Contact interactions in Path Integral Monte Carlo simulations

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We develop a Path Integral Monte Carlo (PIMC) code capable of simulating systems consisting of mixtures of two different Bose gases in thermal equilibrium in one dimension. We apply it to the study of the total energy per particle, looking how it behaves at different temperatures and densities, and for different interaction strengths.

In the PIMC formalism, quantum particles are mapped to a classical system of closed polymers [1], with a number of beads $M$ increasing with temperature, harmonically coupled as:

$$\rho_{bc} = \left( \frac{\mu}{2\pi \hbar^2} \right)^{1/2} \exp \left( -\frac{\mu (x-x_0)^2}{2\hbar} \right) \quad [2]$$

With $\tau = \beta / M$. From the Hamiltonian with zero range (contact) interaction in one dimension

$$H = -\hbar^2 \frac{\partial^2}{\partial x^2} + \delta(x) \quad [3]$$

We obtain the normalized relative density matrix:

$$\rho_{rel} = 1 - \exp \left( -\mu x y + \frac{\mu^2}{2\hbar^2} \right) \frac{\hbar}{\pi \mu \tau} \text{erf}(u) \exp(u^2) \quad [4]$$

With $u = \frac{\mu |x| + |y| + \mu \tau}{\hbar}$ and $g$ the interaction strength. We construct the total thermal density matrix by means of the pair product approximation. We use the thermodynamic estimator for the total energy per particle [5].

WEAK INTERACTION REGIME

For any given interaction strength, we can observe an ideal gas regime for sufficiently large temperatures, since interaction energy is much less significant than thermal one

$$E \approx \frac{1}{2} k_B T$$

For $g \to 0$, we have $E \approx k_B T + \frac{1}{2} g n$

In contact interactions in one dimension we can observe two different regimes: transmission and total-reflecting. By increasing the interaction strength, we can see in a world-line diagram how the particles collide without any transmission:

STRONG INTERACTION REGIME

We observe a saturation of the total energy per particle, higher with increasing density and temperature. This point marks the transition between high and low interaction regimes.

CONCLUSIONS

We recover better results for weak interactions. We can also observe the two different regimes corresponding to high and low (total reflecting and partially transmitting) interparticle interaction strength.