Drude Weight, Meissner Weight, Rotational Inertia of Bosonic Superfluids: How Are They Distinguished?

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Abstract

The Drude weight, the quantity which distinguishes metals from insulators, is proportional to the second derivative of the ground state energy with respect to a flux at zero flux. The same expression also appears in the definition of the Meissner weight, the quantity which indicates superconductivity, as well as in the definition of non-classical rotational inertia of bosonic superfluids. It is shown that the difference between these quantities depends on the interpretation of the average momentum term, which can be understood as the expectation value of the total momentum (Drude weight), the sum of the expectation values of single momenta (rotational inertia of a superfluid), or the sum over expectation values of momentum pairs (Meissner weight). This distinction appears naturally when the current from which the particular transport quantity is derived is cast in terms of shift operators.

1 Introduction

To distinguish conductors from insulators in the quantum case, the strength of the zero-frequency conductivity was derived by Kohn [1]. The Drude weight is often expressed [1, 2] in terms of the second derivative of the ground state energy with respect to a phase Φ associated with the perturbing field as

$$D^{(c)} = \frac{\pi}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}, \tag{1}$$

where $E(\Phi)$ denotes the perturbed ground state energy. The Meissner weight, which appears in London's phenomenological theory of superconductors is formally identical to the Drude weight. Moreover, the inverse of the rotational inertia of a rotating bosonic superfluid (non-classical rotational inertia (NCRI))is also proportional to the second derivative of the ground state energy, i.e. it is exactly of the same form as Eq. (1), only that in that case Φ is proportional to the angular velocity. Here these quantities will be collectively called transport susceptibilities.

A fundamental question thus arises: there are three distinct physical phenomena, but they appear to be described by a single mathematical expression. Scalapino, White, and Zhang (SWZ) [3, 4] have proposed an interpretation which distinguishes the Drude weight from the Meissner weight. They pointed out that the derivative with respect to the flux is ambiguous. It could refer to the derivative of the ground state eigenvalue of the energy with respect to the perturbation (adiabatic derivative) or the actual ground state as a function of the perturbation ("envelope" derivative). In the absence of level crossings the two are identical. SWZ conclude that the difference between the Drude and superfluid weights is that the former(latter) corresponds to the adiabatic(envelope) derivative. Up to now this appears to be the last word on this topic.

There are a number of weaknesses in this interpretation. In one dimension the level crossings occur at $\Phi = \pi$ even in the thermodynamic limit, hence in that case the Drude and Meissner weights can not be distinguished. Moreover, as discussed in a recent paper of the author [5] and summarized below, the application of these ideas to variational wavefunctions is ambiguous. The usual way [6, 7] to calculate the Drude weight is to take the second derivative of the variational ground state energy. However, this quantity can be cast in terms of an average of the true energy eigenvalues. Turning on the perturbation can cause level crossings. If we insist on SWZ, then these level crossings should be excluded, and the usual approach [6, 7] would be invalidated. In the limit of a perfect variational wavefunction (one which corresponds to the exact ground state for any value of the perturbation) the result would be what according to SWZ is the Meissner weight, not the Drude weight. We stress though that this usual approach would *only be invalidated if we assume SWZ is correct*. In addition the SWZ interpretation does not distinguish the Meissner weight associated with superconductors from the non-classical inertia of rotating superfluids (these two quantities in SWZ belong to the general category of "superfluid weight").

In this paper a different approach to distinguishing the Drude weight, Meissner weight, and the rotational inertia of a superfluid is developed, which does not make any reference to whether the derivative is adiabatic or envelope. First a general expression for the second derivative of the ground state energy is derived, which is of the form

$$\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0} = \frac{N}{m} + \lim_{\Delta\Phi\to 0} \frac{\langle\Psi|\left[e^{-i\Delta\Phi\hat{X}}\hat{K} + \hat{K}e^{i\Delta\Phi\hat{X}}\right]|\Psi\rangle}{m\Delta\Phi}. \tag{2}$$

where $\hat{K} = \sum_{i=1}^{N} \hat{k}_i$. In a periodic system this expression includes an expectation value which can be interpreted in a number of ways. It can be taken to mean (A) the expectation value of the sum over all momenta, (B) the sum over expectation values of single momenta, or (C) any other break up of the total momentum operator (pairs, triplets, etc.). In fact, this ambiguity disappears if the current, from which Eq. (2) is derived, is written in terms of the appropriate Berry phase expression [5]. Case (A) is shown to correspond to the Drude weight, which distinguishes metallic conductors from insulators. It is also shown that metallic conduction can be related to a generalization of the concept of off-diagonal long-range order (ODLRO) [8, 9, 10]. Case (B) is shown to correspond to bosonic superfluids. The justification is based on the fact that the second derivative of the ground state energy with respect to the flux in this case is proportional to the number of particles in a Bose-Einstein condensed state. A direct connection is established between ODLRO associated with the single particle density matrix. Breaking up $\hat{K}$ into pairs is shown to correspond to a condensate of pairs, such as in the case of BCS superconductivity. Here, a direct connection is established between ODLRO associated with the two-particle density matrix. Moreover, this interpretation, unlike SWZ, distinguishes not only conductors from superconductors, but also superfluids with single particle condensates from condensates with other basic groups (two particles, three particles, etc.). Also, unlike SWZ, its applicability is independent of dimensions.

The fact that Eq. (2) is ambiguous may appear surprising, but it can be made obvious by casting the current from which the transport susceptibility is derived in terms of an explicit position shift operator [5]. In that case, as shown below, the distinct transport susceptibilities originate from the limiting cases of different current expressions.

In addition the results of this work solve another open problem. In a recent paper Anderson stated [11] the following:

> *...it has never been demonstrated that ODLRO, and NCRI are synonymous,...*

Below this gap is filled by making this connection explicit.

This paper is organized as follows. The subsequent two sections provide background information, followed by a brief note on current. Section 5 derives the Drude weight. In section 6 the connection of standard conduction with off-diagonal long-range order is presented, the subsequent sections treat the case of simple Bose-Einstein condensation and condensation in a general pairing system. The penultimate section presents a comprehensive theory of conduction, after which the work is concluded.

2 Background

The quantities which in this work will be referred to as transport susceptibilities are the Drude weight, the Meissner weight (the fraction of particles which are in a Bose-Einstein condensate in a superconductor), and the rotational inertia of the superfluid fraction. In this section some general background information on transport susceptibilities is provided.

We consider a system of N identical particles in a periodic potential with Hamiltonian

$$\hat{H}(\Phi) = \sum_{i=1}^{N} \frac{(\hat{k}_i + \Phi)^2}{2m} + \hat{V}, \tag{3}$$

where $\hat{k}_i$ denotes the momentum operator of particle i, m denotes the mass of the particles, Φ denotes a perturbation, and $\hat{V}$ denotes the interaction potential, for which it holds that

$$V(x_1, ..., x_i, ...x_N) = V(x_1, ..., x_i + L, ...x_N) \tag{4}$$

for any i. For most of this article, we will consider the ground state of this Hamiltonian,

$$\hat{H}(\Phi)|\Psi(\Phi)\rangle = E(\Phi)|\Psi(\Phi)\rangle, \tag{5}$$

where $E(\Phi)(|\Psi(\Phi)\rangle)$ denotes the ground state energy (wavefunction) for the perturbed system. In the momentum space representation the unperturbed state can be written as $\Psi(k_1, ..., k_N)$, whereas the perturbed wavefunction takes the form $\Psi(k_1 + \Phi, ..., k_N + \Phi)$. One can also express the pertubed wavefunction in terms of the unpertubed one using the total momentum shift operator [12, 13] as

$$|\Psi(\Phi)\rangle = e^{i\Phi\hat{X}}|\Psi(0)\rangle, \tag{6}$$

where $\hat{X} = \sum_{i=1}^{N} \hat{x}_i$.

The Drude weight was first derived in Ref. [1]. The main results from this work relevant here are that the current and the Drude weight can be obtained in terms of the first and second derivatives (respectively) of the ground state energy with respect to Φ, i.e.

$$\begin{aligned} J(\Phi) &= \frac{\partial E(\Phi)}{\partial \Phi} \qquad (7) \\ D^{(c)} &= \frac{\pi}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}, \end{aligned}$$

$D^{(c)}$ is obtained by assuming Φ to be of the form $\Phi = Ee^{i\omega t}/(i\omega)$. Using this form for the perturbation, the imaginary part of the frequency dependent conductivity $\sigma''(\omega)$ can be calculated and the zero frequency limit of the quantity $\lim_{\omega\to 0}\omega\sigma''(\omega)$ can be taken, resulting in $D^{(c)}$.

The Meissner weight is a result of the phenomenological explanation of the Meissner effect due to London and London. We follow Ref. [14]. We first assume that a superconductor is a perfect conductor, obeying

$$\mathbf{E} = \frac{1}{n^{(s)}}\frac{\partial \mathbf{j}}{\partial t}, \tag{8}$$

where $n^{(s)}$ the density of superconducting charge carriers, $\mathbf{j}$ indicates the current density. Using the Maxwell relation for the curl of the electric field we obtain

$$\frac{\partial}{\partial t}\left[\nabla \times \mathbf{j} + n^{(s)}\mathbf{B}\right] = 0. \tag{9}$$

If the quantity in the square brackets is assumed to equal zero then the Meissner effect can be accounted for and the penetration depth of the magnetic field in a superconductor can be calculated. Using this assumption and the London gauge ($\nabla\chi = 0$) we obtain

$$\mathbf{j} = n^{(s)}\mathbf{A}. \tag{10}$$

Considering one dimension only, and associating the vector potential with the momentum shift we obtain

$$n^{(s)} = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}. \tag{11}$$

One of the main characteristic properties of a bosonic superfluid emerges from the rotating bucket experiment, first discussed by Landau [15] in 1941. When a superfluid below the critical temperature is rotated slowly, its moment of inertia is reduced compared to a normal fluid, since the superfluid fraction remains stationary. We write the total rotational inertia as

$$I = I^{(s)} + I^{(n)}, \tag{12}$$

where $I^{(s)}(I^{(n)})$ corresponds to the rotational inertia associated with the superfluid(normal) fraction. Above the critical temperature, where both fractions rotate, the work to rotate the container would be

$$\Delta W(\Phi) = E(\Phi) - E(0) = I\frac{\Phi^2}{2}. \tag{13}$$

Below the critical temperature only the normal fraction would rotate with the bucket and the work required would be

$$\Delta W^{(n)}(\Phi) = E^{(n)}(\Phi) - E^{(n)}(0) = I^{(n)}\frac{\Phi^2}{2}, \tag{14}$$

where $E^{(n)}(\Phi)$ denotes the ground state energy associated with the normal fluid. From Eqs. (13) and (14) it follows that

$$E^{(s)}(\Phi) - E^{(s)}(0) = I^{(s)}\frac{\Phi^2}{2}, \tag{15}$$

or for small Φ

$$I^{(s)} = \left[\frac{\partial^2 E^{(s)}(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}. \tag{16}$$

All three quantites $D^{(c)}$, $n^{(s)}$, $I^{(s)}$ are proportional to the second derivative of the ground state energy with respect to the perturbation Φ at $\Phi = 0$.

3 The Problems with Distinguishing Transport Susceptibilities Based on Adiabatic or Envelope Derivatives

SWZ suggested [3, 4] that to distinguish the Drude weight from the Meissner weight, one has to consider that the derivative with respect to Φ in the definition of transport susceptibilities is ambiguous. They pointed out that the derivative could refer to the derivative of the ground state energy with respect to the perturbation (adiabatic derivative) or that of the zero temperature limit of the free energy (envelope derivative). In the case of the former level crossings are excluded. SWZ also show that level crossings occur at $\Phi \approx 1/L^{d-1}$, where L is the linear dimension and d is the dimensionality. In one dimension the level crossing occurs at a finite value even in the thermodynamic limit, resulting in no distinction between the Drude and Meissner weights. One could argue that superconductivity is a two-dimensional effect (the Meissner weight is the response of the system to a magnetic field), but this would be incorrect. A superconducting ring is described by a one-dimensional model. Also the analysis of flux quantization by Byers and Yang [16] uses a one-dimensional example (a ring around the cavity).

One can also show that the SWZ interpretation is ambiguous when applied in variational theory. The usual procedure to calculate the Drude weight in variational theory [6, 7] is to take the second derivative of the variational ground state energy, however, as shown below, when this procedure is followed, level crossings are still present, and the derivative can not be considered adiabatic. To see this one can compare variational theory to the finite temperature extension of the Drude weight.

The finite temperature extension of $D^{(c)}$ has been given by Zotos, Castella, and Prelovšek [17] (ZCP). This generalization can be summarized as

$$D_{adb}(T) = \frac{\pi}{V} \sum_n P_n(0) \left[\frac{\partial^2 E_n(\Phi)}{\partial \Phi^2} \right]_{\Phi=0}, \tag{17}$$

where

$$P_n(0) = \frac{\exp\left(-\frac{E_n(0)}{k_B T}\right)}{Q(0)}, \tag{18}$$

and where $Q(0)$ denotes the canonical partition function of the unperturbed system. The important point is that in Eq. (17) the Boltzmann weight factors *remain unchanged as the perturbation* Φ *is turned on.* Thus the effect of level crossings is excluded and the *derivative is the adiabatic one.* Taking the zero temperature limit reproduces Kohn's expression for D (Eq. (1)). Eq. (17) consists of a sum over *adiabatic derivatives* of energies weighted by the Boltzmann factor. Eq. (17) has been applied [18] to calculate the Drude weight in strongly correlated systems.

To define [5] a quantity which in the limit of zero temperature produces Eq. (1), but with the envelope derivative instead of the adiabatic one, one could modify Eq. (17) as

$$D_{env}(T) = \frac{\pi}{V} \left[\frac{\partial^2}{\partial \Phi^2} \langle E(\Phi) \rangle \right]_{\Phi=0} = \frac{\pi}{V} \frac{\partial^2}{\partial \Phi^2} \left[\sum_n P_n(\Phi) E_n(\Phi) \right]_{\Phi=0}, \tag{19}$$

where $\langle E(\Phi) \rangle$ indicates the average energy of the perturbed system. Alternatively, one could also define a quantity based on the free energy as

$$D_{env}(T) = \frac{\pi}{V} \left[\frac{\partial^2 F(\Phi)}{\partial \Phi^2} \right]_{\Phi=0}. \tag{20}$$

In the zero temperature limit both Eqs. (19) and (20) tend to the same expression, Eq. (1) but this time with the *envelope derivative,* since level crossings can in this case alter the state which enters the definition of the derivative.

In a variational theory, when the Drude weight is calculated, usually [6, 7] the second derivative of the variational energy is taken with respect to Φ . Such an assumption is not consistent with the SWZ interpretation for the following reasons. Suppose $|\tilde{\Psi}(\gamma)\rangle$ is a variational wavefunction, where γ denotes a set of variational parameters, which we wish to use to optimize some Hamiltonian $\hat{H}$ with eigenbasis

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle. \tag{21}$$

The estimate for the ground state energy may be written in terms of a density matrix as

$$\langle\tilde{\Psi}(\gamma)|\hat{H}|\tilde{\Psi}(\gamma)\rangle = \sum_n \langle\tilde{\Psi}(\gamma)|\Psi_n\rangle E_n \langle\Psi_n|\tilde{\Psi}(\gamma)\rangle = \sum_n \tilde{P}_n E_n, \tag{22}$$

the probabilities can be written as

$$\tilde{P}_n = |\langle\tilde{\Psi}(\gamma)|\Psi_n\rangle|^2. \tag{23}$$

Comparing with Eq. (17) it is obvious that if the SWZ interpretation is assumed then the correct Drude weight would be defined as

$$D_{adb} = \sum_n \tilde{P}_n(0) \left[\frac{\partial^2 E_n(\Phi)}{\partial\Phi^2}\right]_{\Phi=0}, \tag{24}$$

with $\tilde{P}_n(0)$ independent of the perturbation Φ, since this way we would have a set of weighted adiabatic derivatives. In this case the effect of level crossings on the weights would be excluded.

Instead, the standard way [6, 7] to calculate the Drude weight in variational theory is to take the second derivative of the variational energy with respect to the perturbation, i.e.

$$D_{env} = \frac{\pi}{V}\frac{\partial^2}{\partial\Phi^2}\left[\sum_n P_n(\Phi)E_n(\Phi)\right]_{\Phi=0}, \tag{25}$$

in which case the effect of level crossings are *not excluded*, and which corresponds to an *envelope derivative.* In fact Eq. (25) has the same form as Eq. (19), in both cases the derivatives of the average energy are taken. Millis and Coppersmith [6] conclude based on Eq. (25) that the Gutzwiller projected Fermi sea [19] is a conductor. The equivalent of the zero temperature limit for Eq. (25) would be the limit of a perfect variational wavefunction, which corresponds to the true wavefunction for any value of Φ. In this limit Eq. (25) would corresponds to the *envelope derivative*, in other words, according to the logic of SWZ, the Meissner weight. It needs to be stressed that the statement of this article is not that Eq. (25) corresponds to the Meissner weight, only that it does according to the criteria of SWZ.

Apart from the above, another shortcoming of the SWZ prescription is that it does not explicitly distinguish bosonic superfluids from superconductors (condensation of paired fermions).

4 Berry Phase Expression for the Current in Many-Body Systems with Periodic Boundary Conditions

In Ref. [5] it was shown that for continuous systems with many-particles under periodic boundary conditions the current can be expressed as

$$J_N(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{1}{m\Delta X}\mathrm{Im}\ln\langle\Psi(\Phi)|\exp(i\Delta X\hat{K})|\Psi(\Phi)\rangle. \tag{26}$$

Carrying out the limit $\Delta X \to 0$ results in

$$J_N(\Phi) = \frac{N}{m}\Phi + \frac{1}{m}\langle\Psi(\Phi)|\hat{K}|\Psi(\Phi)\rangle. \tag{27}$$

However, for a system with identical particles one could also write

$$J_1(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{N}{m\Delta X}\mathrm{Im}\ln\langle\Psi(\Phi)|\exp(i\Delta X\hat{k})|\Psi(\Phi)\rangle, \tag{28}$$

where $\hat{k}$ is a single momentum operator, or more generally one has

$$J_p(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{N/p}{m\Delta X}\mathrm{Im}\ln\langle\Psi(\Phi)|\exp\left(i\Delta X\sum_{i=1}^{p}\hat{k}_i\right)|\Psi(\Phi)\rangle. \tag{29}$$

Carrying out the limit in $\Delta X \to 0$ Eqs. (29) and (28) would appear to give identical results similar to Eq. (27).

The difference between $J_p(\Phi)$ for different ps becomes obvious if we cast the second term in terms of the appropriate reduced density matrix (Eq. (43)),

$$J_p(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{N/p}{m\Delta X}\mathrm{Im}\ln\mathrm{Tr}\left\{\hat{\rho}_p\exp\left(i\Delta X\sum_{i=1}^{p}\hat{k}_i\right)\right\}. \tag{30}$$

As shown below the transport susceptibilities derived from a particular definition of current are sensitive to ODLRO [10] in density matrices of different orders. In the examples analyzed below, it will always be assumed that the transport susceptibility is derived from one particular definition of the current, Eq. (30), i.e., a particular value of p. However, to prevent the notation from becoming too cumbersome, we will not write the current in terms of the corresponding shift operators.

5 Expressing $\left[\frac{\partial^2 E(\Phi)}{\partial\Phi^2}\right]_{\Phi=0}$

As our first example we analyze the case $p = N$. The quantities in this section are derived based on $J_N(\Phi)$. The first derivative of the ground state energy with respect to Φ corresponds to the total current, and, after the limit $\Delta X \to 0$ is taken, it can be written as

$$J(\Phi) = \frac{N}{m}\Phi + \frac{\langle\Psi(\Phi)|\hat{K}|\Psi(\Phi)\rangle}{m}. \tag{31}$$

Taking the next derivative results in

$$\frac{\partial^2 E(\Phi)}{\partial\Phi^2} = \frac{N}{m} + \frac{1}{m}\left[\langle\partial_\Phi\Psi(\Phi)|\hat{K}|\Psi(\Phi)\rangle + \langle\Psi(\Phi)|\hat{K}|\partial_\Phi\Psi(\Phi)\rangle\right]. \tag{32}$$

We now multiply and divide the last two terms by $\Delta\Phi$, resulting in

$$\frac{\partial^2 E(\Phi)}{\partial\Phi^2} = \frac{N}{m} + \frac{1}{m\Delta\Phi}\left[\Delta\Phi\langle\partial_\Phi\Psi(\Phi)|\hat{K}|\Psi(\Phi)\rangle + \Delta\Phi\langle\Psi(\Phi)|\hat{K}|\partial_\Phi\Psi(\Phi)\rangle\right]. \tag{33}$$

In the limit $\Delta\Phi \to 0$ it holds that

$$\Delta\Phi\langle\partial_\Phi\Psi(\Phi)| = \langle\Psi(\Phi + \Delta\Phi)| - \langle\Psi(\Phi)|. \tag{34}$$

Using the fact that at $\Phi = 0$ the total current is zero, we obtain

$$\frac{\partial^2 E(\Phi)}{\partial\Phi^2} = \frac{N}{m} + \lim_{\Delta\Phi\to 0}\frac{1}{m\Delta\Phi}\left[\langle\Psi(\Delta\Phi)|\hat{K}|\Psi(0)\rangle + \langle\Psi(0)|\hat{K}|\Psi(\Delta\Phi)\rangle\right]. \tag{35}$$

Applying the definition of the shift operator results in

$$\frac{\partial^2 E(\Phi)}{\partial\Phi^2} = \frac{N}{m} + \lim_{\Delta\Phi\to 0}\frac{1}{m\Delta\Phi}\left[\langle\Psi|e^{-i\Delta\Phi\hat{X}}\hat{K}|\Psi\rangle + \langle\Psi|\hat{K}e^{i\Delta\Phi\hat{X}}|\Psi\rangle\right]. \tag{36}$$

which is the same as Eq. (2).

The interpretation of Eq. (36) is the same as that of the Drude weight derived in Ref. [20]. If the unperturbed wavefunction $|\Psi\rangle$ is an eigenstate of $\hat{K}$, given that it is unperturbed it would have to have an eigenvalue of zero. In this case the second derivative is simply $\frac{N}{m}$. When that is not the case one can expand Eq. (2) in $\Delta\Phi$ and keep the leading term, resulting in

$$\left[\frac{\partial^2 E(\Phi)}{\partial\Phi^2}\right]_{\Phi=0} = \frac{N}{m} + i\frac{\langle\Psi(0)|[\hat{K},\hat{X}]|\Psi(0)\rangle}{m}. \tag{37}$$

The zeroth order term in the expansion in $\Delta\Phi$ corresponds to the expectation value of the total current in the unperturbed state which is zero. Using the definitons of the operators $\hat{K}$ and $\hat{X}$, it is easy to show that

$$[\hat{K},\hat{X}] = \sum_{i=1}^{N}[\hat{k}_i,\hat{x}_i] = iN, \tag{38}$$

and that the second derivative in this case is zero.

6 Off-Diagonal Long-Range Order

One can also cast [21] the criterion for conduction in terms discontinuous features of the distribution of the total momentum K alternatively in terms of a variation on the idea of ODLRO. We define

$$P_N(K) = \int ... \int dk_1...dk_N |\Psi(k_1, ..., k_N)|^2 \delta\left(K - \sum_{i=1}^{N} k_i\right). \tag{39}$$

If Ψ is an eigenstate of the total momentum, $P_N(K)$ is a δ-peak at the origin. For the insulating state $P_N(K)$ is some smooth function, symmetric around the origin. One can define a quantity,

$$\tilde{\rho}_N(X, X') = \int ... \int dx_1...dx_N \Psi(x_1 + X, ..., x_N + X)\Psi^*(x_1 + X', ..., x_N + X'). \tag{40}$$

It is easy to show that

$$\tilde{\rho}_N(X, X') = \int dK P_N(K) e^{iK(X-X')}, \tag{41}$$

and that conduction corresponds to

$$\lim_{|X-X'|\to\infty} \tilde{\rho}_N(X, X') = \text{finite}, \tag{42}$$

whereas insulation corresponds to a decay in $\tilde{\rho}_N(X, X')$ to zero.

In the following we will use the reduced density matrices defined as

$$\rho_p(x_1, ..., x_p; x'_1, ..., x'_p) = \int ... \int dx_{p+1}...dx_N \Psi(x_1, ..., x_p, x_{p+1}, ..., x_N)\Psi(x'_1, ..., x'_p, x_{p+1}, ..., x_N). \tag{43}$$

It is well-known [10] that long-range order in the reduced density matrix corresponds to Bose-Einstein condensation in systems of identical particles at low temperature. For example, if the one-body reduced density matrix exhibits long-range order, i.e.

$$\lim_{|x-x'|\to\infty} \rho_1(x; x') = \text{finite}, \tag{44}$$

then the system exhibits condensation in which the basic group has one particle (superfluidity in bosonic systems, e.g. He^4). Similarly, ODLRO in $\rho_2(x_1, x_2; x'_1, x'_2)$, but not in $\rho_1(x; x')$ corresponds to the condensation where the basic group consists of two particles, as in BCS pairing in superconductors, or superfluidity in He^3. ODLRO in the m-body real-space reduced density matrices corresponds to δ-peaks in the m-body momentum distributions. These results were derived by Yang [10]. Yang has also shown that if off-diagonal long-range order is present in some reduced density matrix ρ_j, then it will also be present in all reduced density matrices ρ_k with $k \geq j$.

7 Bose-Einstein Condensation of Single Particles

We will now interpret Eq. (2) as a sum over single-particle momenta, in other words, we assume that the current expression from which the transport susceptibility originates is $J_1(\Phi)$ (Eq. (28)). The corresponding second derivative is

$$\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0} = \frac{N}{m} + \sum_{j=1}^{N} \lim_{\Delta\Phi \to 0} \frac{\langle \Psi | \left[e^{-i\Delta\Phi \hat{X}} \hat{k}_j + \hat{k}_j e^{i\Delta\Phi \hat{X}} \right] | \Psi \rangle}{m \Delta\Phi}. \tag{45}$$

Equations (2) and (45) appear to be identical, however they are distinct, with different physical meanings. We first expand in $\Delta\Phi$ resulting in

$$\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0} = \frac{N}{m} + i \sum_{j=1}^{N} \frac{\langle \Psi | [\hat{k}_j, \hat{x}_j] | \Psi \rangle}{m}. \tag{46}$$

The second part of Eq. (46) is an average over single particle commutators. This average can be expressed in terms of the one body reduced density matrix as

$$i \sum_{j=1}^{N} \frac{\langle \Psi | [\hat{k}_j, \hat{x}_j] | \Psi \rangle}{m} = \frac{iN}{m} \mathrm{Tr} \hat{\rho}_1 [\hat{k}, \hat{x}]. \tag{47}$$

The one-body reduced density matrix can be diagonalized resulting in

$$\rho_1(x; x') = \sum_j R_j^{(1)} f_j(x) f_j(x'), \tag{48}$$

where $f_j(x)$ are the natural orbitals of the many-body system,

$$\sum_j R_j^{(1)} = 1, \tag{49}$$

and $R_j^{(1)} \geq 0$ for all j. In order to evaluate Eq. (47) we first consider the action of the commutator on a single orbital. In general it will hold that

$$\langle f_j | [\hat{k}, \hat{x}] | f_j \rangle = i, \tag{50}$$

except if $f_j(x)$ is an eigenstate of either the momentum or the position. [22] In particular for the zero momentum state

$$f_j(x) = \frac{1}{\sqrt{V}}, \tag{51}$$

it holds that

$$\langle f_j | [\hat{k}, \hat{x}] | f_j \rangle = 0. \tag{52}$$

Such eigenstates of the reduced density matrix will not contribute to the average in the second term in Eq. (46) so

$$\left[\frac{\partial^2 E(\Phi)}{\partial\Phi^2}\right]_{\Phi=0} = \frac{N}{m}\left(1 - \sum_j{}' R_j\right) = \frac{N_0}{m}, \tag{53}$$

where the prime indicates that the summation is over states which are not zero momentum states. $N_0 \leq N$ can be associated with the number of particles in zero momentum states. In principle it can also occur that an eigenstate of the reduced density matrix is also an eigenstate of the momentum, but with a finite eigenvalue. Such states will contribute to the non-classical rotational inertia, but not to ODLRO. In this sense Bose-Einstein condensation is distinct from superfluidity.

Clearly, the expression for the second derivative of the energy, when interpreted according to Eq. (45), is proportional to the number of single particles in a zero momentum state, in other words the Bose-Einstein condensate, therefore we can interpret the second derivative in this case as the rotational inertia of the superfluid component of a rotating sample ($I^{(s)}$ Eq. (16)). Also, the casting of Eq. (2) in terms of the one-body reduced density matrix establishes the connection between non-classical rotational inertia of a superfluid and off-diagonal long range order, solving a long-standing open problem [11].

8 Bose-Einstein Condensation of Pairs of Particles

One can also break up the total momentum operator into pairs of momenta, rather than only single momenta. We will use first quantization, as we have throughout the paper. Some details of the first quantized notation in the context of indistinguishable particles is given in the appendix.

In this case the current from which the transport susceptibility is derived is of the form $J_2(\Phi)$ (Eq. (29) with $p = 2$). The second derivative of the energy, when the current is taken to mean a sum over pairs, takes the form

$$\left[\frac{\partial^2 E(\Phi)}{\partial\Phi^2}\right]_{\Phi=0} = \frac{N}{m} + \sum_{j=1}^{\frac{N}{2}} \lim_{\Delta\Phi\to 0} \frac{\langle\Psi|\left[e^{-i\Delta\Phi\hat{X}}\hat{k}_j^{(2)} + \hat{k}_j^{(2)}e^{i\Delta\Phi\hat{X}}\right]|\Psi\rangle}{m\Delta\Phi}, \tag{54}$$

where

$$\hat{k}_j^{(2)} = \hat{k}_j + \hat{k}_{j+\frac{N}{2}}. \tag{55}$$

Note that the indices on operators refer to arguments of the wavefunction on which $\hat{k}_j + \hat{k}_{j+\frac{N}{2}}$ operates. Taking the limit $\Delta\Phi \to 0$ leads to

$$\left[\frac{\partial^2 E(\Phi)}{\partial\Phi^2}\right]_{\Phi=0} = \frac{N}{m} + i\sum_{j=1}^{\frac{N}{2}} \frac{\langle\Psi|[\hat{k}_j^{(2)}, \hat{x}_j^{(2)}]|\Psi\rangle}{m}. \tag{56}$$

Due to the indistinguishability of the particles we can cast Eq. (56) in terms of the two-body reduced density matrix,

$$\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0} = \frac{N}{m} + \frac{iN}{2m}\mathrm{Tr}\{\hat{\rho}_2[\hat{k}^{(2)}, \hat{x}^{(2)}]\}. \quad (57)$$

As before we can diagonalize $\hat{\rho}_2$ as

$$\rho_2(x_1, x_2; x_1', x_2') = \sum_j R_j^{(2)} g_j(x_1, x_2) g_j(x_1', x_2'), \quad (58)$$

where

$$\sum_j R_j^{(2)} = 1, \quad (59)$$

with $R_j^{(2)} \geq 0$ for all j. In general it holds that

$$[\hat{k}^{(2)}, \hat{x}^{(2)}] g_j(x_1, x_2) = 2i g_j(x_1, x_2), \quad (60)$$

except for pair-orbitals $g_j(x_1, x_2)$ for which

$$\hat{k}^{(2)} g_j(x_1, x_2) = 0. \quad (61)$$

(This would be the case for BCS pairs, since there the momenta of opposite spin particles cancel.) Again, such pairing states will not contribute to the second derivative of the energy, since

$$\langle g_j | [\hat{k}^{(2)}, \hat{x}^{(2)}] | g_j \rangle = 0, \quad (62)$$

whereas for the rest we can use Eq. (60), resulting in

$$\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0} = \frac{N(1 - \sum_{j=1}' R_j^{(2)})}{m} = \frac{N_{0,p}}{m}. \quad (63)$$

$N_{0,p} \leq N$ can be interpreted as the number of electrons in paired states for which the total momentum is zero, such as Cooper pairs in the BCS theory.

9 A Comprehensive Theory of Transport

Based on the above one can define a generalized transport susceptibility as follows:

$$D_p = \frac{\pi}{V}\left[\frac{\partial J_p(\Phi)}{\partial \Phi}\right]_{\Phi=0} = \frac{\pi}{V}\left(\frac{N}{m} + \sum_{j=1}^{\frac{N}{p}} \lim_{\Delta\Phi \to 0} \frac{\langle \Psi | \left[e^{-i\Delta\Phi\hat{X}}\hat{k}_j^{(p)} + \hat{k}_j^{(p)} e^{i\Delta\Phi\hat{X}}\right] | \Psi \rangle}{m\Delta\Phi}\right), \quad (64)$$

where $\hat{k}_j^{(p)}$ indicates the sum of p distinct momenta. The quantity D_p can be used to distinguish insulators and different types of conductors. Due to the result of Yang [10], that if ODLRO is present in a reduced density matrix of order p, then all higher order density matrices will also exhibit ODLRO, it follows that if D_p is finite, then all D_r's will be finite if $r \geq p$. Hence, in principle, one has to find the smallest value p_m for which D_{p_m} is finite. If p_m is of microscopic magnitude ($p_m = 1$ for bosonic superfluids or perfect conductors, $p_m = 2$ for BCS superconductors) then the system can be classified as a superconductor. If p_m is on the order of the total number of particles in the system, then the system can be classified as a regular conductor. If all $D_p = 0$ then the system is an insulator.

We have defined a large number of D_p, which raises the question: which one is measured experimentally? Experiments detect the motion of particles, charges in conductors, so a finite D_p, for any value of p will be detected as conduction. To decide whether the current corresponds to a Bose-Einstein condensed state (bosonic superfluids, superconductors), information other than conduction is needed (for example Meissner effect, flux quantization, non-classical rotational inertia).

Another interesting aspect of the above results is the overall interpretation of conductivity which follows. Bose-Einstein condensates are independent particles in zero momentum states. Superconductors are pairs of particles in zero momentum states. Normal conduction in a correlated system is a large (thermodynamic) number of particles in zero momentum states. In a superconductor the applied field moves pairs of particles independently, whereas in a normal conductor, a large number of particles are moved together. This is consistent with the fact that a superconductor can sustain a persistent current for a very long time, as well as with Kohn's theory [1] of normal conductors. Kohn's statement is that insulation is a result of many-body localization, the wavefunction is a linear combination of states each of which includes large number of particles which are localized. An equivalent statement is: a conducting state is one in which a large number of particles are simultaneously delocalized [20].

One more aspect of the above needs to be mentioned. It turns out that D_1 is finite for a Fermi sea, since the wavefunction in this case consists of a Slater determinant of eigenstates of the single particle momentum operator (non-interacting system). If an interaction is turned on, however small (for example the case of a Landau Fermi liquid), then one expects that the wavefunction will not consist of a Slater determinant of eigenstates of the single momentum, and D_1 will, in general, not be finite. However the fact that D_1 is finite suggests that the Fermi sea exhibits properties similar to bosonic superfluids. It has recently been suggested by Hirsch [23, 24] that current in a superconductor is carried by free electrons.

The evaluation of a particular D_p consists of the following steps. First the reduced density matrix of order p is calculated, diagonalized, and its eigenstates obtained. Then, for each state it needs to be determined whether it is an eigenstate of the p-body momentum operator, $\hat{K}_p = \sum_{i=1}^{p} \hat{k}_i$. This operator when applied directly to the state will reduce to a sum of single body momenta, so it is essential to use the operator $\exp(i\Delta X\hat{K}_p)$ (which is a partial shift operator). If a particular eigenstate of the reduced density matrix is also an eigenstate of $\exp(i\Delta X\hat{K}_p)$, then it contributes to D_p, otherwise it does not.

On the technical side the main issue is the evaluation and subsequent diagonalization of the reduced density matrix. This already has a history, since it is an important step also in the study of natural orbitals [25], and more recently in the density matrix renormalization group method. [26] These statements are valid for the calculation of actual models, as well as variational theories. In the latter case the first step is the calculation of the reduced density matrix associated with the variational wavefunction.

10 Conclusion

In this paper the problem of transport susceptibilities was considered. It is well-known that the Drude weight, the Meissner weight, and the rotational inertia of a rotating superfluid all have the same mathematical expressions apart from constants factors. This problem was thought to have been solved by Scalapino, White, and Zhang, based on observing an ambiguity in the definition of the derivative of the ground state energy, namely, that the derivative could refer to the adiabatic or the envelope derivatives. This classification is not applicable in one dimension, is cumbersome to apply consistently in a variational setting, and only divides the transport susceptibilities into two categories (conductor and superfluid).

In this paper, it was shown that a more fruitful approach to the problem is to start with the Berry phase expression for the current, and distinguish between currents in which the charge carriers conduct individually, in pairs, or in larger (thermodynamically large) clusters. A particular current and the susceptibility derived from it can be cast in terms of a reduced density matrix of the corresponding order (order one for the individually conducting case, order two for paired systems, etc.), and its value will be sensitive to off-diagonal long range order in the reduced density matrix of the given order. Thus the susceptibility for the case of conduction by thermodynamically large clusters corresponds to the Drude weight, for the paired case to the Meissner weight. For the case of individual particles the non-classical rotational inertia results.

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A Anti-Symmetry and First Quantization

In Eq. (55) a two-body operator is defined in first quantization whose expectation value is subsequently evaluated over a many-body wavefunction of indistinguishable particles. In this appendix a brief discussion of first-quantized operators in the context of indistinguishable particles is presented, for a more complete discussion the reader may consult Ref. [27].

The indices in Eq. (55) refer to the positions of arguments in the wavefunction. To give an example, let us consider a three-particle system of spinless fermions in the state

$$|\Psi(k_1,k_2,k_3)\rangle = \frac{1}{\sqrt{3!}}\left(|k_1,k_2,k_3\rangle - |k_1,k_3,k_2\rangle - |k_2,k_1,k_3\rangle + |k_2,k_3,k_1\rangle + |k_3,k_1,k_2\rangle - |k_3,k_2,k_1\rangle\right). \tag{65}$$

$\Psi(k_1,k_2,k_3)$ is an antisymmetric wavefunction, hence it is a valid wavefunction for three identical fermions.

One can define an operator

$$\hat{k}^{(2)} = \hat{k}_1 + \hat{k}_2, \tag{66}$$

which when it acts on one of the (not antisymmetric) components of Ψ results in the sum of the values of the momenta in the first and second arguments, for example,

$$\hat{k}^{(2)}|k_3,k_2,k_1\rangle = (k_3+k_2)|k_3,k_2,k_1\rangle \tag{67}$$

or

$$\hat{k}^{(2)}|k_1,k_3,k_2\rangle = (k_1+k_3)|k_3,k_2,k_1\rangle. \tag{68}$$

Using this one can easily show that

$$\langle\Psi|\hat{k}^{(2)}|\Psi\rangle = 2\overline{k}, \tag{69}$$

where

$$\overline{k} = \frac{k_1+k_1+k_3}{3}, \tag{70}$$

in other words the average momentum.

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