Fundamental role of mass in 1D ^{1}H, ^{2}H and ^{3}H quantum gases

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Abstract

Out of all atoms, **hydrogen** is the **simplest** one and provides a **fundamental model** for study. The **interatomic potential** of spin polarized hydrogen $H_\downarrow - H_\downarrow$ has been previously obtained almost **exactly** in different works [1, 2] permitting to produce quantitatively exact results.

We find the **ground-state** properties of **one-dimensional** spin polarized ^{1}H, ^{2}H and ^{3}H at **zero temperature** by means of **DMC** [3] calculations. The equations of state (EoS) of the three isotopes are found and compared in a wide range of densities. We also compute the pair correlation function $g(r)$, the static structure factor $S(k)$ and the Luttinger parameter $K(\rho)$, which we interpret within the frame of **Luttinger liquid theory** [4]. We identify different **physical regimes**, including: ***ideal Fermi gas***, ***Bose-gas***, ***super-Tonks-Girardeau*** and ***quasi-crystal*** regime. We show the behaviours of the different isotopes as well as the fundamental role of the mass and quantum fluctuations, increased by the low-dimensional geometry.

Method

The one-dimensional **hydrogen system** can be **described by** the following **Hamiltonian**

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m_H}\sum_n \Delta_n + \sum_{i<j} V\left(|x_i - x_j|\right)$$

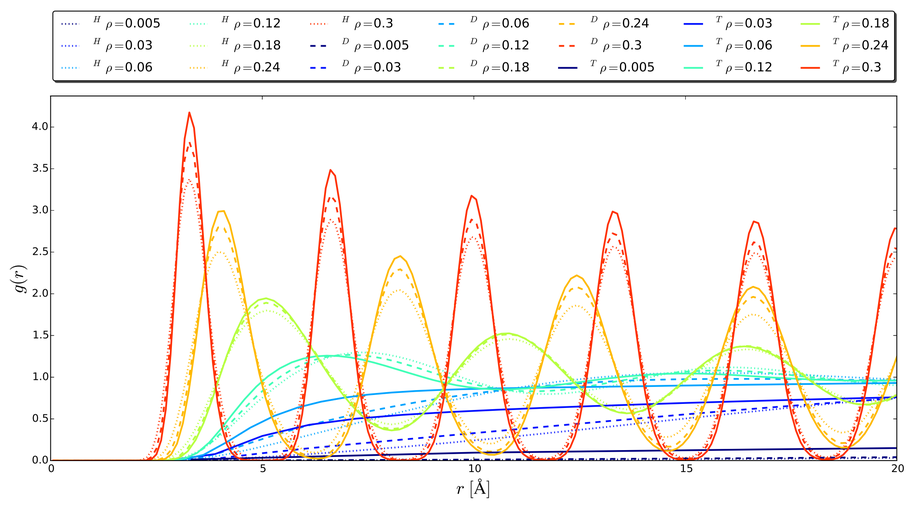
where x_i, $i = 1, N$ are the positions of each atom and N the total number of particles. The **distinguishing factor** is **the mass** of each isotope $m_{1H} = 1.00794u$, $m_{2H} = 2.01410u$ and $m_{3H} = 3.01605u$. We use the JDW potential [2].

We employ the DMC algorithm with importance sampling based on a **guiding wave function** in a pair-product form of

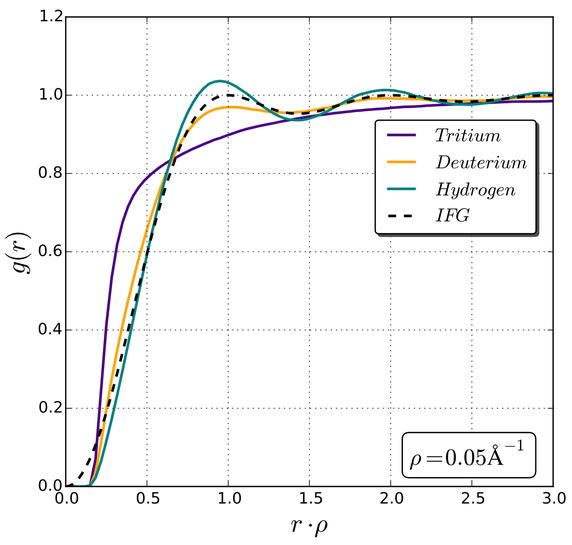
$$\Psi(x_1, \ldots, x_N) = \prod_{i<j} f_2(x_i - x_j)\text{sign}\left(x_i - x_j\right)$$

where the function $f_2(x_{ij})$ is given by the **two body scattering** solution for short distances $x < R_{par}$ and by the **phononic assymptotics** $\left|\sin\left(\frac{\pi x}{L}\right)\right|^{1/K_{par}}$ for large distances $x > R_{par}$. The two **variational parameters** R_{par} and K_{par} are **optimized** using Variational Monte Carlo (**VMC**) **minimizing** the **energy**, which helps to reduce the variance of the results in DMC.

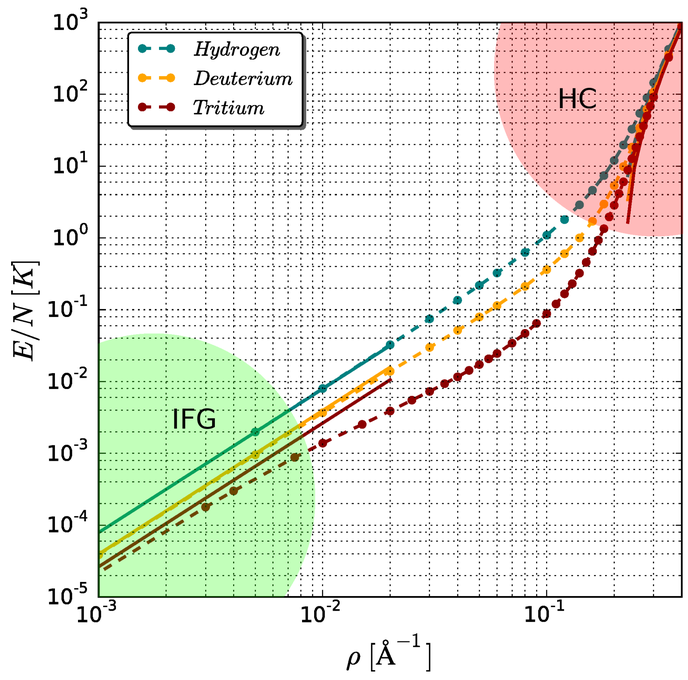
Pair Correlation Function



The **pair correlation function** describes how the density varies around a generic particle in the system. For **large densities** it reminds the one of a **semi-classical crystal**. For **low densities tritium** behaves like a **repulsive Bose gas** while **hydrogen** and **deuterium** like **Fermi gases**.



Energy



The **equation of state** of the system, describing the dependence of the energy on the density, has been computed in a wide range of densities. We see that at **low densities** the system behaves as an **ideal Fermi Gas**, $E/N = \frac{\pi^2\hbar^2\rho^2}{6m}$, while for **high densities** its behaviour is well approximated by the **harmonic crystal**

$$\frac{E}{N} = \sum_{i=1}^{\infty} V(a\cdot i) + \frac{1}{\ell_{BZ}}\int_{BZ}\frac{\hbar\omega(k)}{2}dk$$

where $\omega(k)$ is the **excitation spectrum** that can be computed from

$$\omega^2(k) = \frac{2}{m}\sum_{n=1}^{\infty}\sin^2\left(\frac{kan}{2}\right)\left.\frac{\partial^2 V(x)}{\partial x^2}\right|_{x=an}$$

being $a = \rho^{-1}$ the **inter-atomic** crystal **distance**, and $\ell_{\mathbf{BZ}}$ the size of the **Brillouin zone**.

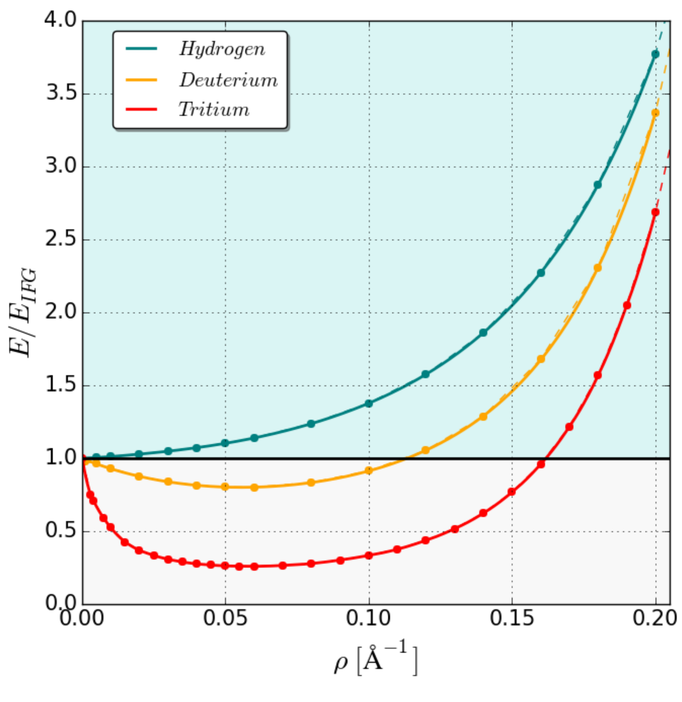
For densities $\rho < 0.2$Å^{-1}, the energy can be fitted with a **polynomial expansion** around the **IFG** energy.

$$\frac{E}{N} = \frac{\pi^2\hbar^2\rho^2}{6m}\left(1 + \sum_{i=1}^{n} a_i\rho^i\right).$$

Using the minimum chi-square fit, we provide the following coefficients

...	a_1 [Å^1]	a_2 [Å^2]	a_3 [Å^3]	a_4 [Å^4]	a_5 [Å^5]	a_6 [Å^6]	a_7 [Å^7]
^1H	$9.51\cdot10^{-1}$	$2.04\cdot10^{1}$	$-2.06\cdot10^{1}$	$1.01\cdot10^{3}$	$5.64\cdot10^{2}$	$-2.00\cdot10^{4}$	$1.11\cdot10^{5}$
^2H	$-7.96\cdot10^{0}$	$8.43\cdot10^{1}$	$2.79\cdot10^{2}$	$-1.24\cdot10^{4}$	$1.29\cdot10^{5}$	$-5.70\cdot10^{5}$	$1.05\cdot10^{6}$
^3H	$-8.07\cdot10^{1}$	$3.43\cdot10^{3}$	$-7.43\cdot10^{4}$	$8.81\cdot10^{5}$	$-5.74\cdot10^{6}$	$1.93\cdot10^{7}$	$-2.59\cdot10^{7}$

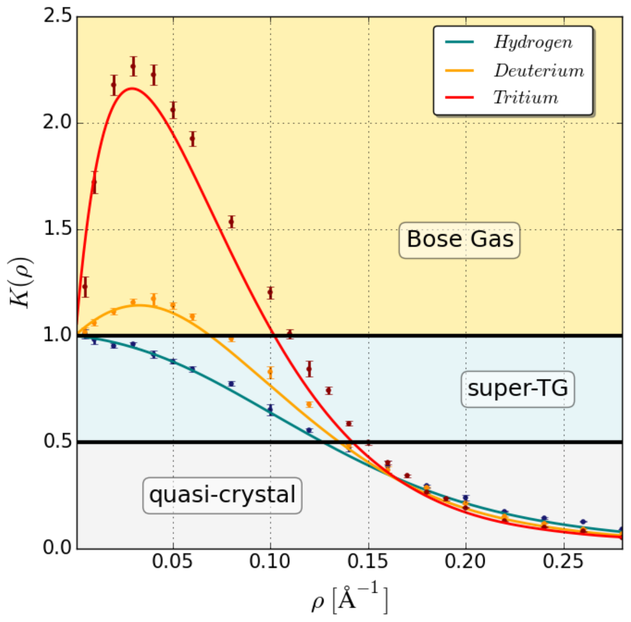
At low densities, **Hydrogen** is close to the IFG in the sense that the first order correction, $\mathbf{a_1}$, is **small** and **positive**. However **Tritium** presents a **strong and negative correction** to the IFG energy and so is the specie with the richest behaviour.



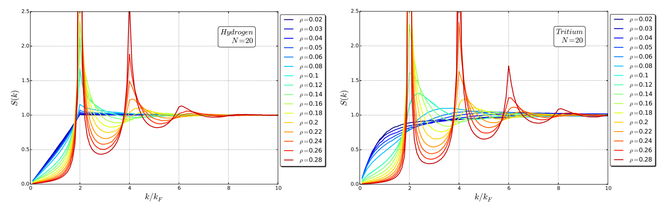
Luttinger Parameter

Quantum one-dimensional systems can be described by a effective Luttinger liquid theory.
The **Luttinger** [4,5] **parameter** is defined as the ratio of the Fermi velocity to the sound velocity in the system, $\mathbf{K}(\rho) = \mathbf{v}_\mathrm{F}/\mathbf{c}$, and can be **obtained** only from a **full man-body calculation from** the **EoS** (solid line) and **from** $S(k)$ (dots)

$$K = \begin{cases} \pi\left(\frac{2}{\rho\epsilon_o}\frac{\partial(E/N)}{\partial\rho} + \frac{1}{\epsilon_o}\frac{\partial^2(E/N)}{\partial\rho^2}\right)^{-1/2} \\ 2\pi\rho\left.\frac{dS_k}{dk}\right|_{k=0} \end{cases}$$



Static Structure Factor



Hydrogen and Deuterium $S(k)$ are qualitatively similar; both present an IFG shape for low densities and **diverging peaks** for **higher densities**. The **slope** of $S(k)$ in **tritium** has a **non-monotonic** dependence on the density, growing at low densities and decreasing at large ones. The presence of growing (diverging) peaks denotes the formation of a **quasi-crystal**.

Conclusions

- The **fundamental role** of the **mass** in the quantum system behaviour is not straightforward
- Hydrogen and deuterium exhibit similar behaviours while **tritium is markedly different** at low densities.
- **Hydrogen** and **deuterium** show the regimes: **IFG**, **STG** and **quasi-crystal**, while **tritium** behaves also like a **Bose gas** at $\rho \sim 0.5$Å^{-1}.
- At **large densities** the **EoS** is well approximated by the harmonic **crystal** description.

References

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