Peierls instability in Heisenberg chains

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Dimerization phase transitions for $S = 1/2$ linear antiferromagnetic chains is investigated by analogy with Peirels transitions in linear conducting chains. This analogy is very close when the fermion representation is used to describe the spin system, and the fermion interactions are treated in the Hartree-Fock approximation. Since the Fermi wave vector can be varied continuously by a magnetic field, the linear antiferromagnetic chain may be a convenient system for studying questions concerning the commensurability of the Fermi wave vector with the underlying lattice which have arisen in connection with the conventional Peierls transition.

I. INTRODUCTION

We consider a lattice of $S = \frac{1}{2}$ linear antiferromagnetic chains with magnetic interactions only along the chains, interacting with three-dimensional phonons. To describe the spin system we use the pseudofermion representation[1,2] in which, essentially, a site with spin-down is said to have a pseudofermion and a site with spin-up is said to be empty. The Hamiltonian obtained in this way is similar to that used to describe Peierls transitions due to the electron-phonon interaction in linear chain conducting systems.[3-5] It differs by the presence of a pseudofermion interaction term which in addition is of the same strength, J, as the one pseudofermion term. However, if the latter interaction is treated in the Hartree-Fock approximation the reduced Hamiltonian becomes formally identical to that used to describe the conventional Peierls transition.

In this paper, the pseudo-fermion-phonon interaction will be treated in the random-phase approximation (RPA) only.[5] The RPA, which is a mean-field theory, neglects the effects of fluctuations and this, as is well known, is a poor approximation for pseudo-one-dimensional systems.[6] For a strictly one-dimensional system, there can be no phase transition at a finite temperature because of the fluctuations. The phonons, however, are three-dimensional, and therefore a phase transition is possible even when there is no direct interchain fermion interactions.[7] The transition temperature is, however, generally much lower than that predicted by RPA.[8] For the conventional Peierls transition there exists a considerable amount of work going beyond RPA much of which can be used in the discussion of the spin-Peierls transition.[9]

That a one-dimensional system can undergo a phase transition when coupled to three-dimensional phonons has been shown rigorously[10] for a model similar to the one considered here, except that the Heisenberg interaction was replaced by an Ising interaction. In the latter case, all the properties of the phase transition can be expressed exactly in terms of a *three-dimensional* pseudo-spin Ising model.

One of the most interesting aspects of the Peierls transition is the prediction of new collective modes which are particularly interesting when the Fermi wave vector is incommensurate with the underlying lattice.[9] While in the usual Peierls transition the Fermi wave vector is determined by the electron density, which is fixed, in the spin case, the Fermi wave vector can be varied continuously by a magnetic field. The antiferromagnetic linear chain may therefore provide a means by which the role of commensurability in the Peierls transition may be examined very directly. In the absence of a magnetic field, the fermion band is half-filled.[11] With increasing field the Fermi level is lowered until for fields larger than a critical field H_c, $g\mu_B H_c = 2J$, the fermion band is empty, corresponding to a ferromagnetic ground state, in which case no Peierls transition can take place.

It should be emphasized that in addition to treating the fermion-phonon interaction in RPA, the fermion-fermion interaction is treated in the Hartree-Fock approximation. For the conventional Peierls transition, the Coulomb interactions can be neglected, at least as a first approximation. This is not possible in the spin case. The fermion interaction is of the same strength, J, as the quadratic fermion term. Neglecting the interaction term changes the symmetry of the problem from the Heisenberg model to an XY model.

It is difficult to assess the validity of the Hartree-Fock approximation. All the results presented below are therefore tentative. A further discussion of the Hartree-Fock approximation is given in Sec. IV.

II. HAMILTONIAN

The exchange interaction along the magnetic chains will be written

$$\mathcal{H}=\sum_l J(l,l+1)\,(\vec{S}_l\cdot\vec{S}_{l+1}-\tfrac{1}{4})\ , \tag{1}$$

where l labels the unit cells. We assume for simplicity that there is only a single magnetic ion per unit cell. Only nearest-neighbor interactions will be considered. We assume that the exchange integral depends on the instantaneous positions of the magnetic ions and expands in terms of the displacements $\vec{u}(l)$ of the magnetic ions,

$$J(l,l+1)=J+\sum[\vec{u}(l)-\vec{u}(l+1)]\cdot\vec{\nabla}_l J(l,l+1)\ . \tag{2}$$

The lattice displacement operators $u(l)$ are expanded in terms of the phonon normal mode coordinates in the usual way:

$$\vec{u}(l)=\sum_{\lambda q}\frac{\vec{e}(\lambda\vec{q})}{(mN)^{1/2}}\,e^{i\vec{q}\cdot\vec{R}_l}\,Q(\lambda\vec{q})\ , \tag{3}$$

where $\vec{e}(\lambda\vec{q})$ is the polarization vector and m the mass of the magnetic ion. The spin system will be described by the fermion operators[1,2]

$$\psi_l=(-2)^{l-1}S_1^z S_2^z\cdots S_{l-1}^z S_l^-\ , \tag{4}$$

defined such that,

$$\{\psi_l,\psi_{l'}^\dagger\}=\delta_{ll'}\ . \tag{5}$$

In terms of these operators

$$S_l^+S_{l+1}^-=\psi_l^\dagger\psi_{l+1}\ , \tag{6}$$

where

$$S^\pm=S_x\pm iS_y\ ,$$

and

$$S_l^z=\tfrac{1}{2}-\psi_l^\dagger\psi_l\ . \tag{7}$$

Making use of Eqs. (1)–(4), the Hamiltonian may be written

$$\mathcal{H}=\sum\epsilon_k\psi_k^\dagger\psi_k+\sum_{k+k'=k''+k'''}v(k'-k'')\psi_k^\dagger\psi_{k'}^\dagger\psi_{k'}\psi_{k'''}+\sum_{kq\lambda}g_1(k\vec{q}\lambda)\,Q(\lambda\vec{q})\,\psi_k^\dagger\psi_{k-q}$$
$$+\sum_{k+k'=k''+k'''-q}g_2(k'-k''\vec{q}\lambda)\,Q(\lambda\vec{q})\psi_k^\dagger\psi_{k'}^\dagger\psi_{k'}\psi_{k'''}\ , \tag{8}$$

where

$$\begin{aligned}
&\epsilon_k=J(\cos ka-1)\ ,\quad v_k=J\cos ka\ ,\\
&g_1(k\vec{q}\lambda)=\tfrac{1}{2}g(\lambda\vec{q})\,(1-e^{-iqa})\,[(e^{ika}-1)\\
&\qquad+e^{iqa}(e^{-ika}-1)]\ ,\\
&g_2(k\vec{q}\lambda)=g(\lambda\vec{q})\,e^{ika}(1-e^{-iqa})\ ,\\
&g(\lambda\vec{q})=\frac{\vec{e}(\lambda\vec{q})}{(mN)^{1/2}}\cdot\vec{\nabla}_l J(l,l+1)\ ,
\end{aligned} \tag{9}$$

and a is the lattice constant along the chain. In the above equations, three-dimensional vectors are boldface and wave vectors along the chain lightface. The first two terms describe the rigid Heisenberg model expressed in terms of fermion operators, while the next two terms describe the coupling to the phonons. To this we add the Hamiltonian describing noninteracting harmonic phonons,

$$\mathcal{H}_{ph}=\frac{1}{2}\sum P(\lambda\vec{q})P(\psi,-\vec{q})+\frac{1}{2}\sum\omega^2(\lambda\vec{q})Q(\lambda\vec{q})Q(\lambda,-\vec{q})\ , \tag{10}$$

where

$$[Q(\lambda\vec{q}),\,P(\lambda'\vec{q}')]=i\delta_{\lambda\lambda'}\delta_{\vec{q}\vec{q}'}\ . \tag{11}$$

The fermion-fermion interactions will be treated in the Hartree-Fock approximation.[1,11] The Hamiltonian Eq. (8) for the uniform chain is then approximated by

$$\mathcal{H}_{\text{H-F}}=\sum_k E_k\psi_k^\dagger\psi_k+\sum g(\lambda\vec{q}k)Q(\lambda\vec{q})\psi_k^\dagger\psi_{k-q}\ , \tag{12}$$

where

$$E_k=pJ\cos ka\ ,\quad g(\lambda\vec{q}k)=2ig(\lambda\vec{q})p\sin ka \tag{13}$$

with p determined by the self-consistency condition

$$p=1-2\sum n_k\cos ka\ , \tag{14}$$

where

$$n_k=\langle\psi_k^\dagger\psi_k\rangle=1/(e^{\beta E_k}+1)\ . \tag{15}$$

The Hartree-Fock Hamiltonian equation (12) is of the same form as that used to describe the conventional Peierls transition in a gas of electrons described in the tight-binding approximation.[5] Furthermore, in the absence of a magnetic field the fermion band is half-filled. This follows from Eq. (7) and the fact that $\langle S^z\rangle=0$ for independent linear chains. Treating the fermion-phonon interaction in RPA, we obtain for the renormalized phonon in the undistorted lattice the dispersion curve

$$\omega^2=\omega_0^2(\lambda\vec{q})+\sum g(k\vec{q}\lambda)\,\frac{g(k-q,\vec{q}\lambda)n_k-g^*(k\vec{q}\lambda)n_{k-q}}{\omega-E_{k-q}+E_k}\ . \tag{16}$$

The stability limit for the uniform phase is determined by setting $q=2k_f$, $\omega=0$ in the expression for the lowest-lying renormalized phonon mode,

$$\omega_0^2(\vec{q}, q = 2kf) = \frac{g^2}{J^2}\frac{2}{\pi}\int_{-Jp}^{Jp} dE\,\frac{[(Jp)^2 - E^2]^{1/2}}{E}\tanh\tfrac{1}{2}\beta_c E\,. \tag{17}$$

In the limit, $kT \ll pJ$, the expression for the transition temperature is of the BCS form

$$kT_c = 1.14pJe^{1/\lambda}\,, \tag{18}$$

where

$$\lambda = 4g^2p^2N_0/\omega_0^2\,,\quad g = g(\lambda\vec{q},\ q = 2k_f)\,, \tag{19}$$

and $N_0 = 1/pJ\pi$ is the density of states at k_f for the fermion band. We note that pJ here plays the role of ϵ_f in the conventional Peierls transition. The effect of the fermion-fermion interaction is contained in the parameter p. It is interesting to note that for T_c given by Eq. (18) $dT_c/dp > 0$ if $p < \alpha$ where $\alpha = 2g^2/\omega_0^2\pi J$, while $dT_c/dp < 0$ if $p > \alpha$.

An approximate description of the low-temperature phase has been given by Beni[12] using Bulaevskii's solution[13] of the alternating Heisenberg chain with

$$J_{1,2} = J(1 \pm \delta)\,. \tag{20}$$

If in Eq. (8) the phonon normal-mode coordinate is replaced by its thermal average

$$Q(\lambda\vec{q}) = \langle Q\rangle\,\delta_{q,2k_f}\,, \tag{21}$$

then

$$\delta = (2g/J)\langle Q\rangle\,. \tag{22}$$

In Bulaevskii's approximation for the alternating Heisenberg chain the fermion interaction terms are treated in a non-self-consistent Hartree-Fock-like approximation. The ground-state energy is given by[12,13]

$$-E_0/J = \frac{1}{2} + \frac{2}{\pi}\,E(\delta) + \frac{2}{\pi^2}\,\frac{1}{1-\delta^2} \times [E^2(\delta) + \delta^2K^2(\delta) - 2\delta^2K(\delta)E(\delta)]\,, \tag{23}$$

where E and K are the complete elliptic integrals of the first and second kind, respectively, of argument $\Delta = (1 - \delta^2)^{1/2}$. In the limit of small distortions the gain in energy on distorting is proportional to $-(\delta\ln\delta)^2$. This differs from the conventional Peirels transition where the leading term is $\delta^2\ln\delta$. The difference is due to the pseudofermion interaction terms. Because the cost in lattice energy is proportional to δ^2, the dimerized chain will have the lower energy. The transition temperature obtained using Bulaevskii's solution with δ given by Eq. (22) is the same as that given by Eq. (17). Thus, when the fermion interactions are treated in the Hartree-Fock approximation and the fermion-phonon interaction in RPA, a dimerization phase transition is predicted.

Further mean-field results will not be given because of the important role of fluctuation in pseudo-one-dimensional phase transitions.

III. FIELD DEPENDENCE OF SPIN PEIERLS TRANSITIONS

The effect of a magnetic field is to shift the Fermi level ϵ_f, measured relative to the center of the band from $\mu = 0$ to[11]

$$\epsilon_f = (2s - h)J\,, \tag{24}$$

where

$$h = g\mu_B H/J\,, \tag{25}$$

and where

$$s = \frac{1}{2} - \frac{1}{N}\sum_k n_k \tag{26}$$

is the reduced magnetization. The Fermi factor is now

$$n_k = 1/(e^{\beta(E_k - \epsilon_f)} + 1)\,. \tag{27}$$

The field lowers the Fermi level and the band is no longer half-filled. The singularity in the fermion susceptibility occurs at a wave vector which can be varied continuously.

At $T = 0$ and for $h \geq 2$, the spins are ferromagnetically aligned:

$$s = \tfrac{1}{2}\,,\quad p = 1\,.$$

Thus $n_k = 0$ for all k and the band is empty. For $h = 0$, $s = 0$, $p = 1 + 2/\pi$, $\epsilon_f = 0$ and the band is half-filled as discussed above. For $0 \leq h < 2$,[11]

$$h = \left(1 + \frac{2}{\pi}\cos\pi s\right)\sin\pi s + 2s\,,\quad p = 1 + \frac{2}{\pi}\cos\pi s\,. \tag{28}$$

Thus, for example, the band is one-third filled for $h \sim 1.1$. For this field the chain may be expected to trimerize rather than to dimerize. For $h \sim 1.5$ the band is one-quarter filled and so on. In the presence of the field, there is a phase boundary connecting the points $h = 2$, $T = 0$, and $h = 0$, $T = T_c$ outside of which the chains remain uniform. The nature of the distorted phase depends on the strength of the field.

The shape of the phase boundary may be very complicated. As discussed by Schrieffer,[14] distortions incommensurate with the lattice are not energetically stable and will lock their wavelength so as to be commensurate with the lattice. Thus, for example, in a weak field such that the band is somewhat less than half-filled, umklapp processes will lock the distortion at π/a. For a sufficiently large wave vector the lattice distortion will jump away from π/a to a value closer to $2k_f$ subject to being a rational fraction of π/a. The stronger the Peierls instability, the larger the deviations of $2k_f$ from π/a, which will be tolerated while still maintaining a distortion of wave vector π/a. RPA calculations as well indicate that the instability remains at π/a until the Fermi level reaches a certain minimum value.[15] The phase boundary may

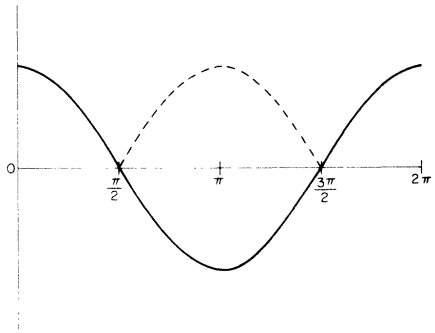

FIG. 1. Pseudofermion band (solid curve) and hole excitation energies (broken curve) for a half-filled band.

therefore be expected to consist of a series of discontinuous steps with the number of steps depending on the strength of the Peierls instability.

In the preceding discussion only the value of $\vec{q}$ along the chain, q, has been considered with $q_\perp$ left arbitrary. The instability will occur at that point in the Brillouin zone for which $g^2(\lambda\vec{q})/\omega^2(\lambda\vec{q})$ has its largest value for fixed q. Thus, the form of the phonon dispersion and the strength of the coupling determine whether the transition occurs at $(\pi/a, 0, 0)$ or $(\pi/a, \pi/a, \pi/a)$, say.

IV. DISCUSSION OF THE HARTREE-FOCK APPROXIMATION

For the antiferromagnetic linear chain a number of exact results have been derived. In this section, these exact results will be compared with those obtained in the Hartree-Fock approximation.

An exact expression for the low-lying spin-wave excitations has been derived by des Cloizeaux and Pearson.[16] The connection between the pseudofermion band as shown in Fig. 1 and the spin-wave spectrum is readily established. The lowest-energy excitations for the pseudofermion system are obtained by adding a particle in the empty part of the band $0 < k < \pi/2a$ and $3\pi/2a < k < 2\pi/a$ or by removing a particle (creating a hole) for $\pi/2a < k < 3\pi/2a$. The latter process gives rise to the excitation energies traced out by the broken curve in Fig. 1. In calculating the k values of these excitations there is a shift in the origin in k space of $\frac{1}{2}\pi$ as shown in Fig. 2.[17] The excitations are described by the spin-wave spectrum[11]

$$\omega_k = Jp\left|\sin\tfrac{1}{2}ka\right| . \tag{29}$$

At $T=0$, $p = 1 + 2/\pi$. This expression should be compared with the exact $T=0$ spin-wave excitation spectrum derived by des Cloizeaux and Pearson,[16]

$$\omega_k = \tfrac{1}{2}J\pi\left|\sin\tfrac{1}{2}ka\right| . \tag{30}$$

The two coefficients $1 + 2/\pi$ and $\frac{1}{2}\pi$ differ by about 4%. This form of the spin-wave dispersion curve has been verified by neutron scattering experiments[18] on the linear antiferromagnet $CuCl_2 \cdot 2NC_5D_5$.

In the Hartree-Fock approximation, the ground-state energy is given by,[1,11]

$$-E_0/J = 0.669 .$$

This differs by about 4% from the exact value derived by Hulthén,[19]

$$-E_0/J + \ln 2 \sim 0.693 .$$

Other approximations have been developed for the uniform Heisenberg chain for which the ground-state energy is closer to the exact value.[20-22] However, these predict a gap in the spin-wave spectrum in contradiction to the exact results of des Cloizeaux and Pearson.

For a sufficiently strong magnetic field the ground state for the linear chain antiferromagnetic will be ferromagnetic. The $T=0$ phase boundary has been calculated exactly by Griffiths,[23]

$$g\mu_B H_c = 2J .$$

This is identical with the result obtained in the Hartree-Fock approximation as discussed above.

The presence of the magnetic field and the associated lowering of the Fermi level have a dramatic effect on the spin-wave spectrum. The pseudofermion band is folded about the Fermi level as in the $H=0$ case. Two branches are obtained. The shift in origin in k space depends on the position of the Fermi level in such a way that the excitations are always zero at $\pm\pi/a$ (for $h \leq 2$). The resulting spin-wave spectra for three different values of the field are shown in Fig. 3. For $H=0$ the exact spin-wave spectrum and that calculated from the pseudofermion Hamiltonian in Hartree-Fock agree to within current experimental accuracy.[18] For $H \neq 0$ no exact calculation of the spin-wave spectra exists. Thus, as a further check on the predictions of the Hartree-Fock approximation it may be of interest to measure the spin-wave spectrum as a function of magnetic field.

For the uniform chain the Hartree-Fock approximation gives quantitatively correct results to within a few percent wherever comparisons with exact results can be made. For the alternating chain

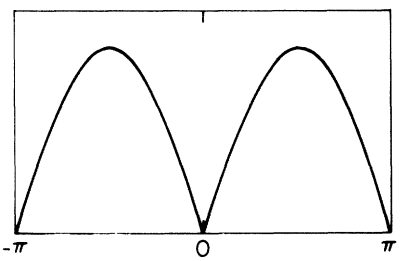

FIG. 2. Spin-wave spectrum for $h=0$.

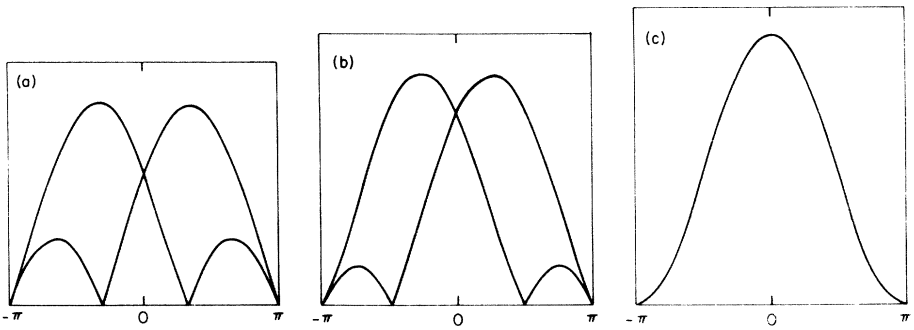

FIG. 3. Field dependence of the spin-wave spectra of the uniform chain (a) for a third-filled band $h \sim 1.1$, (b) a quarter-filled band $h \sim 1.5$, and (c) an empty band $h = 2$.

very few exact results have been derived. In the limit of complete alternation (isolated dimers) $\delta = 1$, $J_1 = 2J$, $J_2 = 0$, the ground-state energy is given by

$$-E_0/J = 1 \ .$$

This limit is correctly reproduced by the Bulaevskii approximation.[13] The ground state of the single dimer is a singlet and the excited state form a triplet. For $J_2 \neq 0$, $J_2 < J$ $(0 < \delta < 1)$, the interaction between dimers gives rise to singlet-triplet exciton bands. However, no exact calculations of these dispersion curves are available. In the Bulaevskii approximation when the chain dimerizes a gap develops in the fermion band at k_f and thus also in the spin-wave spectrum. The unit cell is doubled and singlet-triplet exciton bands are obtained as shown in Fig. 4.

The exact magnetic ground-state energy of the completely dimerized chain is lower than that of the uniform chain. However, as discussed above, it is the behavior of the energy for small δ which determines whether or not a transition will occur. Numerical calculations on finite chains $(N = 10)$ have been carried out by Duffy and Barr,[24] but the small δ regime was not considered in detail.

It is clear that the Hartree-Fock approximation for the uniform chain gives a good description of the ground-state energy and the spin-wave excitations. The important question which remains unanswered is how well the Hartree-Fock wave functions approximate the exact wave functions. The latter are needed in order to calculate the effect of a small lattice distortion on the uniform chain. An exact calculation for the alternating chain is, however, difficult even for small δ. Further finite chain calculations extrapolated to $N \to \infty$ may help determine whether the predictions of the Hartree-Fock approximation are qualitatively correct (still neglecting fluctuations).

The effect of the electron-electron interaction on the conventional Peierls transition has recently been considered for approximations going beyond Hartree-Fock.[25–28] These results are, however, as yet tentative.

V. EXPERIMENTAL SYSTEMS

Two linear-chain Heisenberg antiferromagnets have recently been studied by neutron scattering, $(CD_3)_4NMnCl_3$ (TMMC)[29] and $CuCl_2 \cdot 2NC_5D_5$ (CPC).[18] The former has $S = \frac{5}{2}$ while for the latter $S = \frac{1}{2}$. The spin-wave spectrum of CPC was found to agree with the prediction of des Cloizeaux and Pearson within experimental error.[18] No phase transition has been reported for this material. TMMC, on the other hand, undergoes a phase transition[30] at 0.84 °K. This is believed to be a mag-

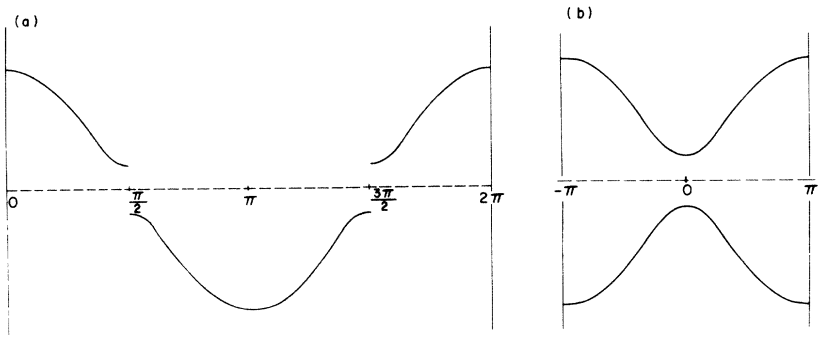

FIG. 4. (a) Pseudofermion band of dimerized chain for $h = 0$, (b) corresponding singlet-triplet excitation bands. Note again change of $\frac{1}{2}\pi$ in origin in k space.

netic transition due to interchain magnetic dipolar coupling.[30,31] Because J plays the same role in the spin-Peierls transition as ϵ_f in the conventional Peierls transition, even the mean-field transition temperature may be expected to be very low. Any three-dimensional ordering temperature would be further lowered due to fluctuations. Thus, only where the interchain magnetic coupling is extremely weak might a spin-Peierls transition be expected to occur before magnetic ordering sets in.

Transitions of the type discussed here may be easier to observe in linear-chain organic systems. These materials have typically very large values of J, $J \sim (300\text{–}4000\,^{\circ}\mathrm{K})$.[32] Consider for example a system in which the electrons along the chain are described by a Hubbard model,[33,34]

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^{\dagger} c_j + U \sum n_{i\uparrow} n_{i\downarrow} , \qquad (31)$$

where c_i, $c_i^{\dagger}$ are annihilation and creation operators for electrons on site i, $n_i = c_i^{\dagger} c_i$. t is the transition integral and U the electron correlation energy of two electrons on the same site. For the limit $U = 0$, we have noninteracting electrons with the dispersion

$$\epsilon_k = -2t \cos ka .$$

When the electrons are coupled to the lattice, a Peierls transition is expected. In the limit $t/U \ll 1$, the leading term in an expansion of Eq. (31) in powers of t/U has the form of a Heisenberg model

$$J \sum_l \vec{S}_l \cdot \vec{S}_{l+1} ,$$

where[35] $J = 2t^2/U$. In this case, the spin-Peierls transition may be thought of as the localized analog of the conventional Peierls transition. If in fact a dimenization phase transition is predicted for the Hubbard model in both limits $t \ll U$ and $t \gg U$, this suggests the interesting but admittedly very speculative possibility that a dimerization transition may occur for any relative value of t and U in the Hubbard model when the coupling to the lattice is included.

Although a number of materials exist which are well described as singlet-triplet exciton systems at low temperature,[32,34] there are, however, at present no known examples of spin-Peierls transitions in organic solids.

ACKNOWLEDGMENTS

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