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Luttinger parameter of quasi-one-dimensional para-H_2

G. Ferré,[1,*] M. C. Gordillo,[2,†] and J. Boronat[1,‡]
[1] *Departament de Física, Universitat Politècnica de Catalunya, Campus Nord B4-B5, E-08034 Barcelona, Spain*
[2] *Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, E-41013 Sevilla, Spain*

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We have studied the ground-state properties of *para*-hydrogen in one dimension and in quasi-one-dimensional configurations using the path-integral ground-state Monte Carlo method. This method produces zero-temperature exact results for a given interaction and geometry. The quasi-one-dimensional setup has been implemented in two forms: the inner channel inside a carbon nanotube coated with H_2 and a harmonic confinement of variable strength. Our main result is the dependence of the Luttinger parameter on the density within the stable regime. Going from one dimension to quasi-one dimension, keeping the linear density constant, produces a systematic increase of the Luttinger parameter. This increase is, however, not enough to reach the superfluid regime and the system always remain in the quasicrystal regime, according to Luttinger liquid theory.

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I. INTRODUCTION

The search for a superfluid phase in molecular *para*-hydrogen (p-H_2) started from the theoretical proposal by Ginzburg and Sobyanin in 1972 [1]. They suggested that p-H_2, with spin 1, should be superfluid under a transition temperature T_λ that they estimated to be $T_\lambda \sim 6$ K using ideal Bose gas theory. This relatively high temperature, compared with the well-known transition temperature in ^{4}He [$T_\lambda(^4\text{He}) = 2.17$ K], was the result of the smaller mass of p-H_2. However, this estimation is too crude because the strong interactions between the p-H_2 molecules are simply ignored. Moreover, the transition temperature for the ideal Bose gas increases with the density ρ as $\rho^{2/3}$, whereas it is known that in superfluid ^{4}He it slightly decreases with ρ. Later on, Apenko [2] proposed a phenomenological theory similar to the Lindemann criterion for classical crystal melting. He concluded that in p-H_2, T_λ should vary between 1.1 and 1.2 K, depending on the density. A recent path-integral Monte Carlo (PIMC) simulation of p-H_2 at low temperatures, in which it was possible to frustrate the formation of the stable crystal, showed that superfluidity appears at temperatures around 1 K [3].

Superfluidity in bulk hydrogen is not observed because it crystallizes in an hcp phase at a temperature $T = 13.8$ K, which is much higher than the estimated transition temperature T_λ. The mean reason is that the intermolecular interaction is around three times more attractive than the one between He atoms. This enhanced attraction dominates over the positive effect produced by the smaller mass of H_2 respect to the ^{4}He one. There have been a number of supercooling attempts to create a metastable liquid phase but even at $T \sim 9$ K the liquid phase freezes quickly into a crystal [4]. One of the *a priori* more interesting options was to confine hydrogen in a porous media, like a vykor glass, with pores in the nanometer scale. However, the lowest temperature at which the system was detected to be liquid was $T \sim 8$ K and so still far from the pursued superfluid [5].

At present, the only experimental signatures of superfluid p-H_2 come from experiments with small doped clusters [6]. By measuring the rotational spectra of the embedded molecule it was possible to determine the effective moment of inertia of the cluster and thus the superfluid fraction. These experiments show significant evidence of superfluidity in clusters made up of $N \leqslant 18$ molecules. Larger clusters of up to $N \sim 10^4$ molecules down to a temperature $T = 2$ K have recently been produced but with no signature of superfluidity due to this still too high temperature [7]. Another way of frustrating the formation of the crystal was the generation of continuous hydrogen filaments of macroscopic dimensions, but again without signature of superfluidity [8].

On the theoretical side, the search for superfluidity in p-H_2 has been intense in the last decades. The well-known radial interaction between the molecules and the progress achieved in quantum Monte Carlo methods have allowed for accurate results in different geometries. To frustrate the crystal formation and reduce the strength of the interactions it was proposed to work with a two-dimensional geometry with some impurities arranged in a periodic lattice [9,10]. First results obtained within this scheme found finite superfluid densities but posterior simulations were not able to reproduce these signatures [11–13]. The greatest effort was devoted to the study of small clusters, both pure [14–23] and doped with impurities [24–26]. There is an overall consensus that p-H_2 becomes superfluid at temperatures smaller than 1–2 K and that the superfluid fraction decreases fast with the number of molecules of the cluster. For $N > 18$–25, the superfluidity vanishes and solidlike structures are observed.

Recently, there has been interest in the study of p-H_2 in quasi-one-dimensional environments [27–29]. Again, the idea is to reduce dimensionality to soften the intermolecular attraction. Quantum Monte Carlo calculations of hydrogen adsorbed inside narrow pores of different size and nature have been performed showing, in some cases, the existence of inner channels which behave as effectively one-dimensional systems. Interestingly, a recent ground-state quantum Monte Carlo calculation [28] has shown that the inner channel of p-H_2 adsorbed inside a (10,10) armchair carbon nanotube is superfluid.

In the present work, we study the one-dimensional character of narrow channels of p-H_2 and determine the Luttinger

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[*] guillem.ferre@upc.edu
[†] cgorbar@upo.es
[‡] jordi.boronat@upc.edu

parameter [30–32] as a function of the linear density. Our method is the path-integral ground state (PIGS), a zero-temperature approach, which is able to generate exact results for the ground-state of the system [33]. We have studied three different cases: a purely 1D array of molecules, p-H$_2$ inside a (10,10) carbon nanotube coated with an incommensurate layer of hydrogen, and p-H$_2$ confined harmonically to move in a channel of different widths. Our results show that moving from 1D to quasi-1D reduces effectively the interaction producing an increase of the Luttinger parameter. However, this slight increment is not enough to achieve the superfluid-like behavior within Luttinger theory. The system breaks its homogeneity when crossing the spinodal point and this happens clearly before of getting superfluity, in contradiction with the recent findings of Ref. [28].

The rest of the paper is organized as follows. In the next section, we briefly discuss the method used in our analysis and describe the properties of the three different studied setups. Our results are reported in Sec. III, mainly the dependence of the Luttinger parameter with the density, within the stability regime of the quasi-1D system. Finally, an account of the main conclusions is given in Sec. IV.

II. METHOD

The ground-state energy and structure properties of quasi-one-dimensional p-H$_2$ have been studied using the path-integral ground-state (PIGS) method [33]. For bosons and a given interaction, this method is exact within controlled statistical noise. The ground-state wave function of the N-body system is obtained from

$$\Psi(\boldsymbol{R}) = \int G(\boldsymbol{R},\boldsymbol{S},\tau)\psi_{\rm m}(\boldsymbol{S})d\boldsymbol{S} \ , \tag{1}$$

with $\boldsymbol{R} = \{\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N\}$, $G(\boldsymbol{R},\boldsymbol{S},\tau)$ the Green's function in imaginary time τ, and $\psi_{\rm m}(\boldsymbol{R})$ a model wave function with the proper Bose symmetry. Obviously, the Green's function for a generic time τ is not known in general but one can build G from its knowledge at short times and then apply its convolution property to arrive to the desired total time τ. This is, in fact, the same method used at finite temperature (the path-integral Monte Carlo method (PIMC)) just changing the imaginary time to inverse of temperature and closing the paths instead of being open as in PIGS.

In our simulations, we approximate the Green's function at short time using the fourth-order splitting proposed by Chin and Chen [34], which in previous calculations has shown high accuracy [35]. The trial wave function $\psi_{\rm m}(\boldsymbol{R})$ in Eq. (1) plays the role of boundary condition of the open paths. As we simulate a Bose system it has to be symmetric under exchange of particles but its specific shape is rather irrelevant, its effect being mainly on the total imaginary time to project out the ground-state wave function [36]. In the present work, we have used a Jastrow model with McMillan correlation factors, $\psi_{\rm m}(\boldsymbol{R}) = \prod_{i<j} \exp[-0.5(b/r_{ij})^5]$, with $b = 3.71$ Å. It is worth noticing that PIGS provides pure (unbiased) estimators of diagonal and nondiagonal operators $\hat{O}$ by calculating them in the center of a symmetric chain with $\psi_{\rm m}$ at both extremes, that is,

$$\langle \hat{O} \rangle = \mathcal{N}^{-1} \, \langle \psi_{\rm m} | G(\tau) \, \hat{O} \, G(\tau) | \psi_{\rm m} \rangle \ , \tag{2}$$

with $\mathcal{N}$ a normalization constant.

The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j}^{N} V(r_{ij}) + \sum_{i=1}^{N} U(r_i) \ , \tag{3}$$

with $V(r)$ the intermolecular interaction and $U(r)$ the confining potential in the quasi-1D simulations. Upon the condition of moderate pressures, it is justified to use a radial interaction between p-H$_2$ molecules because in the *para* state the H$_2$ molecule is in the $J = 0$ rotational state. We use the semiempirical Silvera-Goldman potential [37], which has been extensively used in the past. When the system is not strictly 1D, we include an external potential $U(r)$ which confines in the radial direction. In particular, for the quasi-1D calculations, we have worked on two cases. In a first one, we study the inner channel inside a (10,10) carbon nanotube of radius $R = 6.80$ Å coated with an incommensurate lattice of p-H$_2$ of density $\sigma = 0.112$ Å^{-2}. This configuration is very close to the one obtained in Ref. [28] for the same nanotube. In our case, we obtain the potential $U(r)$ as a sum of the interaction that an H$_2$ molecule located at an r distance to the center would feel due to the C atoms of the nanotube and the H$_2$ molecules of the inert layer. At difference with other approaches, which used the potential inside the nanotube by direct integration of the Lennard-Jones potential [38,39], we include here explicitly the real positions of the atoms and then summed up all to give the total interaction. The C-H$_2$ potential is of Lennard-Jones type, with the same parameters than in Ref. [27]. The second model to study the effects of departing from a strictly 1D geometry is a harmonic potential $U(r) = \hbar^2/(2mr_0^4)\,(x^2 + y^2)$, with r_0 a parameter which controls the strength of the confinement. A similar harmonic model was used recently in a PIMC simulation [29].

We used $N = 30$ in the major part of our simulations; partial runs with larger number of particles were also performed but the results were not significantly different, almost for the quantities of our interest. The time step was $\Delta\tau = 10^{-3}$ K^{-1} and convergence was achieved at imaginary times $\tau \simeq 0.25$ K^{-1}.

III. RESULTS

The energy per particle as a function of the linear density ρ is shown in Fig. 1 for the three studied systems: 1D, (10,10) carbon nanotube (NT), and harmonic confinement (HC). We adjusted the parameter r_0 in the HC case to be close to the particle density profile of the NT case. By taking $r_0 = 0.51$ Å, we obtain in fact very similar density profiles, as shown in Fig. 2. Coming back to the energy results, one can see that near the equilibrium point the equations of state are rather similar (in the NT and HC cases, we have subtracted to the energy per particle the energy of a single molecule in the same environment). The equilibrium densities ρ_0 for 1D, NT, and HC are 0.218(2), 0.224(2), and 0.221(2) Å^{-1}, respectively (numbers within parenthesis are the statistical errors). The possibility of movement in the radial direction makes that the quasi-1D configuration equilibrates at a slightly larger density with respect to the 1D limit. On the other hand, the spinodal point ρ_s, defined as the point

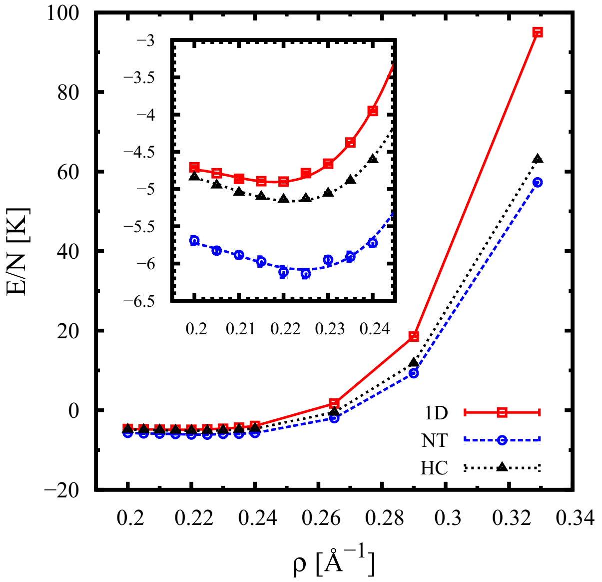

FIG. 1. Energy per particle of p-H$_2$ as a function of the density. The insert shows the same values around the equilibrium density. Harmonic case with $r_0 = 0.51$ Å.

where the speed of sound becomes zero, appears in quasi-1D at densities statistically indistinguishable of the 1D limit, $\rho_s = 0.208(3)$ Å^{-1}. However, the most significant effect of opening the radial direction is produced at large densities in which the growth of the energy with the density is clearly steeper in 1D than in the NT and HC cases.

In 1D systems with gapless excitation spectrum, $\varepsilon(k) = \hbar k c$ when $k \to 0$, one can make use of the Luttinger liquid theory. This phenomenological theory predicts the large-distance (small momenta) of the distribution functions. Within this model, the results are universal in terms of the Luttinger parameter K. In a homogeneous system, like the one we are studying here, K is determined by the Fermi velocity $v_{\rm F} = \hbar k_{\rm F}/m$ and the speed of sound through the relation $K = v_F/c$. In 1D, the Fermi momentum is $k_{\rm F} = \pi\rho$. The estimation of K for different densities requires of a full many-body calculation since the speed of sound depends strongly on the intermolecular interaction.

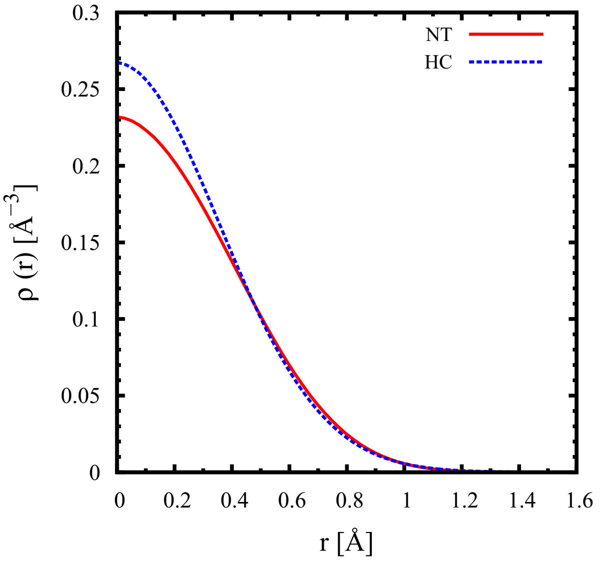

FIG. 2. Radial density profile for NT and HC quasi-1D systems at the equilibrium density. Harmonic case with $r_0 = 0.51$ Å.

According to Luttinger theory [30–32], the pair distribution function in one dimension behaves at large distances as

$$g(z) = 1 - \frac{K}{2(k_{\rm F}z)^2} + \sum_{l=1}^{\infty} A_l \frac{\cos(2lk_{\rm F}z)}{|k_{\rm F}z|^{2l^2K}} , \tag{4}$$

which is a sum of oscillating terms modulated by a power-law decaying amplitude. The exponents of the attenuation are only dependent on the Luttinger parameter K, whereas the amplitudes A_l of each term of the sum are not determined within the Luttinger theory. The oscillations in $g(z)$ (4) can produce divergences at momentum values $k = 2lk_{\rm F}$. This can be observed in the static structure factor $S(k) = \langle \hat\rho(k)\hat\rho(-k)\rangle$, with $\hat\rho(k) = \sum_i \exp(-ikz)$. In fact, the height of the l peak in $S(k)$ is given by

$$S(k = 2lk_{\rm F}) = A_l N^{1-2l^2K} , \tag{5}$$

which diverges with the number of particles N for values $K < 1/(2l^2)$. In particular, the first peak diverges when $K < 1/2$. In Luttinger theory, this regime is termed quasicrystal for the resemblance to Bragg peaks in two and three dimensions. However, a *true* crystal in 2D and 3D shows real Bragg peaks in which the height of the peak increases linearly with N whereas in 1D this only happens when asymptotically $K \to 0$.

In Fig. 3, we report results for the static structure factor $S(k)$ at different densities. From the low-k linear behavior of $S(k)$ we can obtain the speed of sound c,

$$S(k \to 0) = \frac{\hbar k}{2mc} , \tag{6}$$

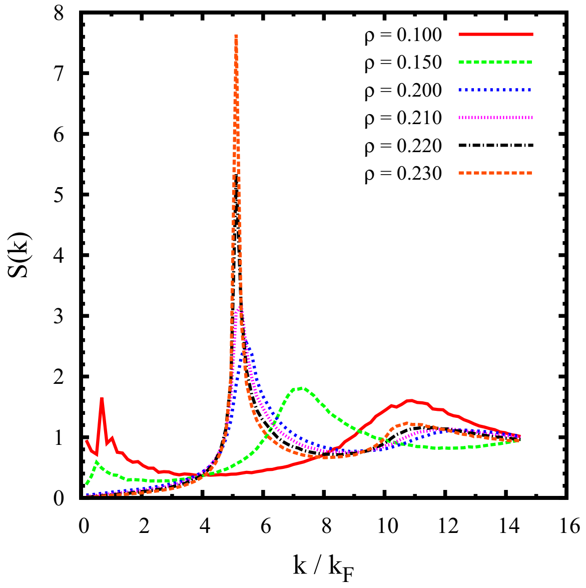

FIG. 3. Static structure factor for one-dimensional H$_2$ at different densities (in Å^{-1}).

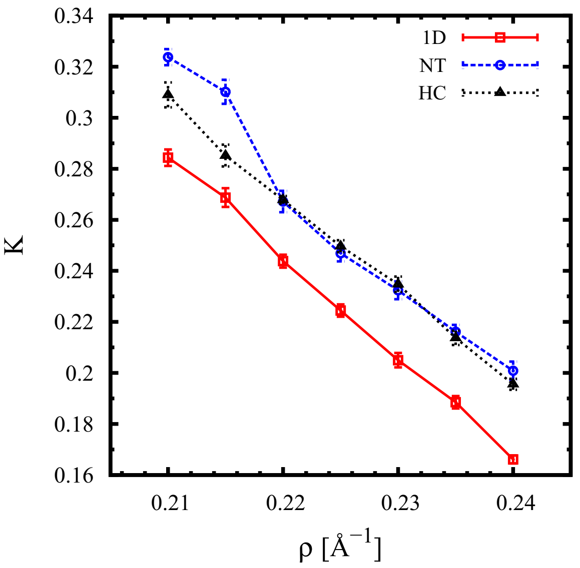

FIG. 4. Luttinger parameter K for the three systems under study as a function of the density.

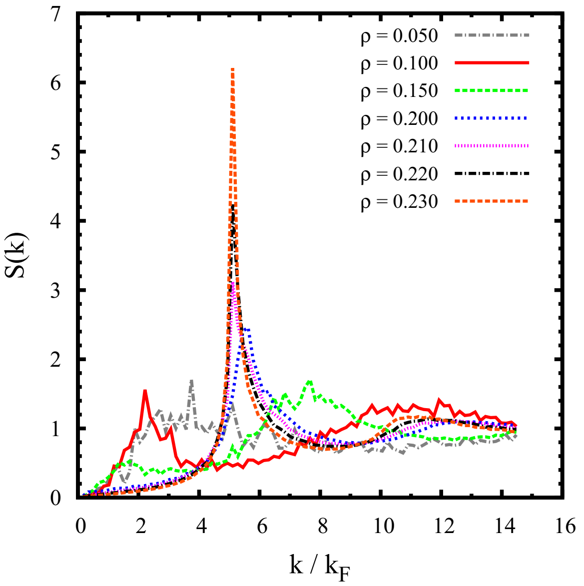

FIG. 5. Static structure factor for quasi-1D H_2 in the NT case at different densities (in Å^{-1}).

and, from it, the Luttinger parameter K. The dependence of K with the density is shown in Fig. 4. It has a value $K \simeq 0.25$ at the equilibrium density and decreases monotonically with ρ. The spinodal point is quite close to ρ_0 and thus 1D p-H_2 remains always in the quasicrystal regime. The limit of stability of the homogeneous phase, signaled by the spinodal point, is clearly shown in the results of $S(k)$ contained in Fig. 3. As one can see, below the spinodal, and when $k \to 0$, the static structure factor shows an anomalous behavior, the linear behavior is lost, and the signal of a divergence is observed. Snapshots of configurations generated along the PIGS runs also show this break of homogeneity.

Results for $S(k)$ along the z direction in the quasi-1D NT case are shown in Fig. 5. Above the spinodal point, the behavior of $S(k)$ is very similar to the purely 1D case shown in Fig. 3, with a clear linear phononic behavior when $k \to 0$. From this behavior, we estimate the speed of sound and the Luttinger parameter K. One can check that the Luttinger liquid theory applies to this quasi-1D system by checking if the asymptotic behavior of the computed $g(z)$ is well reproduced by Eq. (4) using the K value obtained from the low k linear behavior of $S(k)$. As one can see in Fig. 6, the agreement with Luttinger theory is excellent, confirming our premises.

Results obtained for K as a function of the density are shown in Fig. 4. At equal linear density, the K values in the NT configuration are systematically larger than in purely 1D due to the effective reduction of the intermolecular interaction produced by the opening of radial movements. However, it still remains $K < 1/2$, i.e., in the quasicrystal regime. When the density is lowered below the spinodal point the system breaks its homogeneity. As in the previous analyzed 1D case, this instability is clearly shown in the results of $S(k)$ (Fig. 5). In spite of having larger statistical noise than in 1D, due to the radial degree of freedom, one can see as the linear k dependence at low k is lost and a tendency to divergence is observed.

A similar analysis has been carried out in the case of a quasi-1D system with harmonic confinement HC. The PIGS results for $S(k)$ are shown in Fig. 7 at several densities. The observed behavior is quite close to the NT case since the density profiles in both cases are very similar (Fig. 2). One observes the break of homogeneity at the spinodal point and the results for K in this case are also very similar to the NT case. These are shown in Fig. 4; close to the equilibrium density K in HC is slightly smaller than in NT but then both results converge to common values when the density grows.

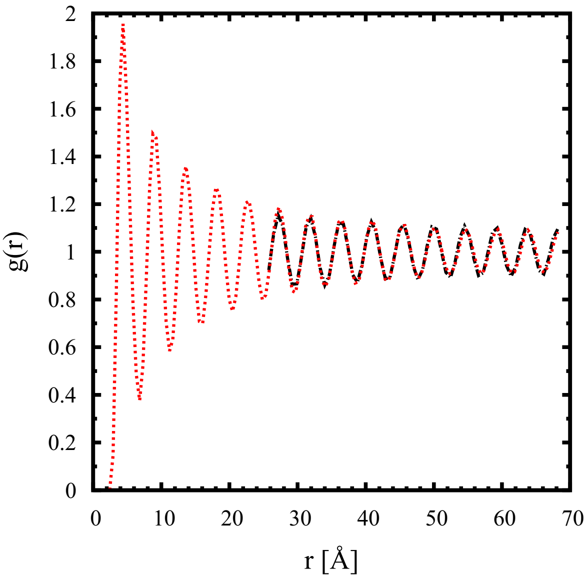

FIG. 6. Two-body distribution function for the NT configuration at the equilibrium density. The red line is the PIGS result and the black one corresponds to the asymptotic behavior predicted by Luttinger theory (4) with K derived from the low $-\,k$ behavior of $S(k)$.

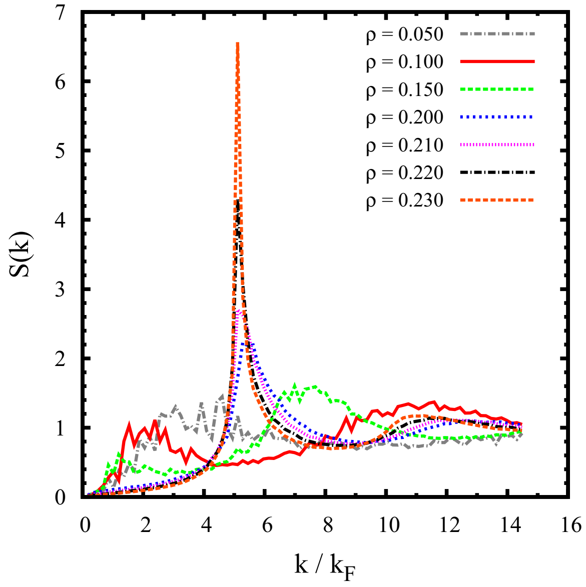

FIG. 7. Static structure factor for quasi-1D H_2 with harmonic confinement HC with $r_0 = 0.51$ Å at different densities (in $\mathring{A}^{-1}$).

The quasi-1D results for the Luttinger parameter show an enhancement of its value with respect the purely 1D geometry. An interesting question is to know if this increase could be even larger if one releases slightly the radial confinement, producing setups that depart more from the 1D constraint. We have explored this possibility by tunning the strength r_0 of the harmonic confinement HC. In Fig. 8, we show results of $S(k)$ for the HC model at a fixed density $\rho = 0.22\ \mathring{A}^{-1}$ and varying the parameter r_0 in the range 0.26-3.83 Å. When the Gaussian potential is narrow enough, $r_0 \leqslant 1.28$ Å, the static structure factor is very similar to the 1D case, with a linear slope at low k and with a strength of the peak decreasing slightly with r_0. However, when $r_0 \geqslant 2$ Å $S(k)$ shows an anomalous behavior, with a main peak located at very small k. This reflects that the system breaks its homogeneity. In fact, we observe in snapshots of the simulations as the system aggregates in clusters of larger density.

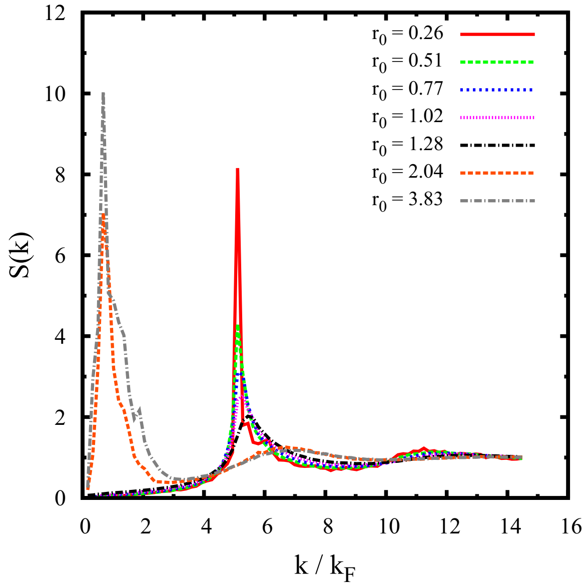

FIG. 8. Static structure factor for the quasi-1D H_2 system with harmonic confinements (HC) of different strength r_0 (in angstroms), at a fixed density $\rho = 0.22\ \mathring{A}^{-1}$.

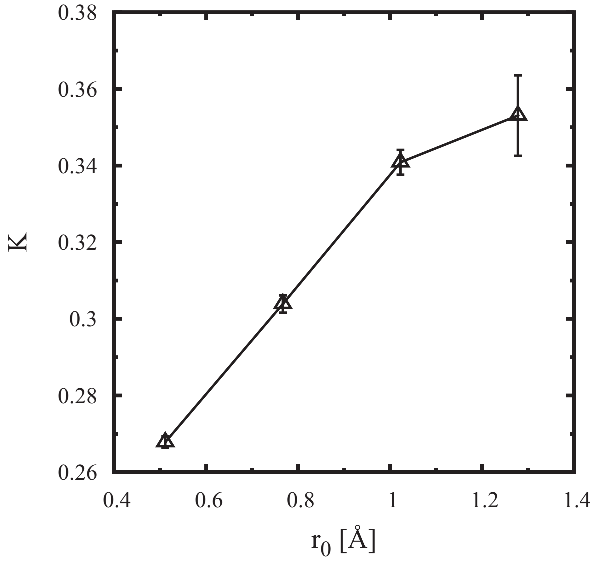

FIG. 9. . Luttinger parameter of the quasi-1D HC model at density $\rho = 0.22\ \mathring{A}^{-1}$ as a function of the strength of the confinement r_0.

In Fig. 9, we show results for K within the HC model as a function of the strength of the confinement r_0. They are obtained at the same linear density $\rho = 0.22\ \mathring{A}^{-1}$ and within the r_0 range in which the system is stable. We observe a linear increase of K with r_0 up to $r_0 \simeq 1$ Å and then it tends to flatten. At $r_0 = 1.28$ Å, we obtain $K = 0.35$ a value which is significantly larger than in 1D at the same density ($K = 0.25$), but still below the threshold for reaching the quasisuperfluid regime.

IV. CONCLUSIONS

By means of the path-integral ground-state Monte Carlo method, we have studied the ground-state (zero temperature) properties of 1D and quasi-1D p-H_2. For the quasi-1D case, we have used two models: the inner channel inside a (10,10) carbon nanotube coated with H_2 and a radial harmonic confinement with variable strength. The calculation of the equations of state in the three cases has allowed for an accurate determination of the equilibrium densities of the three systems. As expected, ρ_0 increases slightly when radial direction opens because the strong H_2-H_2 interaction is effectively reduced. The effect is, however, quite small. The spinodal point of the three problems is indistinguishable within our numerical resolution and remains very close to ρ_0.

From the low-k behavior of the static structure factor, we estimate the speed of sound, and from it, the Luttinger parameter K. In this way, we report results for the evolution of K with the density. K decreases monotonically with ρ in all cases. In all the density regime in which the system is stable, $K < 1/2$ and thus, according to Luttinger theory

p-H_2 is a quasicrystal. For a particular density, we observe as K increases going from strictly 1D to quasi-1D but the effect is not large enough to surpass the quasicrystal threshold.

Our results disagree with the recent findings of Ref. [28] using the same (10,10) nanotube studied here. In that work, the quasi-1D problem is mapped onto a purely 1D one by constructing an effective potential built from the obtained density profiles. The resulting effective potential is more than three times less attractive than the Silvera-Goldman H_2-H_2 potential and thus their calculation leads to the possibility of getting the quasisuperfluid regime because the spinodal density of this effective model is much smaller. Our present results show that this effective potential is not very realistic since a full quasi-1D calculation, accounting for the real interactions C-H_2 and H_2-H_2 shows that the system breaks close to the equilibrium density by spinodal decomposition [40].

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[40] During the completion of our work, we were aware of a preprint from A. Del Maestro and M. Boninsegni, arXiv:1611.03838, which arrives to similar conclusions to ours working with the PIMC method at finite temperature.