Many-body quantum dynamics by adiabatic path-integral molecular dynamics: Disordered Frenkel Kontorova models

Florian R. Krajewski [a,b,1] Martin H. Müser [c,2,*]

[a] Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI Campus, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland
[b] Institut für Physik, WA 331, Universität Mainz, 55099 Mainz, Germany
[c] Department of Applied Mathematics, U.W.O., London, Ontario N6A 5B7, Canada

---

Abstract

The spectral density of quantum mechanical Frenkel Kontorova chains moving in disordered, external potentials is investigated by means of path-integral molecular dynamics. If the second moment of the embedding potential is well defined (roughness exponent $H = 0$), there is one regime in which the chain is pinned (large masses m of chain particles) and one in which it is unpinned (small m). If the embedding potential can be classified as a random walk on large length scales ($H = 1/2$), then the chain is always pinned irrespective of the value of m. For $H = 1/2$, two phonon-like branches appear in the spectra.

Key words: sine Gordon model, many-body quantum dynamics, Luttinger liquid
PACS: 05.60.Gg, 71.10.Pm, 73.43.Jn

---

1. Introduction

The numerical treatment of many-particle quantum systems is an important issue of theoretical condensed matter physics. Quantum effects become relevant when the typical thermal energy of the physical system $k_{\mathrm{B}}T$ is smaller or of the same order as the energy quanta of the microscopic system. Path integral molecular dynamics (PIMD) is a powerful method to calculate accurately static properties of quantum mechanical many-body systems[1]. PIMD has also been used to obtain dynamical information of quantum systems[2], however, it is discussed controversially how precise real time correlation functions can be when evaluated within (adiabatic) PIMD[3–5]. Recently, PIMD has been used by the present authors to simulate the many-body quantum dynamics of the Frenkel Kontorova (FK) model, which can be described as a 1-dimensional elastic chain embedded into a sinusoidal potential[6]. The interest in the FK model and its continuum approximation called the sine Gordon model is due to an abundance of applications of these models arising in various transport phenomena including one-dimensional electronic transport (Luttinger liquids)[7].

The previous PIMD studies of the FK model were mainly concerned with the commensurate case, for which the equilibrium spacing of adjacent particles in the chain equals the lattice constant of the embedding

---

[*] Corresponding Author:
Email address: `mmuser@uwo.ca` (Martin H. Müser).

[1] F.R.K. acknowledges support from the MWFZ Rheinland-Pfalz
[2] M.H.M. acknowledges support from SHARCnet and NSERC

potential $V(x)$. However, there is also interest in disordered systems, in particular in the interplay of disorder and quantum fluctuations [8]. Here, we want to present results on disordered systems, where the disordered potentials are classified by the roughness exponent H, which is defined as

$$\left\langle \{V(x+\Delta x) - V(x)\}^2 \right\rangle \propto \Delta x^{2H}, \qquad (1)$$

where Δx is the distance between two points at which $V(x)$ is evaluated. The two cases that will be considered are $H = 0$, in which case there is a well-defined second moment of the potential energy surface, and $H = 1/2$, which corresponds to a regular random walk on long distances Δx. Since, we employ periodic boundary conditions, Eq. 1 will only be satisfied at distances that are distinctly smaller than half the simulation cell.

2. Model, Method and Results

Model

The Hamiltonian in this study is specified by

$$\hat{H} = \sum_{j=1}^{N} \frac{\hat{p}_j^2}{2m} + \frac{1}{2} K (x_j - x_{j+1})^2 + V(x_j), \qquad (2)$$

where $\hat{p}_j = -i\partial/\partial x_j$ is the momentum of particle j (Planck's constant = unity). K is the stiffness of the springs connecting two adjacent particles in the chain. Periodic boundary conditions are employed after a length $2\pi bN$, where N is the number of particles and b is defined below.

For $H = 0$, $V(x)$ is either zero on a length of πb or - with same probability - it takes the functional form of $V_0\{1 + \cos(x/b)\}$ on an interval of length $-\pi \leq x/b < \pi$. The disordered potential with $H = 1/2$ is constructed in the following way: Patches of the functional form $V_0 \cos(x/b)$ and of the length πb are added where the underlying domain is chosen randomly to be either $[0, \pi b]$ or $[\pi b, 2\pi b]$. The patches are shifted by a constant in a way that no discontinuity in the potential occurs. In the following, we will set V_0 and b to unity. K is chosen throughout to be 0.1. Thus K is much smaller than the maximum curvature (V_0/b^2) of the embedding potential so that the 'phase' $x_j - 2\pi jb$ is not necessarily a smooth function of the index j; hence one may call the chain very discrete. In all simulations, we chose N large enough to be sufficiently close to the thermodynamic limit (typically in the order of 128), and the temperature T was chosen so small that no changes in the density of states could be detected when T was multiplied by a factor of two ($T = 0.064$ turned out to approximate the ground state accurately). Thus, the spectra shown in the following, effectively correspond to ground state spectra.

Method

In this work, we present dispersion relations which are calculated within the centroid dynamics framework. As an implementation adiabatic path integral molecular dynamics is used, which is a special variant of PIMD. Here the 'kinetic' masses of the centroid variables are set to the physical values for the masses and the 'kinetic' masses associated to the internal degrees or freedom of the imaginary time paths are collapsed at a frequency larger than the fastest centroid mode. This allows to observe the motion of the centroid variables on an effective potential surface given by the restricted path integral over all imaginary time paths with fixed center of mass. Because of the special choice of the 'kinetic' masses critical slowing down with increasing Trotter number P is completely eliminated. The spectra $C(\omega, q)$ are calculated from the the velocity autocorrelation functions of the chain's normal modes.

Results for $H = 0$

The numerical analysis of the results for the case $H = 0$ suggests a finite gap for a mass $m > m_c^{(H=0)}$ and zero gap for $m < m_c^{(H=0)}$ (see Fig. 1). The critical value for the mass $m_c^{H=0}$ is larger than the value for the commensurate discrete Frenkel Kontorova model (CDFKM)[6]. For the model potential under consideration, one phonon branch is observed. For masses larger than but in the order of m_c, it forms a broad band. At $m < m_c$, the substrate potential becomes irrelevant and the system shows the same dispersion relation as the CDFKM model in the gapless phase[6]: there is only one relatively narrow branch, which can be well described with the dispersion relation of a free chain

$$\omega(q) = 2\sqrt{\frac{K}{m}} \sin\left(qb/2\right) \ . \tag{3}$$

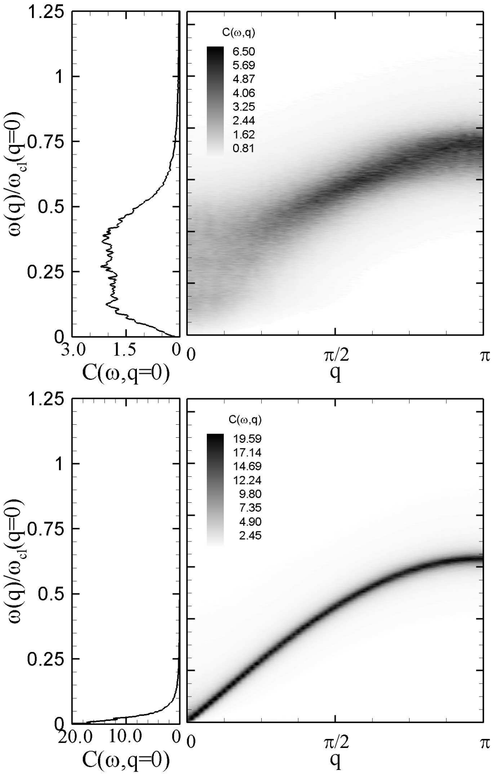

Fig. 1. Quantum ground state spectra of the velocity autocorrelation function for a system with disordered potential with roughness exponent $H = 0$, The results are averages over 12 different realizations of the potential. Top: $m = 0.1$, bottom: $m = 0.02$. For each dispersion relation, the zero wave vector spectrum $C(\omega, q = 0)$ is shown separately on the left. Here $\omega_{\rm cl}(q = 0)$ stands for the classical excitation gap of the elastic chain, which is given by $\omega_{\rm cl}(q\!=\!0) = \sqrt{V_0/(b^2 m)}$.

It is worth mentioning that the behavior for chains with random bond lengths embedded into a regular sinusoidal potential $V_0 \cos(x/b)$ appear to be qualitatively similar to the one discussed above.

Results for $H = 1/2$

The spectra for quantum dispersion relations for $H = 1/2$ are shown in Fig. 2 for a mass of $m = 0.01$. In the CDFKM this value for the mass corresponds to a model in the depinned phase. Despite the small mass, the chain appears to be pinned, as evidenced by the spectral density, which quickly vanishes as the frequency ω approaches zero. A finite-size analysis, which is not shown explicitly, suggests that the $C(\omega = 0, q = 0)$ vanishes quickly with increasing system size N. The quantum spectra are compared to those obtained in a classical simulation, in which the temperature T is chosen such that the classical kinetic energy is equal to the expectation value for the kinetic energy of the corresponding quantum ground state ($T = \frac{2}{k_{\rm B}} \langle \hat{E}_{\rm kin} \rangle_{\rm qm}$). For the classical system, $C(\omega = 0, q = 0)$ does not change dramatically with increasing N, in agreement with the predictions by Chauve et al. [10].

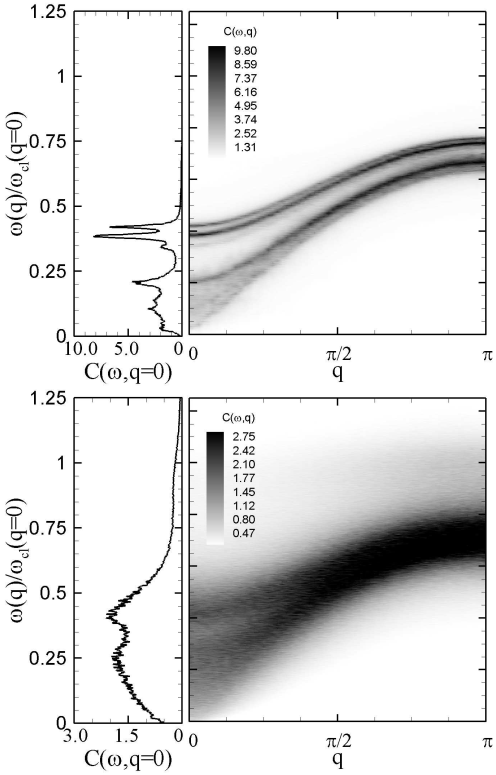

Fig. 2. Same as previous figure but for $H = 1/2$. The top figure is a quantum mechanical calculation for a mass $m = 0.01$. The bottom figure is a classical simulation in which the thermal kinetic energy corresponds to the $m = 0.01$ quantum ground state kinetic energy. The numerical results are the average over 12 different disorder realizations. A single realization shows many individual sharp lines in the quantum case. It appears that the system is not self-averaging.

It is found that the spectra are more complex for disordered potentials with $H > 0$ than for ordered potentials or disordered potentials with $H = 0$. In particular, the (average) spectrum of the quantum system shows two main phonon branches and a complicated substructure for individual realizations of disorder. In these individual realizations, one can even observe the crossing of two individual (very narrow) branches. The occurrence of the second 'optical' branch, which is akin of the dispersion of a classical, commensurate FK model showing a clear gap in the $q = 0$ limit, can be understood when considering the world lines. Due to the random walk nature of $V(x)$, there are some distinct local minima in the potential energy surface. Many particles 'collapse' into those valleys and behave effectively in a classical fashion. In between the areas of high concentration, the chain is stretched and long-wavelength excitations with small, albeit nonzero frequencies occur. A representative graph of the world lines is shown in Fig. 3, confirming the inhomogeneity of the density in self-affine disordered potentials.

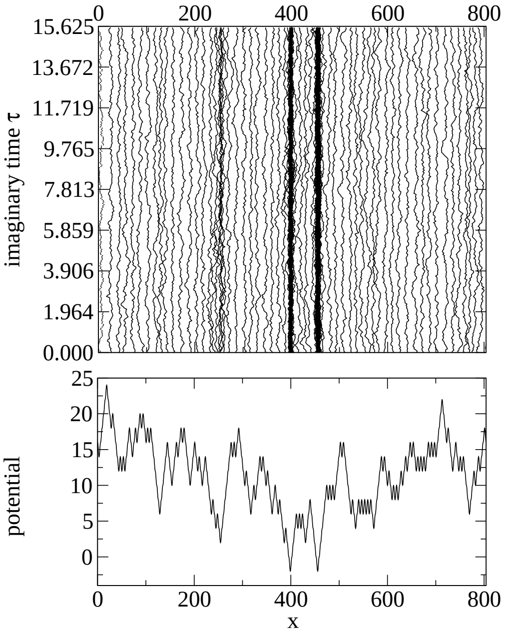

Fig. 3. Above: Snapshot of the imaginary-time trajectories of a typical configuration, calculated with $N = 128$, $T = 0.064$, $P = 256$, $m = 0.01$. Below: Realization of the disordered substrate potential with roughness exponent $H = 1/2$ belonging to the configuration shown above.

Conclusions

In this study, we have investigated the motion of one-dimensional, quantum mechanical and classical elastic manifolds in disordered potentials. For a roughness exponent $H = 0$, we could identify a regime in which the chain appears to be pinned (large values of m) and one in which it appears to be unpinned (small values of m). This result supports the prediction of a critical mass m_c separating a pinned and an unpinned regime [8].

Conversely, for a roughness exponent $H = 1/2$, the quantum mechanical chain seems always pinned, even for values as small as $m = 0.01$. The pinning probably occurs due to the existence of distinct potential energy minima which disable quantum fluctuations to move the chain. Replacing the quantum chains with classical, thermal chains in such a way that both have the same amount of average kinetic energy depins the chain, supporting a renormalization group prediction for thermal, elastic manifolds in external potentials [10]. The reason for this last observation can be understood qualitatively as follows: The quantum system has large local fluctuations as compared to the classical chain. However, the classical chain has the larger long wavelength fluctuations as compared to the quantum system and these are the fluctuations required to move the chain globally.

References

[1] M. E. Tuckerman, B. J. Berne, G. J. Martyna, M. L. Klein, J. Chem. Phys. 99 (1993) 2796.

[2] J. Cao, G. A. Voth, J. Chem. Phys. 99 (1993) 10070.

[3] J. Cao, G. Martyna, J. Chem. Phys. 104 (1996) 2028.

[4] R. Giachetti, R. Maciocco, V. Tognetti, Phys. Lett. A 252 (1999) 157.

[5] G. Krilov, B. J. Berne, J. Chem. Phys. 111 (1999) 9140–9146.

[6] F. R. Krajewski, M. H. Müser, Phys. Rev. Lett. 92 (2004) art.–no. 030601, and to be published.

[7] L. S. Levitov, A. M. Tsvelik, Phys. Rev. Lett. 90 (2003) 016401.

[8] D. A. Gorokhov, D. S. Fisher, G. Blatter, Phys. Rev. B 66 (2002) 214203.

[9] M. H. Müser, Comp. Phys. Comm. 147 (2002) 83.

[10] P. Chauve and T. Giamarchi and P. Le Doussal, Europhys. Lett.44 (1998) 110