

## Comment on “Lattice vibrations in the Frenkel-Kontorova model. I. Phonon dispersion, number density, and energy”

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A recent publication [Q. Meng, L. Wu, D. O. Welch, and Y. Zhu, *Phys. Rev. B* **91**, 224305 (2015)] examines the quantum normal modes of the Frenkel-Kontorova chain. The authors compare their results to those of an older work [A. D. Novaco, *Phys. Rev. B* **22**, 1645 (1980)], attributing the differences to limitations in the numerical analysis of that 1980 paper. We show here that it is not numerical limitations that cause the differences between the two papers, and we argue that the cause of these differences resides with the approaches used in the modeling.

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The article by Meng *et al.* [1] (paper I) explores a quantum treatment for the modes of the Frenkel-Kontorova (FK) problem, and it compares those modes to the classical modes found by Novaco [2] (paper II) using a mass-density-wave (MDW) analysis. There are many similarities between these results, but some differences were found that affect the general conclusions of these papers. The authors of paper I suggest that these differences were due to limitations in the computational analysis used in paper II. To test this suggestion, new results have been generated using higher precision than used in paper II and using Fourier expansions to higher order for the analysis of the structure and normal modes.

The equation for the equilibrium positions of the atoms in the FK chain is a well-known problem in system dynamics known as the Standard Map [3]. This map is a prototypical map for the illustration of chaos, approaching chaos through the generation of nested homoclinic tangles. The general behavior of this map is characterized by one parameter,  $L_0$ , a scaled length that determines the width of the domain walls in the FK chain. In paper II,  $L_0 = 4.0$  was chosen to match the work of Ref. [4].

The original MDW code was single precision (IEEE BINARY32), so the first step was to rewrite the code in double precision (IEEE BINARY64). There are two expansions carried out in the MDW analysis of paper II, the first being a Fourier analysis of the MDW structure and the second being a Bessel function expansion that determines the order of the coupling between the harmonics of that Fourier expansion. In this new analysis, the Fourier expansion includes higher-order harmonics ( $-30$  to  $+30$ ) than in the original analysis ( $-15$  to  $+15$ ), but the maximum coupling order remains the same. This appears justified by the smallness of these higher-order terms in the Bessel function expansion and the smallness of the changes generated by the Bessel function terms of orders 6 and 7.

Paper II looks at the energy of the Frenkel-Kontorova chain for a relative average spacing (RAS) of 0.601, 0.8, and 0.95, comparing the energies to an independent calculation of these same energies using an “exact” method [4]. The reanalysis found little to no deviations from those quoted results (to the precision quoted in paper II). Furthermore, selected case studies were carried out with Fourier expansions using up to the maximum number of harmonics, with no noticeable change

in the results. The normal modes were generated using these same parameters, and little change was observed in the mode structure shown in paper II [5]. The main differences, and there are some, involve the modes in the low density of states region between the lower and upper branches of the spectrum. In particular, these modes are of lower weight than found in paper II, and the mode placement is sensitive to the cutoff in the expansion. Figure 1 shows the recalculated spectrum of Fig. 7 in paper II (RAS of 0.87). In this new figure, the strength of the peak was used to determine the gray scale of the plot, with  $S(q, \omega) = 1.0$  given a gray scale of 0 (black) and  $S(q, \omega) = 0$  given a gray scale of 1 (white or background). Notice that the scattered points between the lower and upper branches of the spectrum found in paper II do not appear here, that is, they are small and barely distinguishable from the background. Also note that the curves in this new figure are smoother than those found in paper II, that is, they have less scatter, but they are otherwise the same.

A sanity check of the work of paper II was done by iterating the Standard Map (STD-Map) in high precision (IEEE BINARY128) and seeing to what extent chaos is important in the cases reported. A return map was constructed by plotting  $\Delta_j - N_{\text{int}}(\Delta_j)$  versus  $X_j - N_{\text{int}}(X_j)$ , where  $X_j$  is the position of the  $j$ th atom,  $\Delta_j = X_j - X_{j-1}$ , and  $N_{\text{int}}$  is the nearest integer function. This was typically done using 100 randomly chosen initial point pairs and iterating each initial pair for 2000 steps. The return map so defined forms a square,  $-0.5$  to  $+0.5$  along each edge, the center point  $(0,0)$  being the 1:1 commensurate phase. For  $L_0 = 4.0$ , chaos is present only near the center, occupying a region roughly 0.1 across. This was further explored by comparing various trajectories using the positions calculated from the MDW analysis versus those from a STD-Map iteration (using the first two positions from the MDW analysis as starting points). For the smaller RAS's in paper II, the MDW map and the STD-Map were nearly the same, with the STD-Map giving close to the correct density after about 2000 iterations. However, for the trajectory with a RAS of 0.95, the final density is sensitive to initial conditions and requires small adjustments to the initial point pair to get close to the average density. This trajectory touches the chaotic region and could pass interior to it. This trajectory is similar to that found for nested homoclinic tangles, so we judge the 0.95 case to be near the edge of chaos or even a bit over the edge. Nevertheless, the MDW map and the STD-Map were very close except near the tangles. It must be noted that the MDW

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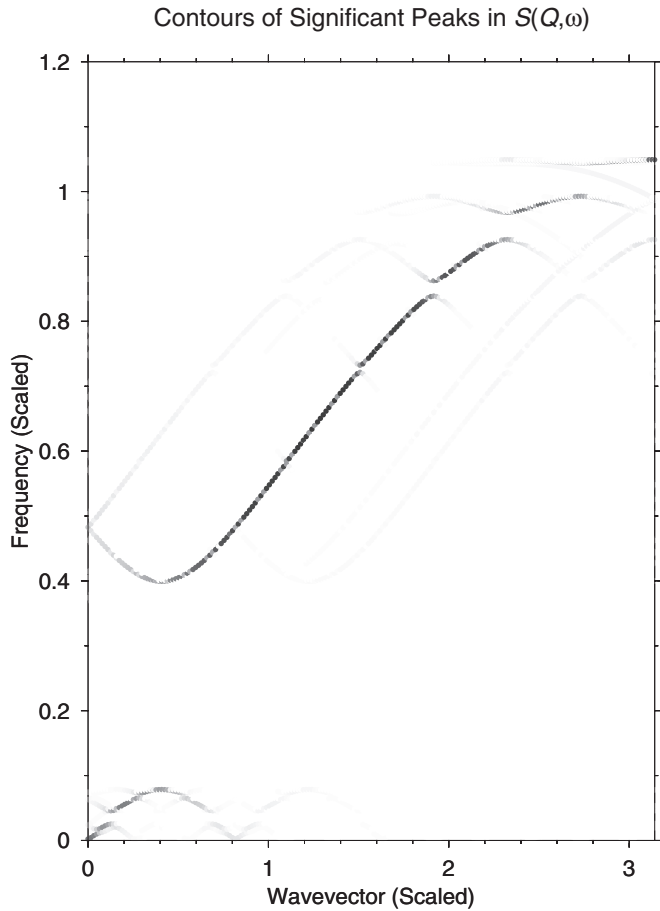


FIG. 1. The MDW dynamics of the case study for  $L_0 = 4.0$  and relative average spacing 0.87. The gray scale is related to the  $S(q, \omega)$  peak height as described in the text.

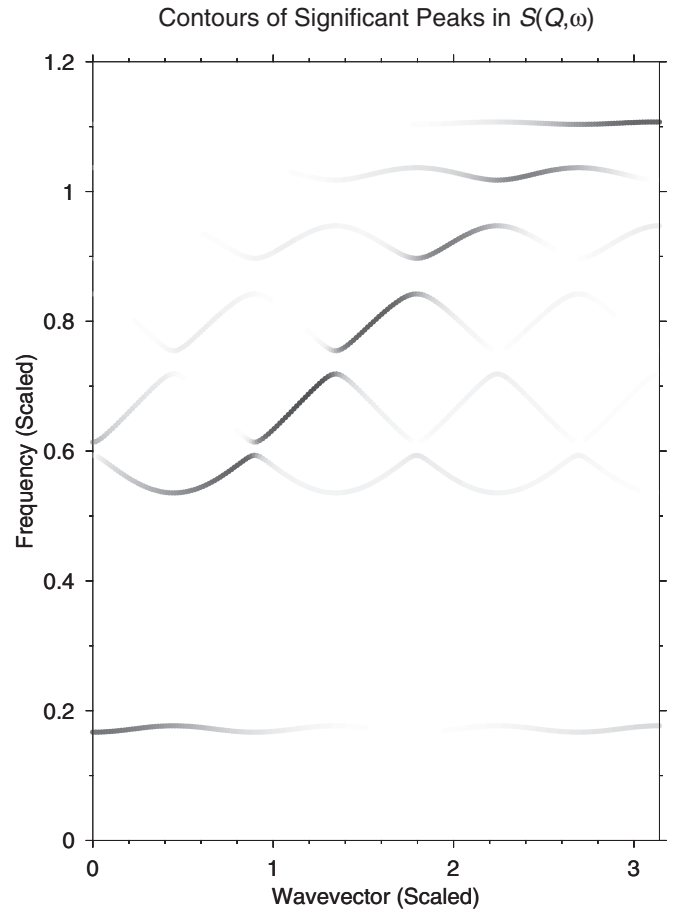


FIG. 2. The MDW dynamics of the case study for  $L_0 = 2.914$  and relative average spacing  $6/7$ . The gray scale is related to the  $S(q, \omega)$  peak height as described in the text.

analysis, when stable solutions are found, forces a periodic or quasiperiodic solution, even when the system is actually chaotic.

The  $L_0$  associated with paper I has a small range of values near 3.0. For values of  $L_0$  near 3.0, the return map for the STD-Map shows about half of the area occupied by chaotic states. We note this not because we claim that the states in paper I are chaotic (I is a quantum calculation) but to point out the danger of comparing the results of paper I to those of paper II in this range. Nevertheless, a MDW calculation of the modes for the cases in paper I shows much similarity between the MDW analysis results and those of paper I. In particular, compare Fig. 2 to Fig. 4(a) in paper I. While the results are similar, there are significant differences. Usually these differences involve one or two modes being significantly “misplaced” relative to the other analysis. Plots of the MDW

structure showed very sharp walls and rather small domains, while the STD-Map showed chaotic behavior.

If numerical limitations are not the source of the differences between papers I and II, they must be due to the differences in either the modeling or the parameter space (the  $L_0$  value). The model in paper I uses a Taylor series expansion of the interaction with the substrate, while paper II does not. On the other hand, paper II uses expansions in both the harmonics and the coupling between these harmonics, while paper I does not. This is most likely the cause of the differences. However, it is also true that paper I uses a quantum analysis and paper II is strictly classical. Furthermore, paper I explores a region where nonlinear effects (as exhibited by the chaos in the classical system) are much stronger than those in paper II. It would be interesting to know if approximations, quantum effects, or simply stronger nonlinear effects are driving the differences in these results.

[1] Q. Meng, L. Wu, D. O. Welch, and Y. Zhu, *Phys. Rev. B* **91**, 224305 (2015).  
 [2] A. D. Novaco, *Phys. Rev. B* **22**, 1645 (1980).

[3] S. N. Rasband, in *Chaotic Dynamics of Nonlinear Systems* (Wiley, New York, 1990), p. 178.  
 [4] J. E. Sacco and J. B. Sokoloff, *Phys. Rev. B* **18**, 6549 (1978).  
 [5] The signs in Table III should be reversed for  $m = 1-5$ .