Probing the optical conductivity of trapped charge-neutral quantum gases

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Abstract – We study a harmonically confined atomic gas which is subjected to an additional external potential such as an optical lattice. Using a linear response formulation, we determine the response of the gas to a small, time-dependent displacement of the harmonic trap and derive a simple exact relation showing that the centre-of-mass position of the atomic cloud is directly related to the global optical conductivity of the system. We demonstrate the usefulness of this approach by calculating the optical conductivity of bosonic atoms in an optical lattice. In the Mott insulating phase, there is clear evidence of an optical Mott gap, providing a proof-of-principle demonstration that the global optical conductivity gives high-quality information about the excitations of strongly correlated quantum gases.

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Introduction. – A major goal in the field of ultracold atomic gases is to use these simple and tuneable systems to simulate strongly correlated electronic systems in order to better understand the properties of the latter. To this end, the field has begun to carry out the same kinds of measurements that have played a crucial role in unravelling the properties of electronic materials. These include high-precision thermodynamics [1], momentum-resolved radio-frequency spectroscopy [2] (the analogue of angle-resolved photo-emission spectroscopy), and transport measurements. The last includes conductance through a narrow channel separating two atomic gas reservoirs [3], as well as transport quantities associated with charge-neutral quantum fluids, namely viscosity [4] and both the longitudinal [5] and transverse [6,7] spin diffusivity.

On the other hand, experiments have yet to probe the analogue of the electrical conductivity \( \sigma \) of quantum gases. Conductivity measurements have played a major role in characterizing peculiar properties of charged quantum materials including the celebrated integer [8] and fractional [9] quantum Hall effects, the mysterious “strange metal” [10] and “pseudogap” [11] phases of the high-\( T_c \) cuprate superconductors, as well as strongly correlated (Mott) insulators [12]. It would obviously be of great interest to be able to observe the analogue of conductivity in neutral quantum gases where novel quantum behaviour can be expected to occur with increasing interaction strength.

In this paper, we propose a way to probe the global optical conductivity in harmonically confined gases and calculate this quantity for a Bose gas in a periodic optical potential. We show that the response of the centre of mass of the gas to a periodic displacement of the harmonic trap directly yields information on the retarded correlation function for the total current \( J = \int \text{d}r \text{d}t j(r,t) \). This opens the door to carrying out detailed measurements of the global optical conductivity tensor \( \Sigma_{\alpha\beta}(\omega) \) for a range of systems, including bosonic Mott insulators [13], the sought-after fermionic Mott insulator [14], strongly interacting fermions in an optical lattice, and fractional quantum Hall systems [15].

Related ideas have been explored experimentally by McKay et al. [16] as well as theoretically by Tokuno and Giamarchi [17] (see also, ref. [18]). In the former, resistive dissipation was observed in the centre-of-mass dynamics of a Bose gas in an optical lattice potential after the trap was suddenly displaced, without resolving the conductivity...
its work builds on this idea by considering a time-dependent periodic displacement of the trap potential. We show that detailed information about the optical conductivity can be obtained by simply measuring the dynamics of the centre of mass of the cloud. In contrast, Tokuno and Gianarchi [17] emphasize the role played by a phase modulation of the optical lattice potential itself in the absence of harmonic confinement. In this case they show that the optical conductivity can be probed by measuring the rate of energy absorption in response to the phase modulation.

To give insight into what information can be inferred from a modulation of the harmonic trapping potential under realistic experimental conditions, we calculate the global optical conductivity for a Bose-Hubbard model in both the deep superfluid and the Mott insulator regimes, without resorting to a local density approximation. Despite the inhomogeneity of the trapped system, sharp signatures of quantum phases are clearly evident in the optical conductivity. In the deep superfluid regime, the global optical conductivity can be probed by measuring the rate of harmonic confinement. In this case they show that the optical conductivity itself. Our work builds on this idea by considering a time-dependent periodic displacement of the trap potential. We show that detailed information about the optical conductivity can be obtained by simply measuring the dynamics of the centre of mass of the cloud. In contrast, Tokuno and Gianarchi [17] emphasize the role played by a phase modulation of the optical lattice potential itself in the absence of harmonic confinement. In this case they show that the optical conductivity can be probed by measuring the rate of energy absorption in response to the phase modulation.

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Measuring the global conductivity. – In charged systems, the local conductivity $\sigma(\omega)$ is measured by applying a uniform electric field varying in time with frequency $\omega$. This generates a frequency-dependent current density $j$ in accordance with Ohm’s law,

$$j_\alpha(\omega) = \sum_\beta \sigma_{\alpha\beta}(\omega) E_\beta(\omega)$$

(1)

(here and throughout this paper $\alpha$ and $\beta$ denote Cartesian components). Microscopically, this leads to the Kubo expression

$$\sigma_{\alpha\beta}(\omega) = (ie^2/\omega N)[(N/m)\delta_{\alpha\beta} - \chi^{\prime\prime}_{\alpha\beta}(\omega)],$$

(2)

for the local conductivity tensor, where $N$ is the total number of conducting electrons, $V$ is the volume of the system and $\chi^{\prime\prime}_{\alpha\beta}(\omega)$ is the Fourier transform of the retarded current correlation function. For a vector operator $\vec{O}$, the correlation function of interest is defined by

$$\chi^0_{\alpha\beta}(t-t') \equiv \frac{i}{\hbar} \Theta(t-t')\langle \vec{O}_\alpha(t), \vec{O}_\beta(t')\rangle.$$  

(3)

Ohm’s law is not restricted to charged systems: it amounts to a statement about the current that arises in response to a force which, in the case of a particle of charge $q$ subjected to an electric field $E$, is $F = qE$. For a charge-neutral quantum gas confined in the harmonic trapping potential $V_{\text{trap}} = \sum_n m\omega_n^2 r_n^2/2$, a small displacement of the trap from its equilibrium position generates a perturbing potential that is proportional to the displacement and hence, acts as a time-dependent uniform “electric field”. For a trap displacement $d\beta(t)$ in the specific direction $\beta$, $\delta V_{\text{trap}}(t, r) = -m\omega_\beta^2 d\beta(t) r_\beta$ (ignoring a dynamically irrelevant constant), and the resulting spatially independent force is $F(t) \equiv -\nabla \delta V_{\text{trap}} \equiv m\omega_\beta^2 d\beta(t) \dot{x}_\beta$.

The trap displacement results in the many-body perturbation $\delta H(t) = -F_\beta(t) \sum_{n=1}^N \dot{r}_\beta = -N F_\beta(t) \dot{R}_\beta$ where $\dot{R} \equiv N^{-1} \sum_{n=1}^N \dot{r}_n = N^{-1} \int d\vec{r} \dot{n}(\vec{r})$ is the centre-of-mass co-ordinate of a cloud of $N$ atoms. For a small displacement an application of linear response theory gives the cloud displacement

$$R_\alpha(t) = N \chi^R_{\alpha\beta}(\omega) F_\beta(t),$$

(4)

where $\chi^R_{\alpha\beta}(\omega)$ and $F_\beta(t)$ are the Fourier transforms of the retarded correlation function defined in (3) for the centre-of-mass position $\vec{R}$ of the trapped gas and the force $F_\beta(t)$. The criterion for the validity of linear response theory depends on the physical context but can generally be taken as the condition that the applied force $F_\beta(t)$ is small in comparison to the characteristic forces experienced by the particles in the system.

To make contact with the optical conductivity, we make use of the exact operator identity

$$N \frac{d\dot{R}_\alpha(t)}{dt} = \dot{J}_\alpha(t),$$

(5)

where $\dot{J}_\alpha(t) \equiv \int d\vec{r} \dot{J}_\alpha(\vec{r}, t)$ is the $\alpha$ component of the total current operator. Combining this with (4) gives

$$J_\alpha(t) = -iN\omega R_\alpha(\omega) = -iN^2 \omega \chi^R_{\alpha\beta}(\omega) F_\beta(t).$$

(6)

If we identify the global conductivity tensor as

$$\Sigma_{\alpha\beta}(\omega) = -iN^2 \omega \chi^R_{\alpha\beta}(\omega),$$

(7)

eq. (6) is precisely Ohm’s law.

The connection between (7) and the usual Kubo formula in terms of the current correlation function follows from the conservation law (5), which gives the exact relation $N^2 \omega^2 \chi^R_{\alpha\beta}(\omega) = (iN/\hbar) \langle [\dot{R}_\alpha(0), \dot{J}_\beta(0)] \rangle + \chi^R_{\alpha\beta}(\omega)$. Using this in (7), the latter reduces to the standard-looking Kubo formula

$$\Sigma_{\alpha\beta}(\omega) = \frac{i}{\omega} \left\{ -\frac{iN}{\hbar} \langle [\dot{R}_\alpha(0), \dot{J}_\beta(0)] \rangle - \chi^R_{\alpha\beta}(\omega) \right\}.$$  

(8)

The diamagnetic term given by the first term in curly brackets determines the sum rule for the frequency integral of the real conductivity: it is equal to $(N/m)\delta_{\alpha\beta}$ for any physical Hamiltonian, even when a trap is present. However, for models with an implicit energy cutoff such as the Bose-Hubbard Hamiltonian we consider below, it assumes a different value (cf. (13)).
If we take the trap displacement to be periodic, \( d_\beta(t) = (d_\beta/2) \exp(-i\omega t) + \text{c.c.} \), the centre-of-mass position of the cloud is given by

\[
R_0(t) = A_0(\omega) \cos[\omega t - \phi_0(\omega)],
\]

where the amplitude \( A_0(\omega) \) is the maximum displacement of the cloud from equilibrium and \( \phi_0(\omega) \) is the phase lag between the oscillation of the cloud and that of the potential. A combination of (4) and (7) then gives the complex conductivity

\[
\Sigma_{\alpha\beta}(\omega) = \frac{2N\omega}{iF_\beta} A_0(\omega)e^{i\phi_0(\omega)}
\]

which is thus completely determined by the dynamics of the centre-of-mass position.

Equation (10) constitutes a major result of this paper. It shows that the centre-of-mass dynamics \( R_0(t) \) provides a measurement of the global optical conductivity tensor for a trapped gas, defined in (8). This tensor will be diagonal unless time-reversal symmetry is broken — as would happen in a rotating gas [20,21] or by creating an artificial gauge field [22]— giving an off-diagonal Hall conductivity diagonal unless time-reversal symmetry is broken — as would happen in a rotating gas [20,21] or by creating an artificial gauge field [22]— giving an off-diagonal Hall conductivity.
Substituting (18) into (17) we thus obtain $\langle \Phi_0 | \hat{R} | \Phi_\text{dip} \rangle = \sqrt{\hbar/2Nm^2\omega^2}$. Using this result in (14) and (7) gives

$$
\Sigma_{xx}(\omega) = i \frac{N}{m^2} \frac{\omega}{\omega^2 - \omega^2 + \eta^2},
$$

(19)

which is analogous to (11). We note that this result for the optical conductivity deep in the superfluid regime obtained within the continuum GP description satisfies the $f$-sum rule (13) with $\langle T \rangle = -2tN = -N\hbar^2/m^2a^2$.

Moving away from the $U/t \to 0$ limit, the continuum GP approximation can no longer be invoked and the Kohn-like response given by (19) does not hold. Specifically, we have confirmed by means of a numerical solution of the discrete BdG equations that, although the pole given by (19) persists, its weight is reduced with increasing $U/t$. By analogy with the optical conductivity of superconductors [19], the weight of the pole provides a measure of the superfluid fraction $N_s/N$; as a result of enhanced quantum fluctuations, $N_s/N < 1$ at $T = 0$. (In a superconductor, both the diamagnetic and paramagnetic current correlation functions contribute Dirac delta functions at $\omega = 0$ to the real part of the optical conductivity (cf. (8)); the net weight of the delta-function contribution provides a definition of the superfluid fraction [26].)

We now consider the deep Mott insulating regime ($t \ll U$) with an occupancy $\bar{n} \approx 1$ near the centre of the trap. We perform numerical diagonalizations of (12) using a truncated Hilbert space to obtain the ground and low-energy excited states of such an insulator. The physically relevant states should include doublons, with energies of order $U$, as well as low-energy excitations involving atoms hopping to empty sites at the edges of the trap. Thus, our truncated Hilbert space is spanned by the Mott insulating ground state in the atomic limit, $|\Phi_0\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$ (where the mid-point in the index range coincides with the trap centre), and the particle-hole excited states $|\varphi_{ij}\rangle = a_j^\dagger a_i |\Phi_0\rangle$ where the index $i$ is one of the occupied sites in $|\Phi_0\rangle$ while $j$ is any possible occupied or empty site. To allow for the latter possibility, we diagonalize (12) using $N = 120$ atoms and $M = 150$ lattice sites.

The complex optical conductivity is shown in fig. 1 for $U/t = 100$. Although this value is beyond what is typically explored in experiments (for the 3D experiment in ref. [13], the Mott insulating transition was observed around $U/t = 36$ while in 1D, it will occur around $U/t = 10$ [27]), it ensures the accuracy of the approximations we have used in our numerical calculations. We expect the behaviour to be qualitatively similar for smaller values $U/t$. For frequencies $\omega \lesssim U/h$, there is clear evidence of a Mott gap in the real part of the conductivity despite the presence of a harmonic trapping potential. Such a feature is expected for untrapped Mott systems and arises from the absence of low-energy excitations in the Mott phase. At higher frequencies $\omega \gtrsim U/h$, doublons corresponding to double-occupancy states can be excited and the real part of the conductivity becomes significant, signifying dissipation. The harmonic trapping potential manifests itself most directly through the presence of low-energy excitations corresponding to atoms being excited from the Mott insulator occupying the centre of the trap to adjacent vacant sites. These give rise to the spectral feature at low frequencies in fig. 1.

The cloud centre-of-mass dynamics corresponding to the conductivity in fig. 1 is shown in fig. 2. Since the right-hand side of (10) contains a factor $\omega$, the dynamics emphasizes the low-energy spectral weight in $\Sigma_{xx}(\omega)$. For this reason, the role of the low-frequency edge excitations is greatly amplified in the centre-of-mass dynamics as compared to the high-frequency doublon contribution. The spectral features in the amplitude and phase associated with these modes can be understood in terms of damped, driven harmonic oscillators. The lower mode corresponding to the edge excitations has a frequency $\omega \sim t$ ($\sim 10^{-2}U/h$ for our parameter values) which is associated with hopping from occupied to unoccupied sites. The “Mott gap” in which insulating behaviour is observed is then bounded by this frequency and the doublon frequency at $\omega \sim U/h$. In this range of frequencies the cloud barely moves ($A(\omega) \approx 0$) in response to the displacement. By the same token, the phase lag becomes $\pi$ since the cloud is being driven at frequencies above the natural resonant frequency of the lower mode (consistent with a purely imaginary conductivity, (10)). When the driving frequency approaches $U/h$, doublons are excited and the cloud once again begins to oscillate and $A(\omega)$ is substantial, corresponding to a nonzero real conductivity. The large degeneracy of the doublons, on the order of the number of lattice sites, opens up a band of width $\gtrsim t$ where dissipation, as given by $dE/dt = Re\Sigma_{xx}(\omega)m^2\omega_0^2\delta^2/4$ (averaged over a period of oscillation), once again becomes significant. Above this
band, the oscillation amplitude $A$ is small and the system is again effectively insulating. Since the driving frequency is above the doublon band, the oscillation of the cloud is out of phase with the driving field ($\phi \sim \pi$).

Although our results are for a 1D Mott insulator, the same primary features will carry over to 3D. The major difference at high frequencies will be a wider doublon band [17,18]. At low frequencies, a pole in the conductivity will arise at $\omega^* = 2\sqrt{\mu_0}/\hbar$ if the atoms at the edge of the cloud are superfluid since they can move around the Mott insulator in 3D.

**Summary.** In this paper we have shown using linear response theory that the centre-of-mass dynamics of an atomic cloud induced by an oscillating trapping potential is a sensitive probe of the optical conductivity of the gas. As an illustration of the potential of conductivity measurements to obtain high-quality information about bulk states of matter, we calculated the optical conductivity of a Bose gas in the Mott insulating phase and the corresponding dynamics of the centre-of-mass of the cloud. Despite the harmonic trap, the large separation $t \ll U$ of energy scales in the Mott insulator means that edge excitations particular to harmonically confined gases do not obscure clear signatures of a bulk Mott gap and doublon excitations. Our scheme should be very useful in obtaining information about the properties of other states of matter, including integer [20] and fractional [15] quantum Hall states, chiral $p$-wave superfluids [28] via measurement of the off-diagonal response $\Sigma_{xy}$, as well as the diagonal spectral response of a strongly interacting Fermi gas in a periodic potential, possibly connecting to spectral features of pseudogap physics [11]. Finally, using a spin-selective perturbing potential, our results for the conductivity immediately carry over to the spin Hall conductivity, the central quantity that characterizes the spin Hall effect [29].

**Appendix: dipole response of a harmonically confined gas in the BdG approximation.** Assuming a real ground-state wave function $\phi(x)$, the BdG equations for excitations on top of the ground state described by the continuum GP equation (16) are

$$ \begin{bmatrix} \mathcal{L} + 2g\phi^2 & -g\phi^2 \\ -g\phi^2 & \mathcal{L} + 2g\phi^2 \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} = \hbar\omega_n \begin{bmatrix} u_n \\ -v_n \end{bmatrix}, $$

where

$$ \mathcal{L} \equiv -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m^* \omega^2 x^2 - \mu^*. $$

The spatially varying Bogoliubov amplitudes $u_n(x)$ and $v_n(x)$ satisfy the orthonormality relations [30]

$$ \int dx [u_n(x)u_n^*(x) - v_n(x)v_n^*(x)] = \delta_{nm} $$

and

$$ \int dx [u_n(x)v_n^*(x) - v_n(x)u_n^*(x)] = 0. $$

Substitution of (18) in the main text into (A.1) confirms that these are the Bogoliubov amplitudes of the dipole mode, with frequency $\omega_{dip} = \omega^*$.

As noted in ref. [25], the BdG equations can be formulated in terms of hydrodynamic variables corresponding to density $\delta \rho_n$ and phase $\theta_n$ fluctuations:

$$ \begin{bmatrix} u_n \\ v_n \end{bmatrix} = \frac{i\delta \theta_n}{\hbar} \pm \frac{\delta \rho_n}{2\phi}. $$

Using this in (A.3) gives

$$ \int dx \delta \rho_n(x)\theta_n^*(x) \propto \delta_{nm}. $$

The dipole mode corresponds to a “rigid-body” motion of the cloud, meaning that the velocity $v \propto \partial_x \theta$ is constant and hence, $\theta_{dip}(x) \propto x$. This is an exact result for systems obeying the generalized Kohn theorem [23], as is the case for the continuum GP model. It can also be seen from (18) and (A.5) that

$$ \theta_{dip}(x) = -i \sqrt{\frac{\hbar m^* x}{2N}}. $$

Using this in (A.6) gives

$$ \int dx \delta \rho_n(x) x \propto \delta_{n,dip}. $$

Using (A.5) to rewrite $\delta \rho_n$ in terms of $u_n$ and $v_n$, this last result becomes

$$ \int dx \phi(x)[u_n(x) - v_n(x)] \propto \delta_{n,dip}. $$

This proves that the matrix element given by (17) in the main text vanishes for all excited states $n$ except for the dipole mode.

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