Quantum creep and quantum creep transitions in 1D sine-Gordon chains

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Discrete sine-Gordon (SG) chains are studied with path-integral molecular dynamics. Chains commensurate with the substrate show the transition from collective quantum creep to pinning at bead masses slightly larger than those predicted from the continuous SG model. Within the creep regime, a field-driven transition from creep to complete depinning is identified. The effects of disorder in the external potential on the chain’s dynamics depend on the potential’s roughness exponent $H$, i.e., quantum and classical fluctuations affect the current self-correlation functions differently for $H = 1/2$.

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The discrete sine-Gordon (SG) chain, also known as Frenkel-Kontorova (FK) model [1, 2], is a generic model for the motion of an elastic object composed of discrete degrees of freedom through an external potential. To name a few of its applications, the SG model is used for the description of driven charge-density waves in solids, coupled Josephson junctions [2], the sliding motion of an adsorbed layer of atoms over a substrate [4], and most recently electronic conductance in nanotubes [5], see also the reviews [6, 7] on electronic transport in one-dimensional structures. A lot of attention has been given to the (discrete) classical FK model both at zero and finite temperatures [2, 3] and the (continuum) quantum-mechanical SG model [1, 2]. However, less is known about the quantum-mechanical properties of the discrete quantum FK (QFK) model, in particular about its dynamical properties. Numerical approaches have led to a clear picture, how quantum fluctuations renormalize the thermal equilibrium structure, but results are often limited to zero (or small) external fields [2] or to variational approaches [10]. While quantum Monte Carlo (QMC) simulations yield numerically exact results for static properties, they only allow one to calculate small-frequency dynamical properties indirectly, i.e., conclusions on the existence of a phonon gap are drawn by studying the temperature dependence of the internal energy [11]. In some cases, more dynamical information can be withdrawn from QMC if the functional form of the low-energy spectrum is known [12].

It is well established for the SG model that the effects due to thermal and those due to quantum fluctuations differ qualitatively. Thermal fluctuations automatically lead to creep, while quantum fluctuations do not. At finite $T$, kink anti-kink pairs will be activated and a small external force will eventually be able to drive the pairs apart, resulting in net mass transport [12]. If one assumes random interaction between the elastic object and the embedding system, thermal creep is also present in higher dimensions, as shown in a sophisticated renormalization group (RG) study [14]. Strictly speaking this implies that the pinning or the static friction force $F_s$ is zero and that the kinetic friction force $F_k$ vanishes linearly with sliding velocity $v_0$ in the limit of $v_0 \to 0$, even though the proportionality coefficient $\gamma_{\text{eff}} = \lim_{v_0 \to 0} F_k/v_0$ may be large. In order for the 1D, quantum sine-Gordon model to creep, it is not sufficient to have arbitrarily small quantum fluctuations, but the effective masses $m$ (defined as density times period of substrate potential) must be less than a certain critical value $m_c$ (at fixed momentum cut-off and fixed substrate strength) [8]. For $m > m_c$, thermal fluctuations and/or finite external forces are required to initiate mass transport. Recent RG studies [15] suggest that $m_c$ is also finite in higher dimensions if the elastic manifold is pinned through an external random potential.

In many of the above mentioned cases, including the quantum SG model, it is necessary to go beyond standard RG theories [14, 15, 16], because otherwise the effect of creep or alternatively the effect of a vanishing excitation gap at zero wave vectors might be artificially removed. It is thus desirable to have numerical techniques which allow one to (i) verify the results of RG studies, (ii) obtain results beyond continuum approximations allowing an accurate determination of critical values such as $m_c$ for discrete systems, and (iii) obtain dynamical responses of the system for arbitrary external forces. In this Letter, we first intend to establish that (adiabatic) path integral molecular dynamics (aPIMD) [17, 18] is a well-suited technique to tackle the many-body dynamics of elastic manifolds moving through embedding systems. We will then study the FK chain’s dynamics as a function of the external field. This analysis includes new results for the quantum dynamics of a FK chain with various types of disordered substrates.

PIMD is a method to calculate static [17] and dynamic [19] properties of many-body quantum systems in thermal equilibrium. It is based on the isomorphism
between the partition function of a quantum mechanical point particle and that of a classical ring polymer. The number of monomers per ring is called Trotter number $P$. Recent progress was made concerning the dynamical interpretation: It was suggested that real time correlation functions $C(t)$ of observables linear in velocity $v$ and/or position $x$ can be calculated exactly with adiabatic PIMD methods [18, 20]. The $C(t)$'s follow from the equivalent correlation functions $C_c(t)$ defined for the ring polymer's centroids (center of mass), provided that the $P-1$ inner degrees of freedom are in full thermodynamic equilibrium for every given position of the centroids. Furthermore, the characteristic time constant of the centroids’ thermostats must be large compared to the intrinsic relaxation time of the system. If these two conditions are satisfied, $C(t)$'s and $C_c(t)$'s Fourier transforms are related through the equation $\tilde{C}(\omega) = \beta \hbar \omega / 2 (\coth(\beta \hbar \omega / 2) + 1) \tilde{C}_c(\omega)$, where $\beta$ is the inverse thermal energy. In the following, only centroid spectra $\tilde{C}_c(\omega)$ will be considered, as they reflect directly the density of states.

While we refer to Ref. [21] and to a future longer-version publication for more details of our implementation, we may note that we used a representation of our system \[\mathcal{H}\] and in the harmonic part of the Hamiltonian \[\tilde{\mathcal{H}}\]. Moreover, higher-order corrections to the high-temperature density matrix were included in our treatment leading to $P^{-4}$ convergence [22]. We made sure that the relative systematic errors of the internal energy with respect to the classical ground state due to the use of finite $P$ was less than $10^{-3}$. While PIMD is a finite-temperature method, it is possible to extract zero-$T$ behavior by analyzing the convergence of the results by decreasing $T$, just like the thermodynamic limit can be approximated from finite-size extrapolations. We will first consider the most simple QFK model, which corresponds to a discrete, elastic chain, which is commensurate with the underlying potential or substrate. The Hamiltonian \[\tilde{\mathcal{H}}\] reads

\[
\tilde{\mathcal{H}} = \sum_{n=1}^{N} \frac{\tilde{p}_n^2}{2m} + \frac{1}{2} k(x_n - x_{n+1})^2 - V_0 \cos(x_n/b),
\]

where $\tilde{p}_n$ and $x_n$ are, respectively momentum and position of particle $n$, $k$ is the stiffness of the spring connecting two neighbor particles, $V_0$ is the coupling strength to the embedding system, and $2\pi b$ is the substrate’s lattice constant. The periodic boundary condition $x_{n+1} = x_n + 2\pi b N$ makes the chain commensurate with the substrate. Our system of units will be defined by $V_0$, $b$, $\hbar$, and Boltzmann’s constant $k_B$. Unless otherwise noted, we vary the mass $m$ but leave the harmonic intrachain coupling $k = 0.1 V_0 / b^2$ constant. This value of $k$ is much smaller than the maximum curvature of the potential max$(\partial^2_x V(x)) = V_0 / b^2$. This challenges the continuum approximations, which assume slow variations of the reduced positions $x_n - 2n\pi b$ with index $n$.

Classically, the dispersion relation of the chain is simply given by

\[
\omega^2(q) = \frac{1}{m} \left[ 4k \sin^2(qb/2) + \tilde{k}_0 \right]
\]

where $q$ denotes the phonon’s wavenumber and $\tilde{k}_0 = V_0 / b^2$. Early calculations [22] suggested that this classical, zero-temperature value is renormalized to a reduced effective coupling $\tilde{k}_0$ due to zero-point and/or thermal fluctuations. Also for the discrete, commensurate 1D QFK model, Eq. (2) with a non-trivial value for $\tilde{k}_0$ turns out to provide an excellent approximation to our calculated phonon spectra. The dispersion relations of our chain are shown in the right-hand side of Fig. 1 for two different masses. (The dispersion relation was obtained by fitting Lorentzians to spectra similar to those shown below in Fig. 4.) In the commensurate system, the lines are much sharper than in the disordered case. The classical zero-temperature dispersion relation is inserted for comparison. Each curve requires only one fit parameter, namely the value for $\tilde{k}_0$. The dispersion relation does not change when particle number $N$ and Trotter number $P$ (sufficiently small but fixed $\beta/P$) are increased. We want to note that all relevant imaginary-time correlation functions could be well reproduced from the centroid spectra $C_c(\omega)$, which made us confident to use the dynamic interpretation of adiabatic PIMD.

The phonon excitation gap apparently becomes zero at a value $m_c \approx 0.02 \hbar^2 / V_0 b^2$, as shown in the left-hand side of Fig. 1. This in turn implies that sliding can be induced with an arbitrarily small external driving force for $m \leq m_c$. As we will show later, the system creeps in the zero-gap regime when subjected to a small external driving force. The discreteness of the
chain alters the value of the mass $m_c$ at which the transition from finite gap (no creep) to zero gap (creep) takes place. The continuum model predicts this transition to occur at $m_c = 0.016 \hbar^2/V_0 b^2$. Thus for $k = 0.1V_0/b^2$, the value for $m_c$ differs by about 20% between the discrete FK and the continuum SG model. This discrepancy will decrease as the spring stiffness within the chain increases as compared to the maximum curvature $k_0 = V_0/b^2$ of the embedding potential. Without showing the data explicitly, we would like to comment again on the imaginary-time behavior, as this behavior does not rely on the correctness of the claims made for adiabatic PIMD. For $m > m_c$, we observe a finite plateau value in the imaginary-time correlation function $G(\Delta n, \Delta \tau) = \langle \{x_{n+\Delta n}(\tau + \Delta \tau) - x_n(\tau) - 2\pi b \Delta n \}^2 \rangle$ for $\Delta n$ and $\Delta \tau \to \infty$. Similar to what one would expect from a (quantum) Berezinski-Kosterlitz-Thouless transition $^{25, 26}$, $G(\Delta n, \Delta \tau)$ increases logarithmically both with $\Delta n$ and $\Delta \tau$ for $m < m_c$. An accurate determination of $m_c$’s value would yet remain much more difficult in terms of an imaginary-time analysis as compared to the one based on centroid dynamics.

To study the response to an externally applied field, a homogeneous force $F$ is applied to each particle by adding a term $-F \sum_n x_n$ to $H$ in Eq. (1). In Fig. 2 the FK chain’s sliding velocity is shown as a function of the driving force for $m = 0.02$. This is the value of $m_c$, where the gap closes. It is found that the response in $v$ is linear with $F$ at very small and very large $F$ with different values for the effective damping coefficient $\gamma_{\text{eff}} = F/v$. While (quantum) continuum approximations predict $\gamma_{\text{eff}}$ to be zero $^7$, the chain’s discreteness is known to change this property in classical systems, because kink-phonon interactions damp solitons $^{27}$. Interestingly, $\gamma_{\text{eff}}$ is independent of temperature $T$ as $T$ approaches zero in both linear regimes. This rules out the possibility that thermal fluctuations assist the system to overcome energy barriers at small $F$. Our observation is yet in partial contrast to the behavior of Luttinger liquids, which show $v/F \propto T^\alpha$ with $\alpha > 0$ $^4$.

Another similarity with the dynamics of the classical (discrete) FK model is seen at an external force $F = 0.02$, where the friction-velocity relation exhibits a cusp, separating a low-friction, low-velocity from a high-friction, high-velocity regime $^{27}$. Finally, at external forces $F > 0.025$, the response crosses over into a completely unpinned regime, in which the motion of the FK chain is mainly opposed by the drag coefficient associated with the heat bath. In that regime, soliton-related dissipation mechanisms become unimportant. Transport of chains consisting of beads with masses $m > m_c$ requires either finite temperatures and/or finite forces. For example for $m = 5m_c$, our numerical data provides an upper bound for the mobility or inverse effective damping $\gamma_{\text{eff}}^{-1}(m = 0.1) < 2 \cdot 10^{-6}\gamma_{\text{eff}}^{-1}(m = 0.02)$.

The previous analysis shows that PIMD can distinguish well between zero gap and finite gap. It is now possible to generalize the treatment for which the quantum mechanical ground state (of the continuum model) is not known analytically. One of the topics of current scientific interest is the interplay of disorder and quantum fluctuations $^{15}$. Here we want to investigate the effect of disorder on the spectral properties of the quantum FK chain. This is done by replacing the external potential $V_0 \cos(x_n/b)$ in Eq. (1) with a random potential $U_H(x)$, which is constructed in the following way: We add patches of the functional form $V_0 \cos(x/b)$ of length $\pi b$ 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 so that no discontinuity in the potential occurs. This leads to $\langle \{V(x + \Delta x) - V(x)\}^2 \rangle \propto \Delta x^{2H}$ on scales $b << \Delta x \ll \pi b N$. The corresponding surface roughness exponent $H$ takes the value $H = 1/2$. In order to construct a random potential with $H = 0$, the potential is either zero on a length of $\pi b$ or - with same probability - it takes the functional form of $V_0 \{1 + \cos(x/b)\}$ on the interval $-\pi \leq x/b < \pi$. Our 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 $m < m_c^{(H=0)}$, in agreement with the predictions by Gorokhov et al. $^{15}$. For the model potential under consideration, one phonon branch is observed at very large $m$, which then forms a broad band for masses larger than but in the order of $m_c$. At $m < m_c$, there is only one relatively narrow branch, which can be well described with Eq. (2) and $\bar{k}_0 = 0$.

The situation is more complex for disordered potentials with roughness $H = 1/2$. In particular, we find that classical and quantum system behave qualitatively different.
different. In agreement with the predictions by Chauve et al. \cite{Chauve}, there is no indication for the classical mobility to become zero at finite temperatures. In contrast, the quantum mechanical mobility always appears to be zero for $H = 1/2$, no matter how small $m$ is. Whenever, we were prompted to believe the quantum $H = 1/2$ system was depinned, doubling the system size dramatically reduced the velocity-velocity spectrum $C(q, \omega)$ near zero wavelengths and zero frequencies. The zero-wavevector spectrum $C(q = 0, \omega)$ for classical and quantum mechanical FK chains is shown in the left-hand side of Fig. 3, where the qualitative difference of $C(q, \omega)$ in the limit $(q, \omega) \to (0, 0)$ is borne out. (Note that due to statistical uncertainties and finite system size, one can never observe $C(0,0) = 0$ in a computer simulation.) The spectrum at finite wavelengths of the quantum system, which is shown on the right-hand-side of Fig. 3 shows two phonon branches. The figure is the average over 12 different disorder realizations. A single realization shows much sharper lines. It appears that the system is not self-averaging.

In conclusion, we find that the regular zero-temperature, discrete, quantum sine Gordon model has an insulating region with $m > m_c$ and finite gap, while for $m \leq m_c$ the gap closes resulting in finite resistance. Similar behaviour is found for a quantum chain on a disordered potential with roughness exponent $H = 0$. However, $H = 1/2$ automatically leads to a zero-temperature insulator, even though small thermal fluctuations are sufficient to induce creep.

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\begin{figure}[h!]
\centering
\includegraphics[width=\linewidth]{figure3}
\caption{Left: Zero wavevector spectrum for the quantum $(m = 0.02$, thick line) and classical $(k_B T = 1.635 V_0$, thin dashed line) FK model embedded in a disordered potential of roughness $H = 1/2$. $T$ was chosen such that the average kinetic energy was the same in the classical as in the quantum case. Right: Full spectrum of the velocity correlation function for the quantum system. Average over 12 different disorder realizations.}
\end{figure}

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