Ultra-cold atomic gases in optical lattices can constitute almost ideal realizations of Hubbard models \cite{1,2} that are fundamental to strongly-correlated physics. Recent experiments on fermionic atoms in lattices have demonstrated both a superfluid pairing \cite{3} and a Mott insulator \cite{4,5}, opening up possibilities for experimental simulation of even more complex strongly-correlated systems, such as antiferromagnetic phases and high-$T_c$ superconductivity. Thermal energy is a major control parameter in fermionic lattice systems and characterizing phase diagrams is fundamentally related to the ability to perform accurate temperature measurements.

Here we show that the temperature of fermionic atoms in a 2D optical lattice can be accurately determined by measurement of the light scattering from the atoms. The diffraction pattern is insensitive to thermal correlations but blocking the diffraction maxima and collecting light scattered outside the diffraction orders using a lens provides a measurable optical signal that reflects thermal and quantum fluctuations of lattice atoms.

The temperature of fermionic atoms in optical-lattice experiments has been deduced indirectly from the temperature of the trapped cloud of atoms before turning up the lattice \cite{4,5}, and by detecting double-occupancy in a two-species gas by converting atom pairs into molecules \cite{4,6}. Other temperature measurements detected atomic shot-noise \cite{7} or the sharpness of interference peaks \cite{8} in absorption images after a ballistic expansion. This existing technology provided vital information about temperature but it has limitations, and there is a clear need for new methods; e.g., detecting atomic shot noise proved inconclusive in some superfluid/thermal lattice systems \cite{8} and it was argued that detecting superfluidity from the sharpness of interference peaks can be ambiguous as even a thermal gas may show misleadingly sharp peaks \cite{9}. Moreover, a range of phenomena occur below the Néel temperatures \cite{10} of these systems, e.g., antiferromagnetic ordering and superfluid pair hopping, but this requires significantly more cooling than current experiments \cite{4,6} further increasing the need for a method to measure ultra-low temperatures. The diffraction of light from regular arrays of atoms in an optical lattice resembles the powerful method of x-ray diffraction from crystalline materials. The diffraction pattern reflects the atomic lattice structure and the overall diffraction envelope the shape of atomic wavefunctions at individual sites. Scattering into angles outside the diffraction orders arises by inelastic processes in which the phonon excitations of atoms in the lattice absorb the recoil kicks from the scattered photons and generate fluctuating shifts in the diffraction pattern which carry information about thermal and quantum correlations of the atoms. Light scattering from optical lattice systems was previously studied theoretically for detecting particle number fractionalization \cite{11}, coupling of atoms to optical cavities \cite{12} and to polarization of light \cite{13}.

We consider a fermionic atomic gas in an optical lattice illuminated by light with the positive frequency compo-
nent of the electric field amplitude $E_{in}^+(r) = \frac{1}{\sqrt{2}} \xi_e e^{i k \cdot r}$, the polarization $\bar{e}_{in}$, and the wave vector $k = k \hat{e}_z$; see Fig. 1. In lattices the atom dynamics can be restricted to 1D (highly-elongated tubes) or 2D (pancake-shaped layers) by optical confinement \[ 14 \]. For light passing through in an appropriate direction such a sample is optically thin and this makes light scattering a more suitable probe than in 3D samples. In the limit of a large frequency detuning $\delta$ of the light from the atomic resonance (compared to the Weisskopf-Wigner linewidth $\gamma$), the dynamics of the electronically excited atomic state may be adiabatically eliminated \[ 15 \]. The scattered light amplitude $E_{sc}^+(r)$ then becomes proportional to the transition amplitude of atoms between the initial and final hyperfine (electronic ground state) states, $g$ and $g'$, and we calculate the scattered light at $r$ (in the far radiation region \[ 16 \]) by integrating over the atomic dipoles residing at $r'$ \[ 16 \]:

$$ E_{sc}^+(r) = CA_g g' \int d^3r' e^{-i \Delta k \cdot r'} \psi_{g'}^{\dagger}(r') \psi_g(r') . \tag{1} $$

Here $\Delta k = k' - k \approx k (\hat{n} - \hat{e}_z)$ is the change of wave vector of light upon scattering ($|\Delta k| = 2k |\sin(\theta/2)|$) with $\hat{n}$ being a unit vector in the direction of the detector from the sample, $C = 3\xi e^{ikr} \gamma / (4\Delta k r)$, $A_g g' = \bar{n} \times (\bar{n} \times d_{eg'}) (\bar{e}_{in} \cdot d_{eg'}) / \mathcal{D}^2$, and $d_{eg} = (d_{eg'})^* = (e|d|g) = \mathcal{D} (e|\sigma|g) e_\sigma$ is the atomic transition dipole matrix element between $g$ and an excited Zeeman state $e$, where $\mathcal{D} = (6\pi \hbar \theta_{0}/a^2) \choose 1/2$. The only contribution to the reduced dipole matrix element $C$ is the Clebsch-Gordan coefficients. Here we use the convention that repeated indices (g, e, $\sigma$, etc.) are summed over.

Ultra-cold atoms only occupy the lowest vibrational state of each lattice site and we can expand the matter field in Eq. (1) in terms of the Wannier functions $w_{g,j}(r) = w_g(r - r_j)$ localized at each site $j$ centered at $r_j$, i.e., we write $\hat{\Psi}_g(r) = \sum w_{g,j}(r) \hat{b}_{gj}$. Here $\hat{b}_{gj}$ denotes the corresponding annihilation operator. We obtain for the scattered light intensity $I(r) = 2\epsilon_0 e^2 (E_{sc}^+ E_{sc}^-)$ which carries information about the atomic correlations

$$ I = M_{g_2g_1}^{g_3g_4} \alpha(\bar{n}) B \sum_{j,l} e^{i \Delta k (r_j - r_l)} \langle \hat{b}_{g_1,j} \hat{b}_{g_2,j} \hat{b}_{g_3,l} \hat{b}_{g_4,l} \rangle . \tag{2} $$

Here $M_{g_2g_1}^{g_3g_4} = \Lambda_{g_2g_1} \Lambda_{g_3g_4}$, and $B = I_{in} (3\gamma / 2\Delta k r)^2$ with $I_{in} = e_0 \xi e^2 / 2$ being the incoming light intensity. The Debye-Waller factor $\alpha(\bar{n})$ depends on the integrals of $w_{g,j}$ and, for the case of a level-independent lattice potential, it is obtained from the Fourier transform of the lattice site density $\alpha = \int d^3r e^{-i \Delta k \cdot r} |w_g(r)|^2 d^3r$.

Equation (2) gives the scattered light intensity for an arbitrary lattice system if the appropriate atomic correlation functions can be evaluated. Here we shall apply it to a single-component, non-interacting FD gas in a 2D square lattice, as illustrated in Fig. 1—inelastic scattering events that carry information about thermal and quantum fluctuations of atoms are mapped onto the light field, hence providing a sensitive in situ thermometer.

We assume that atoms initially occupy only one hyperfine level and that atoms scatter back to the same level (cycling transition). Consequently, we drop any explicit reference to hyperfine levels $g$. We consider a $\sigma^+$-polarized light beam, with wavelength 766.5 nm, driving $|1\rangle \equiv |4S_1/2; F = 9/2, m_F = 9/2 \rangle \rightarrow |2\rangle \equiv |4P_3/2, 11/2, 11/2\rangle$ transition of $^{40}$K, so that $d_{12} = D \hat{e}_{z} \pm 1$ and $M_{11,1}^{11,1} = (3 + \cos 2\theta) / 4$. In a single-component fermionic gas s-wave scattering between ground state atoms is forbidden and, at low temperatures, the atoms can be considered as non-interacting.

We consider a uniform 2D square lattice with periodicity $a$, potential $V = sE_R [\sin^2(\pi x/a) + \sin^2(\pi y/a)]$, and the lattice-photon recoil energy $E_R = \pi^2 \hbar^2 / (2ma^2)$. The atom dynamics along the $z$-axis is assumed to be frozen out by strong confinement. The Wannier functions $w_{j}(r)$ can be approximated by ground state harmonic oscillator wave functions with frequencies $\omega_{z}$ and $\omega_{xy} = 2\sqrt{\hbar E_R / \hbar}$, obtained by expanding the potential at the lattice site minimum. Then $\alpha(\bar{n}) = \prod_{i=x,y,z} e^{-((\Delta k_i)^2 l_i^2 / 2)}$, with $l_i = (\hbar / m a_i)^{1/2}$. The only contribution to the Hamiltonian $\hat{H} = -J \sum \hat{b}_{ij} \hat{b}_{ij}^\dagger + \hat{b}_{ij}^\dagger \hat{b}_{ij}$ arises from the hopping $J \approx 4a^3 / 4 e^{-2\sqrt{\hbar E_R / \sqrt{\pi}}}$. Where the summation is over adjacent sites only.

The Hamiltonian is diagonalized in the quasi-momentum space by $\hat{b}_{ij} = (1/N_s) \sum q \hat{b}_{ij}^q e^{i q \cdot r}$, where the amplitudes $|u_q| = 1$, and $N_s$ is the number of sites in each direction (both $x$ and $y$). The energy is given $E_{q_{xy}} = 4J \{ \sin^2 (q_{xy} a / 2) + \sin^2 (q_{xy} a / 2) \}$, with $q_{xy} = (q_x, q_y) = (2\pi / N_s a)(j_x, j_y)$, where the integers may be chosen as $j_{x,y} = -N_s / 2, \ldots, (N_s / 2 - 1)$. We may now calculate the intensity in Eq. (2) by evaluating $\langle \hat{b}_{ij}^\dagger \hat{b}_{ij} \rangle$ using the phonon operators, $\hat{a}_q$, to give

$$ I / \mathcal{A} = f^2 / 2 \sum_{k} \mathcal{A}_{\Delta k} \sum_{q,q'} \bar{n}_{q} (1 - \bar{n}_{q'}) \mathcal{A}_{\Delta k + q' - q} , \tag{3} $$

where $A = M_{11,1}^{11,1} \alpha(\bar{n}) B$, $f = N / N_s^2 \leq 1$ is the filling fraction of the lattice with $N$ being the total number of atoms, $\bar{n}_{q}$ denotes the occupation numbers of the ideal FD distribution, and

$$ \mathcal{A}_{\Delta k} = \prod_{j=x,y} \sin^2 \left( \frac{N_s \Delta k_j a / 2}{\sin^2 \left( \Delta k_j a / 2 \right)} \right) , \tag{4} $$

is the diffraction pattern from a 2D square array of $N_s \times N_s$ diffracting apertures; where $\Delta k$ is the change in the wave vector of light on the $xy$-plane.

The first term in Eq. (3), proportional to $f^2$, is the elastic scattering contribution where an atom scatters back to its original c.m. state. It generates the diffraction pattern from a non-fluctuating atom density; see Fig. 1. For a large number of sites, this gives rise to sharp diffraction peaks of small angular spread with significantly weaker intensity between the orders. The second term in Eq. (3)
represents inelastic scattering where an atom is excited from a quasi-momentum state $q$ and scatters to a different state $q'$. It is this term that contains the effect of the FD statistics, in both (a) the quasi-momentum distribution $\tilde{n}_q$ that obeys the quantum statistics, and (b) the product of the occupation numbers that describes the Fermi inhibition: scattering events in which an atom would recoil into an already occupied state are forbidden by the Pauli exclusion principle. Importantly, this inelastic term leads to scattering outside the diffraction orders—phonon excitations lead to a deflection of the light since an atomic recoil $\Delta q = q' - q$ is associated with an equal and opposite change of photon momentum. In a sequence of experimental realizations the values of $\tilde{n}_q$ fluctuate according to the FD statistics. Therefore the second term in Eq. (3) generates, on the top of the diffraction pattern envelope determined by the internal atomic level structure and the lattice site wave function (hence does not give information about the FD statistics). Elastic scattering exhibits a diffraction peak in the forward direction which we block using a suitable stop (Fig. 1), together with any unscattered part of the incident beam; this light does not provide any information about the atom statistics.

In Fig. 3 we show the number of collected photons/second by the lens with the numerical aperture $\theta_{\text{max}} = 0.48$ for $I_{\text{in}} = 5$ W m$^{-2}$ and $\delta = 20\gamma$. We use a square stop of half-diagonal angular width of 0.05 rad with its diagonals oriented along the $x$ and $y$ axes, and a cross-shaped stop, $|\theta_x| < \Theta$, $|\theta_y| < \Theta$, for $\Theta = 0.01$ and 0.05 rad to block most of the elastically scattered light without dramatically reducing the detection of inelastically scattered photons.

In each inelastic scattering process an atom absorbs a recoil kick which changes its c.m. state. This affects the temperature (heats the sample) and limits the maximum number of inelastic scattering events $W$ in a single experimental realization of the lattice system to be a small fraction $W/N$ of the total number of atoms (otherwise the measurement perturbs the ground state significantly). Only a fraction $\eta(T)$ of all the inelastically scattered photons are collected by the lens, so $N_{e}^{in}(T) = \eta(T) W$ is the number of detected inelastically scattered photons in each realization (assuming 100% detector efficiency). In experiments the lattice system can be prepared and measured $\tau$ times so that the total number of detected photons is $\tau N_{e} = \tau [N_{e}^{in}(T) + N_{e}^{el}(T)]$, where $N_{e}^{el}$ denotes the number of detected, elastically scattered photons in a single realization. For far off-resonant light, the fluctuations of the number of scattered photons are Poissonian, so to distinguish between two different optical responses corresponding to temperatures $T_1$ and $T_2$ (with $T_2 > T_1$), the difference between the number of detected photons in the two cases must be of order $\sqrt{\tau N_{e}(T_2)}$. 

![FIG. 2](image1.png)

**FIG. 2:** (Color online) The angular distribution of the intensity (in units of $B$ defined under Eq. 2) for elastic scattering (left on a logarithmic scale) at scattering angles $\phi = 0, 0.025, 0.1 \text{rad}$ (top to bottom); and for inelastic scattering (right on a linear scale) showing the effect of fermionic statistics at temperatures $T/T_F = 0.01, 0.05, 0.25, 0.5$ (bottom to top) with $T_F = 64 \text{ nK}$ and $\phi = 0$. Elastic scattering falls off faster in directions away from the $x$ and $y$ axes (Fig. 1) therefore quantitative comparison with the inelastic scattering requires integration over the collected angles (Fig. 3).

![FIG. 3](image2.png)

**FIG. 3:** (Color online) Left: The total number of collected photons/second (elastic + inelastic) as a function of temperature for a square stop (solid line), a cross-shaped stop of angular width 0.01 rad (dashed line) and 0.05 rad (dashed-dotted). Right: The required number of experimental repetitions needed to measure temperature to certain relative precision ($\Delta T/T_2$), with solid (dashed) lines for the square (0.01 rad cross-shaped) stop and temperatures of $T/T_F = 0.02, 0.05, 0.15, 0.25$ (top to bottom).
Thus the number of repetitions of the measurement required for an uncertainty of $\Delta T = T_2 - T_1$ in the determination of temperature is the value of $\sigma$ which satisfies $\tau(N_c(T_2) - N_c(T_1)) \approx \sqrt{7\tau N_c(T_2)}$.

For simplicity, we set $W/N = 0.1$. Figure 3 shows the number of experimental realizations of the lattice system required to achieve an accuracy $\Delta T / T_2$, e.g., $T / T_F = 0.1, 0.25$ can be measured within 5% by preparing the system 98 and 14 times respectively, providing a highly sensitive thermometer for atoms [20]. In Refs. [4] a Mott insulator state was observed at $T \approx 0.28 T_F$. The fraction $\eta(T)$ of inelastically scattered photons collected by the lens is large in Fig. 3 (varying from 18 to 37%). This arises because (a) the intensity in the forward direction is twice the intensity in the transverse direction for $\sigma$-polarized light (a well-known feature of the Zeeman effect); and (b) the size of the lattice site wave function generates an overall envelope for the diffraction pattern that suppresses radiation at large angles. We found that the signal-to-noise ratio is not improved with a larger aperture lens (NA=0.75), but would be increased by using a stack of several identical 2D lattice layers, provided that the system remains optically thin.

In typical experiments atoms are confined in an optical lattice plus harmonic trap—to check that this does not render our method inaccurate we carried out calculations for a 1D lattice system with a harmonic potential of frequency $\Omega$. This affects the plane wave basis used in Eq. 3 when the variation of the trap energy over the sample is greater than the hopping energy: $m\Omega^2(N_c\alpha)^2 \gtrsim J$; which for our parameters occurs when $\Omega \gtrsim 2 \pi \times 7 \text{ Hz}$ ($l_h = \sqrt{\hbar/m\Omega} \lesssim 6 \mu m$). In a trapping potential we diagonalize the Hamiltonian $H = \sum_j [(\epsilon_j^0 \hat{b}_j^\dagger \hat{b}_j) - J(\hat{b}_{j+1}^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_{j+1})]$, with $\zeta = (a^2/\pi l_h^2)^2 E_R$, and use the eigenfunctions as a new basis to evaluate Eq. 2. For the same parameters as in the 2D case ($N_s = 150$ with the lattice along the x axis and $l_y, z = 63 \text{ nm}$) we find that the angular distribution of the scattered light for a trap with $l_h = 6 \mu m$ is modified very slightly (less than 2% difference at any point), whereas the results for an additional potential in which $l_h = 2 \mu m$ are shown in Fig. 4. The temperature variation in the trap is notably stronger than for a translationally invariant lattice because the inelastic scattering depends on temperature at all angles. Thus the temperature sensitivity of the measured signal is enhanced.

In conclusion, we propose an efficient optical thermometer for fermionic atoms in a lattice. The general scattering formula 2 may easily be applied also to multi-species systems [3, 4, 5], provided that the atomic correlation functions can be evaluated.

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[20] Elastic scattering depends only on the total atom number in the lattice system (constant during each experimental realization) and does not alter the state of the atoms, as long as the intensity variation of the incoming light beam is small over the atomic sample—this is analogous to the effect of a quantum non-demolition measurement.