## Comments

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# Comment on "Peierls instability in the two-dimensional half-filled Hubbard model"

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The analyses of the two-dimensional Peierls-Hubbard model by Tang and Hirsch and by the present author are compared. While there is agreement with the principal conclusion of Tang and Hirsch, viz., that the effects of the Hubbard interaction on the Peierls bond alternation are different in one and two dimensions, I disagree on three related issues. First, the $(\pi,\pi)$ phonon which dominates in the uncorrelated limit is different from the one Tang and Hirsch believe wins [$(\pi,\pi)$ along $x$ axis]. Second, the energy crossing between the $(\pi,\pi)$ and $(\pi,0)$ phonons found by Tang and Hirsch for large magnitudes of the Hubbard interaction can occur only in the unrealistic limit of very strong bond alternation where the strength of the weak bond is close to zero. Finally, the disappearance of the bond alternation due to the Hubbard interaction is much more rapid than that calculated by Tang and Hirsch—the bond alternation should become weaker even at small $U$. This suppression of the bond alternation is indeed related to the long-range antiferromagnetism in two dimensions, as surmised by Tang and Hirsch.

The two-dimensional (2D) Peierls-Hubbard model has recently been investigated numerically by Tang and Hirsch.[1] The same Hamiltonian has also been studied by Mazumdar[2] and Zhang and Prelovsek.[3] While Ref. 3 investigates the limit of infinite onsite Coulomb repulsion (i.e., the 2D Heisenberg model), both Refs. 1 and 2 investigate the model for arbitrary values of the Coulomb parameter, but several of the conclusions are different. Since the 2D Hubbard Hamiltonian is still being widely investigated as a possible model for high-temperature superconductivity, and since any lattice distortion will affect fermion pairing, we believe it is important to understand the origins of these differences. Specifically, we disagree with three separate conclusions of Ref. 1, and elaborate on those here.

The model Hamiltonian for a square lattice is written as

$$H = H_{1e} + H_{ee} , \tag{1a}$$

$$H_{1e} = \sum_{i,j,\sigma} t_0[1 - \alpha \hat{\mathbf{j}}\cdot(\mathbf{u}_i - \mathbf{u}_{i+j})](c^{\dagger}_{i\sigma}c_{i+j,\sigma} + \text{H.c.}) + \tfrac{1}{2}K\sum_{i,j}(\mathbf{u}_i - \mathbf{u}_{i+j})^2 , \tag{1b}$$

and

$$H_{ee} = U\sum_i n_{i\uparrow}n_{i\downarrow} . \tag{1c}$$

Here $H_{1e}$ and $H_{ee}$ are the one-electron and many-electron parts of the Hamiltonian, $i$ and $i+j$ are nearest neighbors, and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$. Unlike in one dimension (1D), there are now several possible bond alternation patterns, as discussed by Tang and Hirsch[1] and shown in Fig. 1. In the limit $U=0$, analytic expressions for $H_{1e}$ are obtained; from these it is easily shown that the distortions corresponding to cases (1) and (2) in Fig. 1 are not unconditional, i.e., they do not occur in the limit $\alpha^2/Kt_0 \rightarrow 0^+$. The electronic band energies $E_k(3)$ and $E_k(4)$ corresponding to cases (3) and (4) are given by[1]

$$E_k(3) = 2[(\cos k_x + \cos k_y)^2 + \delta^2(\sin k_x + \sin k_y)^2]^{1/2} , \tag{2a}$$

$$E_k(4) = 2[(\cos k_x + \cos k_y)^2 + \delta^2 \sin^2 k_x]^{1/2} , \tag{2b}$$

where $t_0 = 1$, $|\delta| = 2\alpha u_0$, and $u_0$ is the mean displacement of the $i$th atom along any axis. Then in the limit of $\delta \rightarrow 0^+$, the electronic energy gain from dimerization contains the well-known term $\delta^2 \ln\delta$ in both cases (3) and (4), showing that arbitrarily large K is unable to prevent the distortion in the limit $N \rightarrow \infty$. This is understandable physically: cases (1) and (2) correspond to phonons with wave vectors $(\pi,0)$ and $(0,\pi)$ [both for case (1), only one of them in case (2)], while cases (3) and (4) correspond to phonons with wave vector $(\pi,\pi)$, which is the $2\mathbf{K}_F$ in the present case.

Since the elastic restoring force in case (3) is twice that in case (4), in which only half the bonds are distorted, Tang and Hirsch compare $|\Delta E_{ee}(3)|$ and $2|\Delta E_{ee}(4)|$ to determine which pattern of bond alternation dominates. Here $\Delta E_{ee}$ is the total electronic energy gain on bond alternation. Since $2|\Delta E_{ee}(4)|$ is found to be larger than $|\Delta E_{ee}(3)|$, they conclude that case (4) will dominate

 

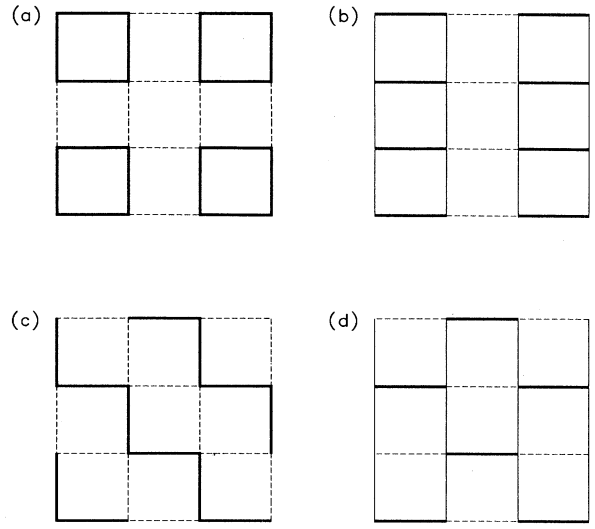


FIG. 1. Bond alternation patterns due to coupling to different phonons (same as Fig. 1 of Tang and Hirsch). Here a thick solid line corresponds to a strong bond with hopping integral $t_0(1+\delta)$, a dashed line corresponds to a weak bond with hopping integral $t_0(1-\delta)$, and a thin solid line corresponds to a normal bond with hopping $t_0$. (a) Case (1) with two phonons with wave vectors $(\pi,0)$ and $(0,\pi)$. In the limit of $\delta\rightarrow 1$, $2\times 2$ plaquettes are formed. (b) Case (2) with a longitudinal phonon $(\pi,0)$. (c) Case (3), one longitudinal phonon of wave vector $(\pi,\pi)$. Staircaselike chains are formed at $\delta\rightarrow 1$. This is the dominating configuration according to Ref. 3. (d) Case (4), one phonon with wave vector $(\pi,\pi)$ and polarization along $x$ axis. The dominating configuration at $U=0$, according to Ref. 4.

over (3). This is the same conclusion that is also reached by Zhang and Prelovsek,[3] while Mazumdar[2] and Barisic, Batistic, and Friedel[4] focus only on case (3). If indeed case (4) dominated over case (3), it would be surprising since, after all, these are *electronic* instabilities; therefore, at $N\rightarrow\infty$ (though not necessarily in finite systems) the distortion driven by larger absolute electronic energy gain should dominate. In the present case, the proper comparison is between $|\Delta E_{ee}(3)|-4NKu_0^2$ and $|\Delta E_{ee}(4)|-2NKu_0^2$, where $4NKu_0^2$ and $2NKu_0^2$ are the harmonic restoring forces, and the former is always larger than the latter, indicating that case (3) dominates over (4). This is expected, since $|\Delta E_{ee}(3)|-|\Delta E_{ee}(4)|$ is also logarithmic and grows faster than quadratic.

The above remains true for arbitrary $U$ and, therefore, also applies to the conclusion of Zhang and Prelovsek,[3] who postulate that case (4) dominates over (3) in the Heisenberg limit. For arbitrary $U$, case (3) dominates, but finite-size effects have to be taken into consideration in numerical simulations done for large $U$. In 1D, for a given $\alpha^2/Kt_0$, bond alternation is seen only in finite lattices $N>N_c$, where $N_c$ depends on the dimensionless electron-phonon coupling constant. In 2D there are two critical sizes $N_{c1}$ and $N_{c2}$. For $N_{c1}<N<N_{c2}$, case (4) dominates, but for $N>N_{c2}$, case (3) dominates.

The second issue over which we disagree with Tang and Hirsch is the crossover between the state(s) with $(\pi,0)$ distortion and the state(s) with $(\pi,\pi)$ distortion. For $\delta=1$, case (3) corresponds to isolated staircaselike 1D chains, while case (1) corresponds to $2\times 2$ plaquettes. Tang and Hirsch compare the energies of the infinite chain and the $2\times 2$ plaquette as a function of $U$ (see Fig. 7 of Ref. 1) and find that while for $U/t_0\lesssim 15$, $\varepsilon(1)>\varepsilon(3)$, $\varepsilon(1)<\varepsilon(3)$ for $U/t_0\gtrsim 15$, where $\varepsilon(1)$ and $\varepsilon(3)$ are the electronic energies per site for cases (1) and (3), respectively. From the numerical data at $\delta=1$, they conclude that case (1) begins to dominate over case (3) [and hence, presumably, case (2) dominates over case (4)] at $U>U_c=15t_0$, while from a perturbative calculation around $\delta=1$, they conclude that $U_c$ *decreases* as $\delta$ decreases (to $U_c\sim 7.5t_0$ for $\delta\rightarrow 0$).

We believe that the above effect is related simply to the behavior of finite $4n$ rings, where $n$ is an integer. At $U=0$, such systems have occupied states at the Fermi level, which do not contribute to the total energy. Thus at small $U$, the energies of $4n$ periodic rings converge to $N\rightarrow\infty$ from above, while those of $4n+2$ rings converge from below. At large $U$, however, the single-particle description is no longer valid and *both* $4n$ and $4n+2$ rings converge from below in the Heisenberg Hamiltonian in 1D, the $N\rightarrow\infty$ result being now bounded by open chains and closed rings.[5] It is thus no coincidence that for $U>U_c$ Tang and Hirsch find that the ground-state energy goes as $1/U$ and resembles the Heisenberg model.

What about $\delta<1$? We do not believe that $U_c$ decreases at small $\delta$ because of the following reason. Consider the $2\times 2$ plaquettes in Fig. 1(a), as the strength of the weak bonds is gradually made finite. At $U=0$ we expect a splitting of all one-electron levels as the interactions $t_0(1-\delta)$ are turned on with $\delta\rightarrow 1-\varepsilon$. Such splittings will lower half the states which were previously at the Fermi level and were *singly* occupied. These are now below the Fermi level and doubly occupied. Such an argument indicates that $U_c$ *increases* for $\delta\rightarrow 1-\varepsilon$, while for any realistic $\delta$ there is no crossing at all. Thus, once again, case (3) should dominate even at large $U$ (although this instability itself has become conditional here).

The final point we want to discuss is the effect of finite $U$ on bond alternation. In Ref. 2 we have argued that $U$ decreases the bond alternation in 2D, and this agrees, therefore, with the principal conclusion of Tang and Hirsch. However, we believe that the rate at which the bond alternation disappears with $U$ is much faster than that calculated by Tang and Hirsch (see Fig. 10 of Ref. 1). This is not an insignificant issue, as the appearance of the much-discussed long-range antiferromagnetism in the 2D Hubbard model coincides with the disappearance of the bond order wave instability.[6] In the present case, we expect antiferromagnetism to appear at $U$ much smaller than $U_c$. Numerical calculation seems to indicate that the energy gained on 2D bond alternation remains largely unaffected until a very large value of $U$ is reached.[1] We believe that this result is a finite-size effect, as well as perhaps being related to the special eight-site lattice studied. In the absence of specific numerical calculations, we can only present a valence-bond argument[2] for this viewpoint.

In Ref. 2 and previous papers, we have shown how a

given broken symmetry can be associated with a single, real-space many-electron configuration (and configurations that are related to it by symmetry operations). Spatial broken symmetry implies that real-space configurations can be classified as $L$ and $R$, where $L$ and $R$ stand for "left" and "right" and favor different phases of the broken symmetry in question. In an infinite system, $L$ configurations can be further classified into $L_1, L_2, L_3, \ldots$, etc., where $L_1$ favors the left phase most strongly, $L_2$ slightly less strongly, and so on. The same applies to the $R$ configurations, which are classified into $R_1, R_2, \ldots$. Thus, if $\sigma$ is the symmetry operation that is lost when the broken symmetry state is reached, $\sigma|L_i\rangle = |R_i\rangle$. If $L_1$ and $R_1$, which are unique, are chosen correctly, it is seen that one may construct paths of the type

$$L_1 \rightarrow L_2 \dashrightarrow S \dashrightarrow R_2 \rightarrow R_1 ,$$

where each arrow represents a single application of $H_{1e}$ and the broken arrow represents $(N/2-1)$ applications. Here $S$ stands for "symmetric," and $\sigma|S\rangle = |S\rangle$. If now $H_{ii} < H_{jj}$ for $i<j$, where $H_{ii} = \langle L_i|H_{ee}|L_i\rangle = \langle R_i|H_{ee}|R_i\rangle$, broken symmetry is enhanced by $H_{ee}$. If $H_{ii} > H_{jj}$, the opposite is true. Clearly this works only because $L_1$ and $R_1$ are unique.

In the case of bond alternation in 2D, we have shown[2] why $L_1$ (or $R_1$) is the many-electron configuration shown in Fig. 2, where the numbers 2 and 0 signify site occupancies. The argument is simple. Since $L_1$ is the extreme configuration favoring bond alternation (at least the left phase of it) most strongly, it must lead to the largest possible *differences* in charge transfers $\langle c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\rangle$ between consecutive bonds. The configuration in Fig. 2(a) does exactly this, as no charge transfer is possible between nearest neighbors with occupancies 2,2 or 0,0, while maximum possible charge transfer occurs between occupancies 2,0.

The significances of these are as follows. First, since $L_1$ and $R_1$ contain the *maximum* possible double occupancies, for any finite $U$, $H_{11} > H_{22} > \cdots H_{SS}$, and we expect $U$ to *rapidly* destroy the bond alternation. This does not occur in 1D since in the infinite 1D system (as well as in finite $4n+2$ rings) the natures of $L_1$ and $R_1$ are different. The behavior of the smallest $4n$ periodic rings should be similar to the 2D systems at small $U$, and there such a rapid destruction is found. Second, from the nature of $L_1$ and $R_1$, here we do not expect coexistence between the bond alternation and a spin-density wave, as occurs in 1D. The configuration in Fig. 1 is orthogonal to the Néel configuration. In this sense, the behavior of the bond order wave and the site diagonal charge-density wave are somewhat similar. A rapid suppression of the charge-density wave with $U$ is the norm. From Monte Carlo simulations, Hirsch[7] finds that antiferromagnetic order sets in at relatively small values of $U$, which, according to arguments given in the above, would indicate that the bond alternation has disappeared. Once again then, these latter calculations suggest that $U$ suppresses the 2D bond alternation very rapidly.

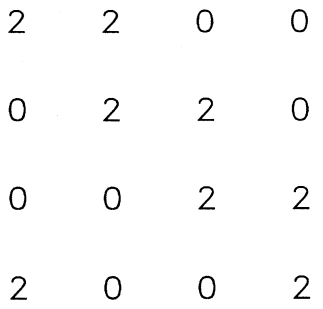


FIG. 2. The real-space many-electron configuration that favors the bond alternation pattern of case (3) most strongly. Other symmetry-related configurations are also possible.

To sum up, we agree with the major conclusion of Refs. 1 and 3, but we believe that (a) the bond alternation pattern (3) in Fig. 1 dominates over all other patterns at both $U=0$ and large $U$, and (b) finite $U$ destroys the bond alternation very rapidly. Clearly, Monte Carlo or exact calculations over large lattices would be useful in this context.

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