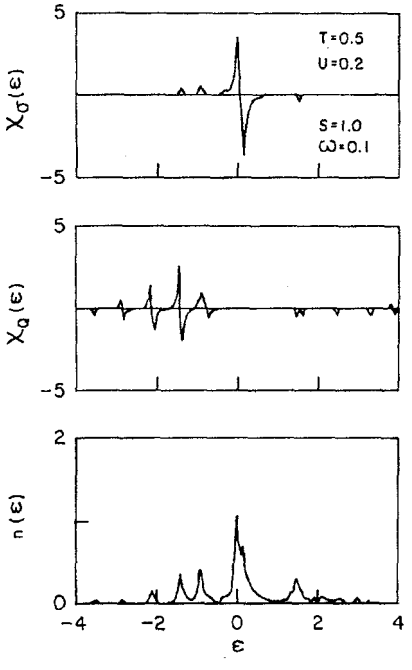

Figure 5: $n(\varepsilon), \chi_Q(\varepsilon) and \chi_\sigma(\varepsilon)$, for the parameter set T = $0.5, U = 0.2, \mathrm{S} = 1.0$ and $w = 0.1$.

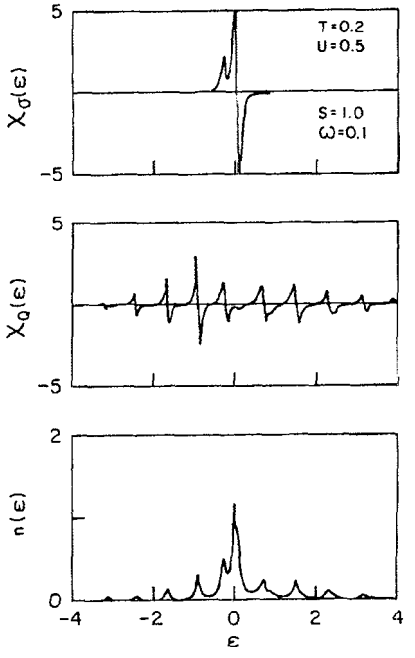

Figure 6: $n(\varepsilon), \chi_Q(\varepsilon) and \chi_\sigma(\varepsilon)$, for tlie parameter set T = $0.2, U = 0.5, S = 1.0$ and $\omega = 0.1$.

Tlie "raw" results $n(\varepsilon), \chi_{Q(\mathrm{E})}, \chi_\sigma(\varepsilon)$ in Figures 1-6 are a rather cumbersome picture of tlie results, if we need to extract from them tlie actual sequeiice of eigenvalues states and/or tlie actual weight of tlie several delta functions. Tlie value 0.05 for tlie imaginary part of tlie energy seems to be adequate for a pictorial view, of course smaller values of 6 will improve tlie accuracy but will generate also a scaling problem for tlie several weights, also increasing the computing time. If tliese "raw" results were needed then it is necessary to appeal to devices such as tlie analytic continuation algorithm mentioned above[27]. We assert tliat tlie latter procedure is not needed beyond the calculation of tlie ground state, since as remarked above the Spin/Charge discriminator is a weak function of S. We notice too tliat a finite value of δ blurs out information, nevertheless by computing many observables this loss is partially retrieved, namely: in Figures 1 and 2, there are 4 eigenstates (see $n(\varepsilon)$), from tlie susceptibilities; in Figure 1, eigenstates 2 and 3 are blurred into one state (tliey have tlie same parity), in Figure 2 eigenstates 3 and 4 are blurred into one state on tlie spin susceptibility, similarly eigenstates 1 and 2 on tlie cliarge susceptibility; so all three observables are needed to have a full view of the results, for our choice of 6. In Figure 4 tlie peak near the origin for $n(\varepsilon)$ seems to be a single heavy weiglit state (a much smaller δ will show to be two eigenstates closely arranged), tlie spin susceptibility indicates this peak to be indeed two states with opposite parity and the charge susceptibility indicates tliese states to be clearly of the type STS. Therefore, if some information is lost due to the finite value of δ (but making the results both ainenable to a pictorial

view and computationally fast), tliis loss is retrieved by computing other observables.

Finally in Figure 7 we present a Spin/Charge phase diagram for tlie diagonal case ($\kappa = 0$, see ref [28]). We plot tlie Spin/Charge interphase curve projected on tlie plane $\mathrm{T} + \mathrm{U} + S = 1$ (in suitable dimensionless units) for $w = 0.1$. Tlie $C(S)$ label refer to tlie Cliarge (Spin) phase, tlie transition is smooth at tlie iiiterpliase. Tlie interphase curve intersects tlie $\mathrm{U} - S$ line at $U = 1/3, S = 2/3, T = 0$, as predicted from tlie small polaron transformation (see ref. [20] for exact results at $\mathrm{T} = 0$). These results were obtained for $\delta = 0.001$, and remain insensitive as δ is decreased.

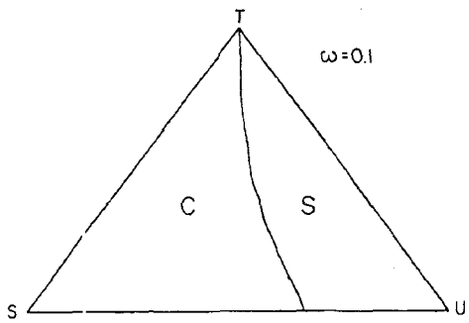

Figure 7: The Spin/Charge phase diagram projected on tlie plane $T + U + S = 1$ with $w = 0.1$.

V. Concluding Remarks

We presented a general method to solve Finite Peierls-Hubbard Systeins and particularized to tlie diagonal phonon dimer. Our conclusions are summarized as follows:

i) our method proved to be advantageous over direct diagonalization[23–26]. Our calculations involved 4 x 4 matrices and up to 30 continued fractions (in the probed region of parameter space). Direct diagonalization[23–26] involves typical 300 x 300 inatrices. To extend the latter metliod for the 3-site 3-electron 1-mode cluster (tlie smallest cluster to exhib t frustration and Jahn-Teller effects[29], with the same degree of accuracy involves 2000 × 2000 inatrices, for tlie 4-site 4-electron 1-mode cluster (solved in tlie adiabatic limit[30]) will involve 7000 × 7000 matrices. Our method will deal at most with 20 x 20 and 70 x 70 inatrices, respectively. If all lattice modes are to be included our metliod yields no increase in the matrices' dimensionality, but direct diagonalization will require 20000 x 20000 and 700000 × 700000 matrices, respectively. Thus, by increasing tlie cluster size to 4,6,8 sites, the matrices involved in our method sre within manageable dimensions, not so for tlie direct diagonalization inetliod. Furthermore our method allows for tlie inclusion of more than one mode via a tested approximation[12–14], and without any heavy increase of computational time. Beyond one mode, tlie direct diagonalization inetliod becomes proliibitive.

ii) our susceptibilities allow, at tlie cost of little extra coinputation, tlie study of tlie STS or QTS character of both tlie ground and tlie low lying excited states, related but not identical to tlie lattice deformation probed by direct diagonalization[23–26]. In fact our bond strength parameter ξ (eq. (16)) plus our Spin/Charge discriminator ρ (eq.(15)) can completely probe both tlie STS/QTS character and lattice deformation for our system[31]. Clearly a strong lattice deforinatioii means a QTS and tlie converse is true for no deforinatioii at all; nevertheless it is not clear for wliat intermediate lattice deformation value the system goes from a charge to a spin regime. Our inetliod provides an unambiguous answer[31].

iii) our inetliod when appliecl to clusters of increased size, will provide a systematic tool to probe tlie diverse approximations available for infinite systems, such as tlie adiabatic and mean field approximations.

iv) tlie diiner case, is not a coinpletely solved case, neither an uninteresting one (see for example[29], wliere solely electronic correlatioiis were considered), it stands as a particularly simple case displaying ill full power tlie aclvantages of tlie metliod presented liere.

v) as for work in progress, we are probing tlie dimer with both diagonal and off-diagonal electron-lattice interactions for a full system characterization[31].

vi) as a final comment, we remark that our method might reminisce other methods hinging on continued fractions tecliniques. recurrence relations and the like (for example, Lanczos' Method, Mori's Approach, Haydock's Representation and so forth[17]), nevertlieless tlie present formalism should not be confused with the former ones, our's being substantially different and inuch more powerful, because even in the zeroth approximation (absence of phonon degrees of freedoin) all fermionic correlations are accounted for.

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