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Universal Thermometry for Quantum Simulation

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Quantum simulation is a highly ambitious program in cold atom research currently being pursued in laboratories worldwide. The goal is to use cold atoms in optical lattices to simulate models for unsolved strongly correlated systems, so as to deduce their properties directly from experimental data. An important step in this effort is to determine the temperature of the system, which is essential for deducing all thermodynamic functions. This step, however, remains difficult for lattice systems at the moment. Here, we propose a method based on a generalized fluctuation-dissipation theorem. It does not rely on numerical simulations and gives a universal thermometry scheme for quantum gas systems including mixtures and spinor gases, provided that the local density approximation is valid.

At present, there is a worldwide experimental effort to simulate theoretical models for strongly correlated quantum systems using cold atoms in optical lattices[1–5]. If successful, these simulations will provide detailed thermodynamic information for many models whose solutions are unknown, even though some of them (such as 2D fermion Hubbard model) have been studied for decades. To deduce the thermodynamic properties of these models directly from experiments, it is necessary to determine three quantities accurately : the density n, chemical potential μ, and temperature T[6, 7]. The recent experiment of Cheng Chin's group[8] using the in-situ density profile to identify directly the thermodynamic phases of the boson Hubbard model is a very important step toward realizing the full power of quantum simulation[6]. The prospect of this realization is further enhanced by the impressive improvement in resolution of density imaging recently developed in Markus Griener's group[9]. The next crucial step is to develope an accurate means of determining the temperature.

Often, the temperature of a lattice gas is estimated by assuming the lattice is turned on adiabatically. One then equates the entropy of the final state $S_f(T_f)$ to that of the initial state $S_i(T_i)$ (i.e. the state before the lattice is switched on), and then deduces the final temperature T_f from the initial temperature T_i through this relation. This procedure neglects intrinsic heating caused by spontaneous emission as the optical lattice is turned on and during the time the experiment is performed[16]. To make matters worse, the entropy function $S_f(T)$ of many systems of interest remains unknown.

For quantum gases in a single trap without an optical lattice, the temperature can be deduced from the density profile at the surface, which has the Boltzmann form. In principle, one can apply the same method to lattice quantum gases, since interaction effects become unimportant near the surface. However, an accurate determination requires repeating the experiment many times in order to achieve a good signal to noise ratio. To get around this, many experimental studies resort to the aforementioned adiabatic assumption to determine temperature. However, this relies on numerical input for the entropy of the strongly interacting system in the lattice $S_f(T_f)$, the exact form of which is unknown in many models of interest. It is thus desirable to have an alternative scheme which is free from all the problems mentioned above. We also note that by studying the density at the surface, one can not determine whether the entire sample is in global equilibrium.

In this paper, we present a new scheme to determine the temperature of trapped quantum gases based on the fluctuation-dissipation theorem *for non-uniform systems.* This method applies to all quantum gas systems (single component gases, mixtures, spinor gases). Compared with traditional schemes, it has a number of advantages. (1) It is based on general thermodynamic principles and is model independent; (2) it makes use of the density of the whole sample, and hence does not suffer the signal to noise problem for thermometry based on surface densities; (3) Unlike traditional methods, our scheme can determine whether the whole system is in global equilibrium.

A. The proposal: We begin with two basic assumptions used in most experiments on quantum gases which have been justified in many cases. The first is that the density $n(\mathbf{r})$ of a quantum gas in a trap $V(\mathbf{r})$ can be calculated in the grand canonical ensemble , i.e. $n(\mathbf{r}) = n(\mathbf{r}; T, \mu)$, where

$$n(\mathbf{r}; T, \mu) = \frac{\mathrm{Tr}\hat{n}(\mathbf{r})e^{-\beta(\hat{H}+\hat{V}-\mu\hat{N})}}{\mathrm{Tr}e^{-\beta(\hat{H}+\hat{V}-\mu\hat{N})}} \equiv \langle \hat{n}(\mathbf{r})\rangle_{T,\mu}. \quad (1)$$

where $\beta = 1/(k_BT)$, $\hat{H}$ is the Hamiltonian without trapping potential, $\hat{V} = \int d^3r V(\mathbf{r})\hat{n}(\mathbf{r})$, T is the temperature and μ is the chemical potential. The second is that $n(\mathbf{r}; T, \mu)$ is given accurately by the local density approximation (LDA),

$$n(\mathbf{r}; T, \mu) = n_o(\mu(\mathbf{r}), T), \quad \mu(\mathbf{r}) = \mu - V(\mathbf{r}), \quad (2)$$

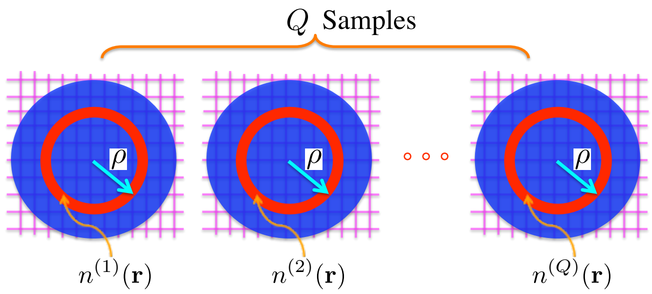

FIG. 1: Demonstration of our scheme. Blue clouds represent Q samples in the repeated experiments. Magenta grids represent the optical lattice. The density of the ith sample at position $\mathbf{r}$ is represented as $n^{(i)}(\mathbf{r})$. Azimuthal averaging of $n^{(i)}(\mathbf{r})$ in each sample is done in the region represented by the red ring to obtain $\zeta(\rho)$ and $\eta(\rho)$.

where $n_o(\nu, T)$ is the density of a homogeneous system with hamiltonian $\hat{H}$ and chemical potential ν, i.e. $n_o(\nu, T) = \mathrm{Tr}e^{-\beta(\hat{H}-\nu\hat{N})}\hat{N}/(\Omega\mathrm{Tr}e^{-\beta(\hat{H}-\nu\hat{N})})$, and Ω is the volume of the homogenous system. For LDA to be valid in lattice quantum gases, it is necessary that the variation of the trapping potential between neighboring sites is small compared with the hopping matrix element [11]. Eq.(1) implies

$$k_B T\frac{\partial\langle\hat{n}(\mathbf{r})\rangle}{\partial\mu} = \int \mathrm{d}\mathbf{r}' \left[\langle\hat{n}(\mathbf{r})\hat{n}(\mathbf{r}')\rangle - \langle\hat{n}(\mathbf{r})\rangle\langle\hat{n}(\mathbf{r}')\rangle\right], \quad (3)$$

where $\langle ...\rangle = \langle ...\rangle_{T,\mu}$. For an isotropic harmonic trap $V(\mathbf{r}) = \frac{1}{2}M\omega^2 r^2$ with frequency ω and $r = |\mathbf{r}|$, Eq.(3) becomes

$$-\frac{k_B T}{M\omega^2 r}\frac{\partial\langle\hat{n}(\mathbf{r})\rangle}{\partial r} = \int \mathrm{d}\mathbf{r}' \left[\langle\hat{n}(\mathbf{r})\hat{n}(\mathbf{r}')\rangle - \langle\hat{n}(\mathbf{r})\rangle\langle\hat{n}(\mathbf{r}')\rangle\right], \quad (4)$$

or simply

$$-\frac{k_B T}{M\omega^2 r}\frac{\partial\langle\hat{n}(\mathbf{r})\rangle}{\partial r} = \langle\hat{n}(\mathbf{r})\hat{N}\rangle - \langle\hat{n}(\mathbf{r})\rangle\langle\hat{N}\rangle. \quad (5)$$

Eq.(5) suggests a convenient way to determine temperature. Suppose we repeat an experiment Q times, labeling the measured quantities of each sample by the superscript $i = 1, 2, 3, ...Q$, as shown in Fig.1. Let $n^{(i)}(\mathbf{r})$ be the density profile of the i-th sample, and $N^{(i)} = \int n^{(i)}(\mathbf{r})$ be the total number of particles in that sample. The averages of these quantities over all Q samples will be denoted as $\overline{n(\mathbf{r})}$ and $\overline{N}$, where $\overline{x} \equiv \sum_{i=1}^{Q} x^{(i)}/Q$. In the limit where $Q >> 1$, Eq.(5) can be written as $L(\mathbf{r}) = R(\mathbf{r})$, where $R(\mathbf{r}) = \overline{n(\mathbf{r})N} - \overline{n(\mathbf{r})}\;\overline{N}$, or

$$R(\mathbf{r}) = Q^{-1}\sum_{i=1}^{Q} n^{(i)}(\mathbf{r})N^{(i)} + Q^{-2}\sum_{i,j=1}^{Q} n^{(i)}(\mathbf{r})N^{(j)}; \quad (6)$$

$$L(\mathbf{r}) = -Q^{-1}\sum_{i=1}^{Q}\frac{k_B T^{(i)}}{M\omega^2 r}\frac{\partial n^{(i)}(\mathbf{r})}{\partial r}. \quad (7)$$

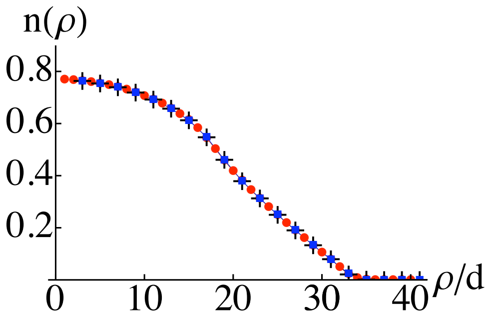

FIG. 2: Density profile in the trap. Red dots: Ensemble averaging over 2000 configurations. Blue boxes:LDA. Black crosses: Exact density in the trap.

That we label temperature T with a superscript i is because in real experiments, there are fluctuations in temperature in each of the samples due to the initial evaporation process. In the following, we shall assume that the temperature fluctuations from sample to sample are sufficiently small compared to the mean temperature that they can be ignored. In this case, we can set $T^{(i)}$ to its mean value, which we simply denote as T, and Eq.(7) becomes

$$L(\mathbf{r}) = T\mathcal{L}(\mathbf{r}), \quad \mathcal{L}(\mathbf{r}) = -\frac{k_B}{M\omega^2 r}\frac{\partial\overline{n(\mathbf{r})}}{\partial r}. \quad (8)$$

Eq.(5) then implies $T = R(\mathbf{r})/\mathcal{L}(\mathbf{r})$ at any position $\mathbf{r}$.

There is, of course, the practical matter of how many samples is needed to average over to reach the thermal average. A very large value of Q will not be practical. To achieve fast convergence, one can suppress the noise by averaging over a ring of thickness ϵ. This is justified since all points on the same ring in an isotropic trap have identical chemical potential. Applying $\frac{1}{\Omega(\rho)}\int_{\rho}^{\rho+\epsilon} d\rho\rho\int_0^{2\pi} d\theta$ on both side of Eq.(5), it results in a function (say, in the 2D case) $\zeta(\rho) = \int_{\rho}^{\rho+\epsilon}\eta(\rho')\rho'\mathrm{d}\rho'/\Omega(\rho)$, where $\eta(\rho) = \int_0^{2\pi}\mathrm{d}\theta\, n(\rho,\theta)$ is the azimuth integrated density at radius ρ, $\Omega(\rho) = \pi[(\rho+\epsilon)^2 - \rho^2]$ is the area of the ring being averaged over, and $(\rho,\theta) \equiv \mathbf{r}$ are polar coordinates. Eq.(5) can be written as

$$T = \mathcal{R}(\rho)/\mathcal{L}(\rho), \quad (9)$$

$$\mathcal{R}(\rho) = \overline{\zeta(\rho)N} - \overline{\zeta(\rho)}\;\overline{N}, \quad (10)$$

$$\mathcal{L}(\rho) = -\left(\frac{k_B}{M\omega^2\Omega(\rho)}\right)\int_{\rho}^{\rho+\epsilon}\mathrm{d}s\frac{\mathrm{d}\overline{\eta(s)}}{\mathrm{d}s}. \quad (11)$$

Eq.(9) holds for all radii ρ. In the 3D case, the quantity most easily accessible is the column integrated density. The corresponding expressions for the temperature are found by replacing $\zeta(\rho)$ and $\eta(\rho)$ by their column integrated analogs $a(\rho)$ and $b(\rho)$, where $a(\rho) =$

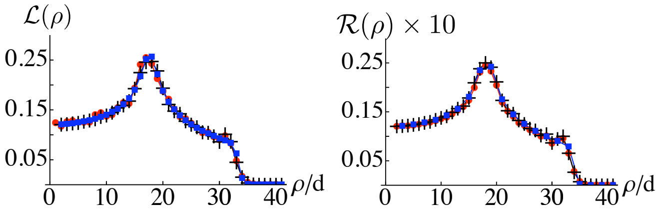

FIG. 3: Compressibility (left) and number fluctuations (right) in the trap. Red dots: averaging over 50 configurations. Black crosses: Exact results in the trap. Blue boxes: LDA.

$\int_\rho^{\rho+\epsilon} \rho' b(\rho')\mathrm{d}\rho'/\Omega(\rho)$, $b(\rho) = \int_0^{2\pi} \mathrm{d}\theta \int dz\ n(\rho,\theta,z)$, and (ρ,θ,z) are cylindrical coordinates.

To illustrate the feasibility of Eq.(9), we consider a 2D ideal Fermi gas in a square lattice with Hamiltonian $\hat{H} = -t\sum_{\langle \mathbf{R},\mathbf{R}'\rangle,\sigma} c^\dagger_{\mathbf{R},\sigma} c_{\mathbf{R}',\sigma}$ confined in harmonic potential $\hat{V} = \frac{1}{2}\sum_{\mathbf{R}} M\omega^2\mathbf{R}^2 c^\dagger_{\mathbf{R}} c_{\mathbf{R}}$ with frequency ω. Here, $\mathbf{R}$ is the lattice site index, t is the hopping matrix element, $\langle \mathbf{R},\mathbf{R}'\rangle$ denotes neighboring sites, and $c^\dagger_{\mathbf{R},\sigma}$ creates a fermion at site $\mathbf{R}$ with spin σ. The equilibrium density of this non-uniform system is $\langle \hat{n}(\mathbf{R})\rangle = \sum_\alpha |u_\alpha(\mathbf{R})|^2 f(E_\alpha)$, where $f(x) = (e^{(x-\mu)/k_BT}+1)^{-1}$ is the Fermi distribution function, E_α and $u_\alpha(\mathbf{R})$ are eigen-energies and eigen-functions of the system $H+V$.

In Figure 2, we show the equilibrium density of a system with temperature $T/t = 0.1$ and a chemical potential μ adjusted so that the number of particles is $N = 1200$. We also show on the same plot the LDA result, which differs from the grand canonical result by less than 0.1% and is invisible in the figure [12]. To generate an equilibrium ensemble, we start with an arbitrary assignment of 0 and 1 of the occupation numbers $\{n_\alpha\}$ of the energy levels $\{E_\alpha\}$ up to a very large cutoff Λ, and evolve the set $\{n_\alpha\}$ using a Monte Carlo scheme. To verify that the resulting states compose an equilibrium ensemble, we calculated the average the occupation numbers n_α, and confirmed that they match their correct values (given by Fermi distribution) to 99.9% accuracy. Moreover, we ensured that there are no correlations between the occupations of different energy levels, as must be true for an equilibrium ideal gas.

Using this equilibrium ensemble, we randomly selected Q configurations, *which corresponds to Q measured samples in experiments.* The level occupation of these configurations will be labeled as $\{n_\alpha^{(i)}\}$, $i = 1$ to Q. The analogs of the experimentally measured density and number fluctuation at $\mathbf{R}$ are then

$$\begin{aligned} \overline{n(\mathbf{R})} &= \textstyle\sum_\alpha |u_\alpha(\mathbf{R})|^2 \overline{n_\alpha}, \\ \overline{n(\mathbf{R})N} - \overline{n(\mathbf{R})}\ \overline{N} &= \textstyle\sum_\alpha |u_\alpha(\mathbf{R})|^2 (\overline{n_\alpha^2} - \overline{n_\alpha}^2), \end{aligned} \quad (12)$$

where $\overline{n_\alpha} = Q^{-1}\sum_{i=1}^{i=Q} n_\alpha^{(i)}$ and $\overline{n_\alpha^2} = Q^{-1}\sum_{i=1}^{i=Q} n_\alpha^{(i)2}$. The density profile after angular averaging $\overline{n(\rho)}$ obtained from averaging over $Q = 50$ samples is shown in Figure 2 together with the LDA result. The differences between these two densities are less than 0.1% and is invisible on the plot. From the "measured" density, we construct the quantities $(\mathcal{R}(\rho), \mathcal{L}(\rho))$. After angular averaging, the radial dependence is shown in Figure 3 [14]. Figure 4 displays the pairs $(\mathcal{R}(\rho), \mathcal{L}(\rho))$ in the $\mathcal{L}-\mathcal{R}$ plot, which form a straight line as Eq.(9) predicts. Using these 50 samples, the temperature obtained from the slope of Figure 4 agrees with the actual temperature within 3%. If we increase Q to 200, the accuracy in temperature increases to 1%. We have repeated our calculation for the same system at lower temperature $T/t = 0.02$ and have found the same accuracy in temperature determination.

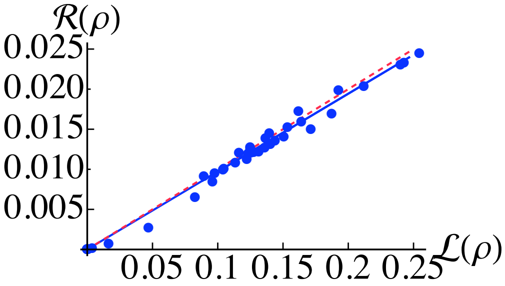

FIG. 4: Linear fit for $\{\mathcal{L}(\rho), \mathcal{R}(\rho)\}$ to extract T. Blue dots are the results of $\mathcal{L}(\rho)$ and $\mathcal{R}(\rho)$ from averaging 50 configurations. Blue straight line is the fitting results. Red straight dashed line represents the real temperature $T = 0.1t$.

We stress that the angular averaging is crucial for our scheme. Due to the self-averaging property of the equilibrium ensemble, the angular average enhances signal to noise significantly, and amounts to a significant increase in the number of configurations averaged. The high accuracy of temperature determination by averaging only 50 samples makes our scheme practical. We would also like to point out that if the system is not in global equilibrium, but was able to establish different temperatures in different parts of the sample[**13**], then the points in the $\mathcal{R}$-$\mathcal{L}$ plot will fall onto a few straight lines with different slopes.

B. Fluctuations in μ and T: In current experiments, the density profile of an atomic gas is obtained by averaging over many samples, each of which has slightly different particle number and energy due to the preparation process, which in turn lead to slightly different chemical potentials and different temperatures. However, it is well known that the density profile averaged over these samples are well described by the prediction of the grand canonical ensemble with chemical potential μ and temperature T obtained by averaging over all these samples. The reason is that as long as the fluctuations in particle number and energy (ΔN and ΔE) are much less than their mean, denoted as N and E, different samples are simply members of different grand canonical ensembles with slightly different chemical potentials and temperatures. Thus, averaging over the experimental samples is the same as averaging over different canonical ensembles of slightly different chemical potentials and temperatures. In the case $\Delta\mu << \mu$ and $\Delta T << T$, the latter can be well approximated by the average of a single grand canonical ensemble with chemical potential μ and temperature T.

To demonstrate the effect of fluctuations in μ and T (which are caused by the preparation process), we generated density profiles of equilibrium ensembles at different temperatures while keeping μ and ω fixed. We find that with 1% (5%) temperature fluctuations, the accuracy for temperature determination after averaging 50 samples remains at 5% (10%). We repeated our calculations for similar fluctuations in μ (which amounts up to 5% fluctuations in particle number), and have found similar results. This shows our scheme is robust against fluctuations in T and μ on the order of a few percent, and that Eq.(8) is justified within this accuracy.

C. Local density fluctuation : The scheme described in section A is very general. However, it requires measuring density correlations in different positions in the trap, i.e., $G_{\mathbf{r},\mathbf{r}'} = \langle n_{\mathbf{r}} n_{\mathbf{r}'}\rangle - \langle n_{\mathbf{r}}\rangle\langle n_{\mathbf{r}'}\rangle$. In this section, we will describe a simplified version of the scheme in section A, which makes use of the region in the trap where only local density correlation are present, i.e., $G_{\mathbf{r},\mathbf{r}'} = \delta_{\mathbf{r},\mathbf{r}'}$

We again consider the 2D case. Eq.(3) can be rewritten as

$$TC_{\mathbf{r}} = D_{\mathbf{r}} + F_{\mathbf{r}}, \tag{13}$$

where $C_{\mathbf{r}}$ and $D_{\mathbf{r}}$ are the local compressibility and local density fluctuation,

$$C_{\mathbf{r}} = -\frac{k_B}{M\omega^2 r}\frac{\partial\langle n_{\mathbf{r}}\rangle}{\partial r}, \quad D_{\mathbf{r}} = (\langle n_{\mathbf{r}}^2\rangle - \langle n_{\mathbf{r}}\rangle^2)\Omega_0, \tag{14}$$

$F_{\mathbf{r}} = \int_{\mathbf{r}'\neq\mathbf{r}} G_{\mathbf{r},\mathbf{r}'}$ is the fluctuation due to the density correlation at different positions. Ω_0 is the volume of an unit cell, which amounts to d^3 in the lattice case where d is the lattice spacing. If the range of $G_{\mathbf{r},\mathbf{r}'}$ at $\mathbf{r}$ happens to be very short, which may occur if the system at $\mathbf{r}$ is in the Mott phase or the normal phase, then $F_{\mathbf{r}} \sim 0$ and Eq.(13) implies that temperature is simply the ratio $T = D_{\mathbf{r}}/C_{\mathbf{r}}$. Thus, if we plot $D_r = \int_\theta D_{\mathbf{r}}$ against $C_r = \int_\theta C_{\mathbf{r}}$, where $\int_\theta$ denotes the angular average, we will find that many points (C_r, D_r) in the $C - D$ plot fall onto a straight line while many other points do not. *The former comes from the regions of* $\{r\}$ *with short range density correlations, while the latter from regions with longer range correlations.* This suggests a simple way to use local density fluctuation to determine temperature: As long as the points (C_r, D_r) fall onto a portion of a straight line, one can deduce the temperature T from the slope of this straight line portion[15]. In the case that correlations are not exactly local, but only exist within a certain length scale ξ, the integration on the right hand side of Eq.(3) can be carried out only in the region $|\mathbf{r} - \mathbf{r}'| < \xi$, since non-local correlations vanish for $|\mathbf{r} - \mathbf{r}'| > \xi$ and give no contribution to Eq.(3). This can actually improves the accuracy of our method[16].

Conclusion: We have shown that density fluctuation measurements give a powerful way to determine the temperature of a trapped gas. It is clear from our derivation that this method applies to other systems such as mixtures and spinor gases. The fact that the temperature can be determined by the fluctuation at every point in the sample provides considerable cross checks on the accuracy of the result. Our method can also reveal situations where different regions of the sample are in equilibrium within themselves but not with each other. At present, all methods of thermometry requires the input of specific theoretical modeling. Our method relies only on basic postulates of thermodynamics. It is therefore immune from errors of theoretical modeling, and is in line with the true spirit of quantum simulation, i.e. obtaining information about unsolved models without specific theoretical input.

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[11] When there are different phases in the trap, LDA fails in the vicinity of the transition point, which takes place on a closed surface inside the sample. However, the majority of the sample is non-critical and LDA applies in most of the sample.

[12] LDA has been justified by many cold atom experiments and numerical calculations (see Yean-an Liao et al., arXiv:0912.0092(2009) for examples). Our calculation for the 2D ideal lattice Fermi gas again shows its validity for a non-interacting system.

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[14] The sharp rise at the surface ($\rho/d \sim 34$) and the peak like structure at $\rho/d \sim 18$ are due to the Van Hove singularities of the spectrum.

[15] From Fig. 3 and Fig.4 in ref.[8], which plots (C_r vs n_r) and (D_r vs n_r) respectively, one can see that a straight line portion emerges in the (C_r-D_r) plot.

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