Density Matrix Renormalization Group Applied to the Ground State of the XY-Spin-Peierls System.

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Abstract

We use the density matrix renormalization group (DMRG) to map out the ground state of a XY-spin chain coupled to dispersionless phonons of frequency $\omega$. We confirm the existence of a critical spin-phonon coupling $\alpha_c \propto \omega^{0.7}$ for the onset of the spin gap bearing the signature of a Kosterlitz-Thouless transition. We also observe a classical-quantum crossover when the spin-Peierls gap $\Delta$ is of order $\omega$. In the classical regime, $\Delta > \omega$, the mean-field parameters are strongly renormalized by non-adiabatic corrections. This is the first application of the DMRG to phonons.
The spin-Peierls state \[1\] in quasi-one-dimensional materials has attracted renewed attention lately because of its discovery in the organic series \[2\] \[3\] \((BCPTTF)_2X\), with \((X = AsF_6, PF_6)\), and in the cuprate compound \[4\] \(CuGeO_3\). Our own interest in this field stems from earlier findings on non-adiabatic effects or quantum lattice fluctuations on the transition temperature \(T_c\) of the closely related (through the Wigner-Jordan transformation \[1\]) electron-phonon problem. These generally tend to decrease \(T_c\) \[5\] \[6\] and the order parameter \[6\] \[7\] and can even destroy it for spinless fermions when the phonon frequency gets appreciably larger than the gap \[8\]. The existence of this adiabatic-quantum crossover has thus far remained only a theoretical concept. Moreover, there are predictions of a Kosterlitz-Thouless (K-T) transition in the quantum regime \[9\] which yet need to be confirmed. With the advent of the density matrix renormalization group (DMRG) \[10\], numerical calculations of the ground state properties of large scale systems has now become a reality. Although phonons have not yet been approached by this method, we will show the feasibility of such calculations.

We propose to study a XY-spin chain whose magnetic interaction depends on the bond length. The reason is twofold. First, the uniform spin chain enjoys an exact solution. It can be mapped into a half-filled non-interacting spinless fermions (pseudo-electrons) chain of width \(2J\) using the Wigner-Jordan transformation \[11\]. Second, the model contains the essential elements for a spin-Peierls transition, that is coupling to inter-molecular motion. We have chosen a dispersionless vibrational spectra for the molecular motion along the chain direction. This is quite acceptable as it is well known that it is the phonons at the zone edge that couple to the spins. This also circumvents the contribution of the hydrodynamic modes to the molecular displacements which increase logarithmically with chain length. This is especially annoying if one wishes to study the thermodynamic limit of the system as one has to go to long chain lengths. We start from the following Hamiltonian

\[
H = \sum_{\ell} \left\{ \omega b_\ell^\dagger b_\ell + \left[ J + \alpha \left( b_\ell^\dagger + b_\ell - b_{\ell+1}^\dagger - b_{\ell+1} \right) \right] \left( S_{\ell}^X S_{\ell+1}^X + S_{\ell}^Y S_{\ell+1}^Y \right) \right\}
\]

in which \(\omega\) is the vibrational energy (or frequency as \(\hbar = 1\) throughout), \(b_\ell\) \((b_\ell^\dagger)\) is the
annihilation (creation) operator for a vibration on molecule \( \ell \), \( J \) is the magnetic interaction, \( \alpha = g/\sqrt{2\omega} \) where \( g = (\partial J_{\ell,\ell+1}/\partial \ell) \) is the standard spin-phonon interaction in the classical paper of Bray et al. [1], and \( S_\ell \) is the local XY spin of value \( \frac{1}{2} \).

The expected crossover and the nature of the different regimes warrants further examination at this time. In the two-cutoff analysis [8], the natural energy cutoff for the pseudo-electrons is the bandwidth for characteristic energies (e.g. the gap \( \Delta \)) larger than \( \omega \). This is the classical regime in which the adiabatic approximation prevails. But for characteristic energies less than \( \omega \), there is a new cutoff \( \omega \) and the pseudo-electron-phonon coupling generates instantaneous backward-scattering \( g_1 \approx -8\alpha^2/(\omega_\pi v_F) \) and Umklapp \( g_3 \approx -g_1 \) couplings (in the renormalization group notation [11] [12] [13]), where \( v_F \) is the Fermi velocity of the pseudo-electrons. This is the quantum regime in which the interactions are unretarded and quantum fluctuations impregnate the ground state. It turns out that, for spinless fermions, the local character of the backward scattering cancels out. It is only the non-local character (wave number dependence) that can give rise to non-trivial effects. The renormalization equations [3] [14] show that unless the non-local contribution to \( g_3 \) has the right sign and has a bare (initial) value larger than a certain threshold, the Umklapp processes are irrelevant (\( g_3 \) renormalizes to zero) and the quantum system is gapless. If the threshold condition is met, the Umklapp processes and the vertex function grow to infinity. This signals the onset of a gap in the excitations. The transition is believed to be of the K-T type [15] [9]. We thus propose to look for a threshold value \( \alpha_c \) for the appearance of a gap and for the signature of the Kosterlitz-Thouless transition. The formula derived by Baxter [16] for the order parameter \( P \) is of the form \( P \propto \lambda^{-1} \exp(-\lambda^{-1}) \) where \( \lambda \propto (T_c - T)^{1/2} \) for a thermodynamic transition. For a ground state transition, identifying \( T \) with \( g_1 \propto \alpha^2 \) suggests \( \lambda \propto (\alpha^2 - \alpha_c^2)^{1/2} \). We shall refer to this last form as the effective K-T coupling.

We now turn to the use of the DMRG. Its inherent difficulty in dealing with vibrations is the infinite dimension of the Hilbert space for phonons. The most direct way around this problem is to truncate the space. This is obviously unsatisfactory whenever the average molecular displacements involve too many virtual phonons \( n_\ell = |\langle b_\ell \rangle|^2 \). A crude estimate
for this can be obtained by equating the increase in elastic energy to half the decrease in electronic energy $U$. For single electrons, as in the polaron problem, one gets $n_\ell \approx U/2\omega$, which obviously precludes any serious study of the deep adiabatic region $\omega \ll U$ [17] with a limited phonon space. In the case of a collective state, such as the spin-Peierls (or Peierls) modulated state, the same analysis for non-interacting pseudo-electrons leads, in a mean-field type analysis, to the criterion $n_\ell \approx \Delta^2 \ln(J/\Delta)/2\omega \pi J$. One gains a factor $\Delta \ln(J/\Delta)/\pi J$ over the single-electron situation, allowing a deeper incursion into the adiabatic region $\omega \ll \Delta$.

In our case, we typically kept $n_\ell$ less than 3 and $\omega$ was as small as $\Delta/25$ under the best conditions.

In the DMRG procedure a set of internal sites are coupled, via the inter-site part of the Hamiltonian, to environmental blocks. The DMRG proposes an iteration algorithm for the growth of the environmental blocks and thus, for the size of the system. Our adaptation of the method, for each set of parameters ($\alpha/J, \omega/J$), was the following. At each iteration, we considered a single site coupled to the environment blocks generated by the previous iteration. This central site had two spin states and $M_v$ vibration states, equal to anywhere from three (at small gaps) to twenty (for the larger values of $\alpha$). $M_v$ could be estimated by requiring that the local vibration subspace properly describe a coherent state of $n_v$ phonons, that is with an error much less than the allowed DMRG truncation error. The total number of sites in the chain was chosen to be even such that, with open boundary conditions, the chain would relax to a unique broken-symmetry state. Consequently, the number of sites of the bordering environment blocks differed by one, there being one long block and a one-site shorter block. We kept $M_b$ state in each block, a number varying from 60 to 120 (for the smaller gaps), and the corresponding matrix elements of all operators coupling the central site to the bordering sites of each block. We targeted the four lowest energy states in the superblock using the Davidson-Liu [18] algorithm, two in each of the total spin subspaces having $S^Z = 0, 1$. This way, we were able to reliably access the spin gap energy on the ansatz that, in the spin-Peierls state, the ground state is a singlet $S = 0$ state and the spin gap is to an $S = 1$ state. These four target states were then used to project out the density matrix $\rho_{ij}$.
of the two new blocks formed by the direct product of the spaces of the left (right) block and the added site. The z component of the spin being a good quantum number, we used it to fragment the block spaces into more manageable sizes. The density matrix was diagonalized and the $M_b$ highest energy eigenstates were kept. The truncation error $Tr \rho - \sum_{i=1}^{M_b} \rho_{ii}$, which was used as a minimal error indicator, was kept at a few times $10^{-5}$ or less. The block sizes thus increased by one and the chain length, by two sites at each iteration. The total length varied from 100 to 600 sites at the smaller gaps. At the longer chain lengths, the numerical accuracy on the gap greatly suffered and finite size scaling arguments were used to analyze the data. The error on the gap is estimated to be 10% under these strained conditions.

Fig. 1 shows typical values of the gap plotted in such a fashion as to bring out the characteristic K-T form $\Delta \propto (\alpha^2 - \alpha_c^2)^{-0.5} \exp(-b(\alpha^2 - \alpha_c^2)^{-0.5})$. The signature is clear and there is indeed a critical spin-phonon (pseudo-electron-phonon) coupling $\alpha_c$ for the onset or long-range order. Its values are obtained by least-squares fitting and are plotted in Fig. 2. This phase diagram identifies, for the first time, the existence of a power-law relationship $\alpha_c \sim \omega^{0.7}$. The average molecular displacement $u = |\langle b_t^+ + b_t \rangle|$ also seems to obey a similar law although the fit is less reliable as $u$ varies much more slowly. Fig. 3 hints to the probable existence of a power relationship between $\Delta$ and $u$ which one should expect if both parameters follow the K-T formula. We could not define one unambiguously.

Fig. 3 points to the identification of a crossover between two regimes. One, on the left of Fig. 3, is characterized by a rapid increase of $\Delta/\alpha u$ and the other one, on the right, shows a rather flat dependence $\Delta/\alpha u \sim 1$. As a matter of comparison, the mean-field solution predicts $\Delta/\alpha u = 2$. It is thus tempting to identify this latter region, which has a mean-field like behavior, as the classical or adiabatic regime described earlier. Fig. 4 confirms this assignment. It shows a crossover from a classical region, with a gap of the mean-field form $\Delta = \Delta_0 \exp(-AJ\omega/\alpha^2)$, into another regime, the K-T one of Fig. 1. Moreover, this crossover occurs at the expected value $\Delta \approx \omega$ (at the position of the arrows in Fig. 4). This crossover is also shown in the phase diagram (Fig. 2). The classical region is obviously
limited to $\Delta < \omega$. We have found the gap to saturate at a value very near $J$ for large $\omega$. This is why the adiabatic regime is restricted to $\omega < J$ in Fig. 4. The gap prefactor $\Delta_o$ and the leading coefficient $A$ in the exponential are strongly frequency dependent as shown in Fig. 5. We find that $A$ extrapolates to 0.44 and $\Delta_o$ to $1.3J$ at zero frequency (calculations cannot be performed at $\omega \to 0$ since the number of virtual phonons goes to infinity). These values are close to the expected mean-field ones of $\pi/8$ and $4J/e$, respectively \[ \text{[1]} \text{[9]}. The difference is significant, however, in view of a least-squares error of order 2% for these parameters. It is perhaps our linear extrapolation from finite frequencies which is improper. This conclusion is borne out by the plot in Fig. 5 of the plateau value of $\Delta/\alpha u$ in Fig. 3 (an average value in the classical region). It clearly shows that the classical regime does not satisfy the mean-field condition \[ \text{[1]} \Delta/\alpha u = 2 \] and that the extrapolation to $\omega \to 0$ is surely far from linear. It is however likely that this ratio can reach the value of 2 and that our results are consistent with the mean-field limit at $\omega = 0$. The parameters $\Delta_o$ and $A$ in the classical regime expression for the gap are seen in Fig. 5 to be strongly renormalized by non-adiabatic phonon contributions. Moreover, there seems to be a crossover, within the classical regime, between two behaviors. For $\omega \leq 0.05J$, the renormalization of $\Delta_o$ and $A$ are identical. This suggests a common origin to the renormalization, i.e. that it is the magnetic interaction $J$ which changes at these smaller frequencies. For $J > \omega > 0.05J$, these two parameters evolve differently, the extra renormalization of $A$ coming seemingly from vertex corrections to $\alpha$. The reason for this peculiar behavior is unclear.

We were also able to monitor the change in phonon frequency in the classical regime. We find, as Wu \textit{et al.} \[ \text{[19]} \] did, that the renormalized phonon frequency $\omega_r$ decreases as $\Lambda = 8\alpha^2/\pi \omega J$ does. For instance, we find at the crossover $\omega/\Delta = 1$ that $\omega_r/\omega \approx 0.5, 0.7$ for $\omega = 0.025, 0.3$ or $\Lambda \approx 0.3, 1.3$. This renormalization is stronger than the one Wu \textit{et al.} found for spin $1/2$ fermions.

In conclusion, we have not only verified the predictions of a Kosterlitz-Thouless transition and of a classical-quantum crossover in the spinless-fermion-phonon problem but we have also been able to produce a quantitative phase diagram of the spin-Peierls system and deduce
a power law dependence of the critical spin-phonon coupling on the phonon frequency. We have also shown that the DMRG can be used advantageously on phonon problems be they only dispersionless in this paper.

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FIGURES

FIG. 1. Semi-log plot of the spin gap $\Delta$ as a function of the reciprocal of the effective K-T coupling, for two values of the phonon frequency. The lines, as well as the quoted values of $\alpha_c$, are least squares fits to the formula of Baxter in the quantum region.

FIG. 2. Phase diagram of the system. The full line is a fit of the Kosterlitz-Thouless transition line. It has the power-law dependence $\alpha_c^{-2} \propto \omega^{-1.4}$. The dashed line straddles the classical-quantum crossover $\Delta \approx \omega$ and ends at $\omega \approx J$.

FIG. 3. Ratio of the spin gap $\Delta$ to the lattice modulation amplitude $u$ times the spin-phonon coupling $\alpha$ as a function of the square of the effective K-T coupling, for two values of the phonon frequency. The arrows point to the axis each data set refers to.

FIG. 4. Semi-log plot of the spin gap $\Delta$ as a function of the reciprocal square of the spin-phonon coupling $\alpha$, for two values of the phonon frequency. The straight lines are least squares fits to the mean-field like expression in the classical regime. The arrows point to the axis each data set refers to and also indicate where the classical-quantum crossover occurs.

FIG. 5. Evolution of the parameters $\Delta_o$ and $A$ of the mean-field type expression for the spin gap $\Delta$ as a function of frequency $\omega$, normalized to their zero frequency values $\Delta_o(0)$ and $A(0)$ which were linearly extrapolated from the data at finite frequencies. Also shown is the frequency dependence of the average value of $\Delta_o(\omega)/\alpha u$ in the classical region, where $\alpha$ the spin-phonon coupling and $u$ is the average molecular displacement. This latter ratio should equal 2 in a mean-field solution. The arrows point to the axis each data set refers to.
\[ \Delta / J = \frac{J(\alpha^2 - \alpha_c^2)^{-0.5}}{\omega} \]

- \( \omega = 0.025 \text{ J}, \alpha_c = 0.041 \text{ J} \)
- \( \omega = 0.3 \text{ J}, \alpha_c = 0.24 \text{ J} \)
\( J^2 \alpha^{-2} \)

\[ \frac{\omega}{J} \]

- gapless quantum
- classical
- quantum with gap
\[ \Delta / \alpha u = \frac{(\alpha^2 - \alpha_c^2)}{J^2} \]
