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## Spin stiffness in the Hubbard model

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**Abstract.** The spin stiffness  $\rho_s$  of the repulsive Hubbard model that occurs in the hydrodynamic theory of antiferromagnetic spin waves is shown to be the same as the thermodynamically defined stiffness involved in twisting the order parameter. New expressions for  $\rho_s$  are derived, which facilitate the interpretation, and connections with superconducting weight and gauge invariance are discussed.

### 1. Introduction

When a continuous symmetry is broken a Goldstone mode appears, which has to be considered as a slow variable and which necessitates an extension of the hydrodynamic equations [1]. The most famous example of this phenomenon is the case of superfluidity, where the Goldstone mode leads to second sound. The second-sound velocity is governed by the superfluid density  $\rho_s$ , which is a measure of the stiffness of the superfluid order parameter against spatial variations. This situation has a perfect analogy in antiferromagnetic ordering, where the Goldstone mode is a spin wave and  $\rho_s$  a spin stiffness. A third member in this family is superconductivity, where  $\rho_s$  may be viewed as the density of superconducting carriers. In the last example, one can relate  $\rho_s$  also to the response to an electromagnetic field: it is inversely proportional to the square of the London penetration depth in the Meissner effect [2].

In this paper, we analyse the antiferromagnetic ordering and the associated spin waves in the context of the Hubbard model. However, our considerations are applicable to a larger class of quantum lattice models; the Hubbard model merely serves as an example and an opportunity to give explicit formulae. The purpose of reconsidering this well known theory is that it enables us to establish, on a microscopic basis, the general connection between spin-wave velocity and the stiffness  $\rho_s$  [3]. In doing so, we find new expressions for  $\rho_s$  which reveal more clearly the nature of  $\rho_s$  than does the rather formal definition in terms of a twist in the order parameter [4]. By using the Hubbard model as an example we can easily make the connection with the superconducting language, by means of a transformation between repulsive and attractive Hubbard models. This gives us the opportunity to clarify some misunderstanding in the literature concerning gauge invariance. In general, the spirit of the paper is an articulation for the Hubbard model of the analysis by Forster [1] of the connection between broken symmetry, correlation functions and hydrodynamics.

We have organized the paper as follows: we start with a brief discussion of the tools needed for the analysis. Then we show how  $\rho_s$  enters in the (hydrodynamic) equations for the spin waves. In section 4, we work out the (thermodynamic) definition of  $\rho_s$  in terms of a twist in the order parameter and subsequently we demonstrate in section 5 that the

hydrodynamic  $\rho_s$  is indeed the spin stiffness. In section 6, we draw the analogy with  $\rho_s$  as the response function between the current and the inducing gauge field as it appears in the theory of superconductivity. In section 7, we comment on formal manipulations with the expression for  $\rho_s$  and derive new expressions which are more transparent. We close with a brief discussion.

## 2. Preliminaries

### 2.1. The Hubbard model

The Hubbard model is represented by the Hamiltonian [5]

$$\mathcal{H}_h = -t \sum_{j,\delta,\sigma} c_{j+\delta,\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (2.1)$$

where  $c_{j\sigma}^{(\dagger)}$  are electron annihilation (creation) operators for site  $j$  with spin  $\sigma$  ( $\sigma = \uparrow, \downarrow$  corresponds to  $+1, -1$ , respectively, if it does not occur as an index). Neighbouring sites of site  $j$  are denoted by  $j + \delta$ . We consider a bipartite lattice, such that hops from site  $j$  to site  $j + \delta$  are always from one sublattice to the other.  $t$  is the exchange or hopping integral,  $U$  is the on-site interaction between electrons of opposite spin, and  $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$  is the occupation number operator.

$\mathcal{H}_h$  has a rich set of symmetries. For our purpose it suffices to mention the magnetic symmetry:

$$[\mathcal{H}_h, M] = 0 \quad (2.2)$$

where  $M$  is the total magnetization operator:

$$M = \sum_j s_j \quad (2.3)$$

with  $s_j$  the local magnetization operator:

$$s_j = \frac{1}{2} \sum_{\sigma,\sigma'} c_{j\sigma}^\dagger \sigma_{\sigma\sigma'} c_{j\sigma'} \quad (2.4)$$

and with  $\sigma$  the set of the three Pauli matrices.

### 2.2. Averages and operator inner products

Averages are based on a (grand) canonical ensemble described by a Hamiltonian  $\mathcal{H}$ . The partition function gives the free energy  $F$  according to

$$F = -\frac{1}{\beta} \ln \text{tr} e^{-\beta\mathcal{H}} \quad (2.5)$$

where  $\beta = 1/k_B T$ . Averages are taken with respect to the canonical weight:

$$\langle \mathcal{A} \rangle = e^{\beta F} \text{tr} e^{-\beta\mathcal{H}} \mathcal{A}. \quad (2.6)$$

We will need an inner product in operator space, for which we take [6, 1]

$$\langle \mathcal{A}, \mathcal{B} \rangle = \frac{1}{\beta} \int_0^\beta d\lambda \{ \langle \mathcal{A}^\dagger e^{-\lambda\mathcal{H}} \mathcal{B} e^{\lambda\mathcal{H}} \rangle - \langle \mathcal{A}^\dagger \rangle \langle \mathcal{B} \rangle \}. \quad (2.7)$$

In addition to having all the properties of an inner product this definition has a few more desirable aspects. If the Hamiltonian  $\mathcal{H}$  is perturbed by adding the operator  $\delta\mathcal{H}$ , the linear response of an operator  $\mathcal{J}$  is given by

$$\delta \langle \mathcal{J} \rangle \equiv \langle \mathcal{J} \rangle_{\mathcal{H}+\delta\mathcal{H}} - \langle \mathcal{J} \rangle = -\beta \langle \delta\mathcal{H}^\dagger, \mathcal{J} \rangle. \quad (2.8)$$

The change in the free energy is, to second order in  $\delta\mathcal{H}$ ,

$$\delta F = \langle \delta\mathcal{H} \rangle - \frac{\beta}{2} \langle \delta\mathcal{H}^\dagger, \delta\mathcal{H} \rangle. \quad (2.9)$$

The last two equations are derived in the appendix.

Another property of the inner product that we will use concerns the Heisenberg operators:

$$\mathcal{A}(t) = e^{i\tau\mathcal{H}/\hbar} \mathcal{A} e^{-i\tau\mathcal{H}/\hbar} \quad (2.10)$$

and their time derivatives

$$\dot{\mathcal{A}}(t) = \frac{i}{\hbar} [\mathcal{H}, \mathcal{A}(t)]. \quad (2.11)$$

Using the invariance of the trace under cyclic permutation of the operators one easily proves the relation

$$\langle \mathcal{B}, \dot{\mathcal{A}}(t) \rangle = \frac{i}{\beta\hbar} \langle [\mathcal{B}^\dagger, \mathcal{A}(t)] \rangle. \quad (2.12)$$

### 2.3. Hydrodynamic equations

Linear hydrodynamic equations are obtained by first identifying the set of hydrodynamic variables  $\mathcal{A}_j$  [1]. They span a hydrodynamic subspace (using the operator inner product defined above). Projection on the hydrodynamic subspace is achieved by the projection operators:

$$\mathbb{P}\mathcal{O} = \sum_{j,m} \mathcal{A}_j P_{jm} (\mathcal{A}_m, \mathcal{O}) \quad (2.13)$$

where the matrix  $P$  is the inverse of the matrix of susceptibilities  $(\mathcal{A}_i, \mathcal{A}_j)$ :

$$\sum_m P_{jm} (\mathcal{A}_m, \mathcal{A}_k) = \delta_{jk} \quad (2.14)$$

where all indices run through the hydrodynamic subspace.

The dissipation-free hydrodynamic equations result from the projections on the hydrodynamic subspace of the time derivatives:

$$\mathbb{P}\dot{\mathcal{A}}_\ell = \sum_j \mathcal{A}_j \Omega_{j\ell} \quad (2.15)$$

with  $\Omega_{j\ell}$  given by

$$\Omega_{j\ell} = \sum_m P_{jm} (\mathcal{A}_m, \dot{\mathcal{A}}_\ell). \quad (2.16)$$

The hydrodynamic equations then read

$$\frac{d}{dt} \langle \mathcal{A}_\ell(t) \rangle = \sum_j \langle \mathcal{A}_j(t) \rangle \Omega_{j\ell}. \quad (2.17)$$

### 3. Spin stiffness and hydrodynamic spin waves

The slow or hydrodynamic modes derive from the conserved quantities and the Goldstone modes of a broken symmetry [1]. Since the total magnetization is conserved, the Fourier components

$$\mathbf{M}(\mathbf{k}) = \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \mathbf{s}_j \quad (3.1)$$

are slow modes for small  $\mathbf{k}$ . The symmetry breaking that we consider is antiferromagnetic ordering, which occurs in the Hubbard model at low temperatures near half-filling. The staggered magnetization

$$\mathbf{N} = \sum_j (-1)^j \mathbf{s}_j \quad (3.2)$$

then acquires a non-zero average.  $(-1)^j$  equals  $+1$  on one sublattice and  $-1$  on the other sublattice.  $\mathbf{N}$  can be seen as a Fourier component  $\mathbf{M}(\mathbf{Q})$ , where the wavevector  $\mathbf{Q}$  has the property

$$e^{i\mathbf{Q}\cdot\mathbf{r}_j} = (-1)^j. \quad (3.3)$$

The Fourier components  $\mathbf{N}(\mathbf{k}) = \mathbf{M}(\mathbf{k} + \mathbf{Q})$  are the slow modes for small  $\mathbf{k}$  associated with the antiferromagnetic symmetry breaking. We assume that the system orders antiferromagnetically in the  $x$ -direction, i.e.

$$\langle N^x \rangle = M_{\text{st}} \neq 0. \quad (3.4)$$

The spin waves arise from an interplay of the small- $\mathbf{k}$  components of  $\mathbf{M}(\mathbf{k})$  and  $\mathbf{N}(\mathbf{k})$ . Which components play a role can be seen from the general commutation relation

$$[M^\alpha(\mathbf{k}), M^\beta(\mathbf{k}')] = i M^\gamma(\mathbf{k} + \mathbf{k}') \quad (3.5)$$

with  $\alpha, \beta, \gamma$  a cyclic permutation of  $x, y, z$ . Taking  $\gamma = x$ , we see that a non-zero average of  $N^x$  couples  $M^z(\mathbf{k})$  to  $N^y(\mathbf{k})$  and  $M^y(\mathbf{k})$  to  $N^z(\mathbf{k})$ . The two pairs are equivalent and we focus on the first couple. In principle, one should write down the hydrodynamic equations in the combined six-dimensional space of  $\mathbf{M}(\mathbf{k})$  and  $\mathbf{N}(\mathbf{k})$ , but symmetry considerations permit us to restrict the equations to the  $2 \times 2$  subspace of  $M^z(\mathbf{k})$  and  $N^y(\mathbf{k})$ . So we obtain equations of the form [1, 7]

$$\frac{\partial \langle M^z(\mathbf{k}, t) \rangle}{\partial t} = \langle M^z(\mathbf{k}, t) \rangle \Omega_{zz} + \langle N^y(\mathbf{k}, t) \rangle \Omega_{yz} \quad (3.6)$$

$$\frac{\partial \langle N^y(\mathbf{k}, t) \rangle}{\partial t} = \langle M^z(\mathbf{k}, t) \rangle \Omega_{zy} + \langle N^y(\mathbf{k}, t) \rangle \Omega_{yy}. \quad (3.7)$$

The  $\Omega_{j\ell}$  are calculated using (2.16). The entry  $(\mathcal{A}_m, \dot{\mathcal{A}}_\ell)$  is simple, as it can be calculated with (2.12) and (3.5):

$$(M^z(\mathbf{k}), \dot{M}^z(\mathbf{k})) = 0 \quad (M^z(\mathbf{k}), \dot{N}^y(\mathbf{k})) = M_{\text{st}}/\beta\hbar \quad (3.8)$$

$$(N^y(\mathbf{k}), \dot{M}^z(\mathbf{k})) = -M_{\text{st}}/\beta\hbar \quad (N^y(\mathbf{k}), \dot{N}^y(\mathbf{k})) = 0. \quad (3.9)$$

The matrix elements  $P_{jm}$  are obtained from the inverse of  $(\mathcal{A}_m, \mathcal{A}_k)$ , which in turn is interpreted as the response to a perturbation as in (2.8). So we consider first a perturbation

$$\delta\mathcal{H} = -\xi M^z(\mathbf{k}) \quad (3.10)$$

with a small amplitude  $\xi$ . It will induce

$$\delta \langle M^z(\mathbf{k}) \rangle = \beta\xi (M^z(\mathbf{k}), M^z(\mathbf{k})) = N_{\chi\perp}(\mathbf{k})\xi \quad (3.11)$$

where  $N$  is the number of sites. In the second equality we introduce a susceptibility  $\chi_{\perp}$ , where the subscript is a reminder that it concerns a susceptibility perpendicular to the order parameter direction. We may drop the  $\mathbf{k}$ -dependence since we are interested in small  $\mathbf{k}$  and  $\chi_{\perp}(\mathbf{k})$  is expected to be regular for small  $\mathbf{k}$ .

For symmetry reasons the perturbation (3.10) will give no effect  $\delta\langle N^y(\mathbf{k}) \rangle$ . So,

$$\langle M^z(\mathbf{k}), N^y(\mathbf{k}) \rangle = \langle N^y(\mathbf{k}), M^z(\mathbf{k}) \rangle^* = 0. \quad (3.12)$$

The perturbation,

$$\delta\mathcal{H} = -\xi N^y(\mathbf{k}) \quad (3.13)$$

requires a different treatment. It tends to turn the spontaneous order over from the  $x$ -direction to the  $y$ -direction. For small  $\mathbf{k}$  the response will diverge and we will determine the singular behaviour in section 5. For the moment, we use the result

$$\langle N^y(\mathbf{k}), N^y(\mathbf{k}) \rangle = \frac{M_{\text{st}}^2}{\beta N \rho_s k^2} (1 + \mathcal{O}(k)) \quad \mathbf{k} \rightarrow 0. \quad (3.14)$$

One can see (3.14) as the *hydrodynamic* definition of the spin stiffness  $\rho_s$ .

Now all the ingredients for  $\Omega_{j\ell}$  are present and we find

$$\Omega_{zz} = 0 \quad \Omega_{zy} = \frac{M_{\text{st}}}{\hbar N \chi_{\perp}} \quad (3.15)$$

$$\Omega_{yz} = -\frac{N \rho_s k^2}{M_{\text{st}} \hbar} \quad \Omega_{yy} = 0. \quad (3.16)$$

The hydrodynamic equations (3.6) and (3.7) have a solution

$$\langle M^z(\mathbf{k}, t) \rangle = \langle M^z(\mathbf{k}, 0) \rangle e^{\pm i c k t} \quad \langle N^y(\mathbf{k}, t) \rangle = \langle N^y(\mathbf{k}, 0) \rangle e^{\pm i c k t} \quad (3.17)$$

with the spin-wave velocity  $c$  given by

$$c = \frac{1}{\hbar} \sqrt{\frac{\rho_s}{\chi_{\perp}}} \quad (3.18)$$

which is a relation due to Halperin and Hohenberg [3].

#### 4. The spin stiffness and twisted order parameter

The more fundamental definition of the spin stiffness  $\rho_s$  relates it to the increase in the free energy due to imposing a twist in the boundary condition on the order parameter [4]. For example, one can have the order parameter point in the  $x$ -direction at one end of the system and in the  $y$ -direction at the other end. For a continuous symmetry the twist in the order parameter will spread itself equally over the system. So we imagine that the order parameter slowly rotates around the  $z$ -axis:

$$\langle s_j^x \rangle = m_{\text{st}} \cos((\mathbf{q} + \mathbf{Q}) \cdot \mathbf{r}_j) \quad \langle s_j^y \rangle = m_{\text{st}} \sin((\mathbf{q} + \mathbf{Q}) \cdot \mathbf{r}_j) \quad (4.1)$$

where  $\mathbf{q}$  is the pitch of the twist and  $m_{\text{st}} = M_{\text{st}}/N$ . The two equations (4.1) can be combined into

$$\langle s_j^{\pm} \rangle = m_{\text{st}} \exp(i(\mathbf{q} + \mathbf{Q}) \cdot \mathbf{r}_j) \quad (4.2)$$

with

$$s_j^{\pm} = s_j^x \pm i s_j^y = c_{j\uparrow}^{\dagger} c_{j\downarrow} \quad (4.3)$$

as the spin-raising operator. The condition (4.2) leads to an increment in the free energy which for small  $\mathbf{q}$  can be written as

$$F(\mathbf{q}) = F(0) + \frac{1}{2}N\rho_s q^2 + \dots \quad (4.4)$$

The term linear in  $\mathbf{q}$  is absent due to inversion symmetry. Formula (4.4) has to be considered as the *thermodynamic* definition of the spin stiffness  $\rho_s$  against a twist.

This formal definition does not lead to a simple calculational scheme since it involves the computation of the free energy of a spatially inhomogeneous system. We can, however, map the system with the condition (4.2) onto a different system with an easier constraint via a unitary transformation  $\mathcal{U}$  of the form

$$\mathcal{U} = e^{i\mathbf{q} \cdot \sum_j \mathbf{r}_j s_j^z}. \quad (4.5)$$

$\mathcal{U}$  transforms  $\mathcal{H}$  and the density matrix  $\rho$  as

$$\mathcal{H}' = \mathcal{U} \mathcal{H} \mathcal{U}^\dagger \quad \rho' = \mathcal{U} \rho \mathcal{U}^\dagger \quad (4.6)$$

such that the partition function is invariant:

$$e^{-\beta F} = \text{tr} e^{-\beta \mathcal{H}} = \text{tr} e^{-\beta \mathcal{H}'}. \quad (4.7)$$

Averages in the transformed system (based on  $\rho'$ ) are denoted as  $\langle \dots \rangle'$  and are related to the original averages  $\langle \dots \rangle$  by

$$\langle \mathcal{A} \rangle' = \text{tr} \rho' \mathcal{A} = \text{tr} \mathcal{U} \rho \mathcal{U}^\dagger \mathcal{A} = \text{tr} \rho \mathcal{U}^\dagger \mathcal{A} \mathcal{U} = \langle \mathcal{A}' \rangle \quad (4.8)$$

with

$$\mathcal{A}' = \mathcal{U}^\dagger \mathcal{A} \mathcal{U}. \quad (4.9)$$

$\mathcal{U}$  locally rotates the spins around the  $z$ -axis over an angle  $\mathbf{q} \cdot \mathbf{r}_j$ . Using the properties of spin operators, we have

$$s_j^{z'} = \mathcal{U}^\dagger s_j^z \mathcal{U} = e^{-i\mathbf{q} \cdot \mathbf{r}_j} s_j^z \quad (4.10)$$

such that (4.2) changes into

$$\langle s_j^{z'} \rangle' = \langle s_j^z \rangle = m_{\text{st}} e^{i\mathbf{Q} \cdot \mathbf{r}_j} \quad (4.11)$$

which puts the staggered magnetization in the new system everywhere in the  $x$ -direction. Thus the constraint is simple and homogeneous at the expense of changing the Hamiltonian from  $\mathcal{H}$  to  $\mathcal{H}'$ . It is, however, easy to compute the new Hubbard Hamiltonian  $\mathcal{H}'_h$  by making use of the properties of the  $c_{j\sigma}$  under the transformation  $\mathcal{U}$ :

$$\mathcal{U} c_{j\sigma} \mathcal{U}^\dagger = e^{-i\mathbf{q} \cdot \mathbf{r}_j \sigma / 2} c_{j\sigma}. \quad (4.12)$$

Using (4.6),  $\mathcal{H}'_h$  is

$$\mathcal{H}'_h = -t \sum_{j,\delta,\sigma} e^{i\sigma \mathbf{q} \cdot \mathbf{r}_\delta / 2} c_{j+\delta,\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (4.13)$$

where  $\mathbf{r}_\delta = \mathbf{r}_{j+\delta} - \mathbf{r}_j$  is a vector connecting nearest neighbours. Note that the new Hamiltonian is again spatially homogeneous and of the Hubbard form with a complex hopping integral that depends on the pitch of the twist. So we must evaluate the free energy of  $\mathcal{H}'_h$  under the condition that the order parameter points in the  $x$ -direction. In, e.g., the mean-field approximation one can directly determine  $F(\mathbf{q})$  and then expand  $F(\mathbf{q})$  to obtain  $\rho_s$  [8]. Concrete calculations of  $\rho_s$  starting from the thermodynamic definition (using series expansions) can be found in [9] and [10] for the 2D Heisenberg antiferromagnet and Hubbard model, respectively.

In general we may evaluate  $F(\mathbf{q})$  by expanding  $\mathcal{H}'_h$  in powers of  $i\mathbf{q}$ :

$$\mathcal{H}'_h = \mathcal{H}_h + i\mathbf{q} \cdot \vec{\mathcal{H}}_1 + \frac{1}{2}i\mathbf{q} \cdot \vec{\mathcal{H}}_2 \cdot i\mathbf{q} + \dots \quad (4.14)$$

with

$$\vec{\mathcal{H}}_1 = -\frac{t}{2} \sum_{j,\delta,\sigma} \mathbf{r}_\delta \sigma c_{j+\delta,\sigma}^\dagger c_{j\sigma} = N \mathbf{J}_h^z \quad (4.15)$$

$$\vec{\mathcal{H}}_2 = -\frac{t}{4} \sum_{j,\delta,\sigma} \mathbf{r}_\delta \mathbf{r}_\delta c_{j+\delta,\sigma}^\dagger c_{j\sigma}. \quad (4.16)$$

We note that  $\vec{\mathcal{H}}_1$  is the current of the  $z$ -component of the spin and that  $\vec{\mathcal{H}}_2$  is (for cubic symmetry) a diagonal tensor with the kinetic energy on the diagonal. As  $\mathbf{q}$  is small, the free-energy increment due to  $\mathbf{q}$  can be calculated using perturbation theory with (2.9):

$$F(\mathbf{q}) - F(\mathbf{0}) = \frac{1}{2}i\mathbf{q} \cdot \left\{ \langle \vec{\mathcal{H}}_2 \rangle - \beta \left( \vec{\mathcal{H}}_1^\dagger, \vec{\mathcal{H}}_1 \right) \right\} \cdot i\mathbf{q}. \quad (4.17)$$

Here we use that  $\langle \vec{\mathcal{H}}_1 \rangle = 0$  (no current in the unperturbed state) and we note that  $\vec{\mathcal{H}}_1^\dagger = -\vec{\mathcal{H}}_1$ . So we obtain for  $\bar{\rho}_s$  the expression:

$$\bar{\rho}_s = -\frac{1}{N} \left\{ \langle \vec{\mathcal{H}}_2 \rangle^x + \beta \left( \vec{\mathcal{H}}_1, \vec{\mathcal{H}}_1 \right)^x \right\}. \quad (4.18)$$

For cubic symmetry  $\bar{\rho}_s$  reduces to  $\bar{\rho}_s = \rho_s \bar{I}$ . We stress, by using superscripts  $x$ , that in (4.18) the averages are with respect to an ensemble with the order parameter pointing in the  $x$ -direction (and with  $\mathcal{H}_h$  as the Hamiltonian).

## 5. Equivalence of the two definitions for spin stiffness

We now prove that the hydrodynamic definition (3.14) and the thermodynamic definition (4.4) are equivalent. We do this by considering the response to the perturbation:

$$\delta\mathcal{H} = -\sum_j (-1)^j \xi_j s_j^y \quad (5.1)$$

where the  $\xi_j$  are small and smoothly varying in space, e.g. of the form

$$\xi_j = \xi \cos(\mathbf{q} \cdot \mathbf{r}_j). \quad (5.2)$$

The perturbation is added to the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_h - \xi^x N^x \quad (5.3)$$

where we have introduced a small symmetry-breaking field  $\xi^x N^x$  to guarantee that the reference system has its order parameter pointing in the  $x$ -direction.

Because of the intrinsic stiffness of the system the response to the small perturbation (5.1) will be a local rotation of the spins around the  $z$ -axis over a small angle  $\varphi_j$ :

$$\langle s_j^x \rangle = (-1)^j m_{\text{st}} \cos \varphi_j \quad \langle s_j^y \rangle = (-1)^j m_{\text{st}} \sin \varphi_j \quad (5.4)$$

where  $\varphi_j$  is spatially smooth. The spatial variation (5.2) will induce a similar wave pattern for the  $\varphi_j$ :

$$\varphi_j = A \cos(\mathbf{q} \cdot \mathbf{r}_j) \quad (5.5)$$

with a small amplitude  $A$  proportional to  $\xi$ . Determining this proportionality is the main goal of this section, as it leads directly to the singular behaviour of the inner product (3.14). To see this we write  $\delta\mathcal{H}$  with (5.2) for the  $\xi_j$  as

$$\delta\mathcal{H} = -\frac{1}{2}\xi \left[ N^y(\mathbf{q}) + N^y(-\mathbf{q}) \right]. \quad (5.6)$$



The anticipated response (5.4) gives for the  $y$ -component of  $\mathbf{N}(\mathbf{q})$

$$\frac{1}{2}\langle N^y(\mathbf{q}) + N^y(-\mathbf{q}) \rangle = m_{\text{st}} \sum_j \cos(\mathbf{q} \cdot \mathbf{r}_j) \sin \varphi_j. \quad (5.7)$$

Inserting (5.5) and using the fact that the angles  $\varphi_j$  are small yields

$$\langle N^y(\mathbf{q}) + N^y(-\mathbf{q}) \rangle = 2m_{\text{st}}A \sum_j \cos^2(\mathbf{q} \cdot \mathbf{r}_j) = M_{\text{st}}A. \quad (5.8)$$

On the other hand, linear response theory (see (2.8)) gives

$$\langle N^y(\mathbf{q}) + N^y(-\mathbf{q}) \rangle = \frac{\beta\xi}{2} (N^y(\mathbf{q}) + N^y(-\mathbf{q}), N^y(\mathbf{q}) + N^y(-\mathbf{q})). \quad (5.9)$$

The modes  $\mathbf{q}$  and  $-\mathbf{q}$  have no overlap, so combining (5.8) and (5.9) leads to

$$M_{\text{st}}A = \beta\xi (N^y(\mathbf{q}), N^y(\mathbf{q})). \quad (5.10)$$

Thus the computation of  $A$  gives the inner product which must lead to the hydrodynamic definition of  $\rho_s$ , (3.14). We calculate the  $\varphi_j$  by first determining the increase in the free energy for a set of arbitrary  $\varphi_j$  and then optimize this free energy with respect to the  $\varphi_j$ ; this yields the  $\varphi_j$  resulting from the  $\xi_j$ . As in the previous section, we gauge away the  $\varphi_j$  via a unitary transformation:

$$\mathcal{U} = e^{i\sum_j \varphi_j s_j^z}. \quad (5.11)$$

The averages in the new system are

$$\langle s_j^x \rangle' = \langle \mathcal{U}^\dagger s_j^x \mathcal{U} \rangle = (-1)^j m_{\text{st}} \quad (5.12)$$

$$\langle s_j^y \rangle' = \langle \mathcal{U}^\dagger s_j^y \mathcal{U} \rangle = 0 \quad (5.13)$$

such that in the new system the order parameter points in the  $x$ -direction everywhere. This new constraint has to be combined with the transformed Hamiltonian:

$$\mathcal{H}' = \mathcal{U} \left( \mathcal{H}_h - \xi^x N^x - \sum_j \xi_j (-1)^j s_j^y \right) \mathcal{U}^\dagger. \quad (5.14)$$

We evaluate the free energy by perturbation theory. Therefore we decompose  $\mathcal{H}'$  into

$$\mathcal{H}' = \mathcal{H}_h + \mathcal{H}_a + \mathcal{H}_b \quad (5.15)$$

where  $\mathcal{H}_h$  is taken as the unperturbed Hamiltonian together with the constraints (5.12) and (5.13) on the order parameter. As in the previous section, such averages are denoted by  $\langle \dots \rangle^x$ . The other two parts in (5.15) are given by

$$\mathcal{H}_a = \mathcal{U} \mathcal{H}_h \mathcal{U}^\dagger - \mathcal{H}_h \quad (5.16)$$

$$\mathcal{H}_b = -\mathcal{U} \left[ \xi^x N^x + \sum_j \xi_j (-1)^j s_j^y \right] \mathcal{U}^\dagger. \quad (5.17)$$

These parts will be treated as perturbations on  $\mathcal{H}_h$ .  $\mathcal{H}_a$  can be expanded for small angles as

$$\mathcal{H}_a = i \sum_j \mathcal{H}_j \varphi_j - \frac{1}{2} \sum_{i,j} \varphi_i \mathcal{H}_{ij} \varphi_j + \dots \quad (5.18)$$

where it follows formally from (5.11) that

$$\mathcal{H}_j = [s_j^z, \mathcal{H}_h] \quad (5.19)$$

$$\mathcal{H}_{ij} = [s_i^z, [s_j^z, \mathcal{H}_h]]. \quad (5.20)$$

For the Hubbard Hamiltonian (cf. (4.13)) one can explicitly transform  $\mathcal{H}_h$ :

$$\mathcal{U} \mathcal{H}_h \mathcal{U}^\dagger = -t \sum_{j,\delta,\sigma} e^{i\sigma(\varphi_{j+\delta}-\varphi_j)/2} c_{j+\delta,\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (5.21)$$

which can then be expanded as in (5.18), yielding explicit expressions for  $\mathcal{H}_j$  and  $\mathcal{H}_{ij}$ . The free energy associated with  $\mathcal{H}_a$  can be written as

$$\delta F_a = \frac{1}{2} \sum_{i,j} \varphi_i K_{ij} \varphi_j \quad (5.22)$$

with

$$K_{ij} = -(\mathcal{H}_{ij})^x - \beta (\mathcal{H}_i, \mathcal{H}_j)^x. \quad (5.23)$$

This part of the free-energy increase can be directly related to  $\bar{\rho}_s$  as defined in the previous section.  $K_{ij}$  is translationally invariant, i.e., a function of  $\mathbf{r}_i - \mathbf{r}_j$ . Moreover, we have

$$K_{ij} = K_{ji} \quad \sum_j K_{ij} = 0 \quad (5.24)$$

as a constant rotation angle  $\varphi_j$  will not lead to an increase in the free energy.

Angles with a uniform gradient

$$\varphi_j = \mathbf{q} \cdot \mathbf{r}_j \quad (5.25)$$

have been discussed in the previous section and lead to  $\bar{\rho}_s$ . So

$$\sum_{i,j} (\mathbf{q} \cdot \mathbf{r}_i) K_{ij} (\mathbf{q} \cdot \mathbf{r}_j) = N \mathbf{q} \cdot \bar{\rho}_s \cdot \mathbf{q}. \quad (5.26)$$

We will need the Fourier transform of  $K_{ij}$ , which can be evaluated with (5.24) and (5.26) as

$$\sum_{i,j} K_{ij} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} = N \mathbf{q} \cdot \bar{\rho}_s \cdot \mathbf{q} \quad \mathbf{q} \rightarrow 0. \quad (5.27)$$

The part  $\mathcal{H}_b$  is found as

$$\mathcal{H}_b = - \sum_j (-1)^j \left\{ [\xi^x \cos \varphi_j + \xi_j \sin \varphi_j] s_j^x + [-\xi^x \sin \varphi_j + \xi_j \cos \varphi_j] s_j^y \right\} \quad (5.28)$$

and yields

$$\delta F_b = \langle \mathcal{H}_b \rangle^x = -m_{\text{st}} \sum_j (\xi^x \cos \varphi_j + \xi_j \sin \varphi_j). \quad (5.29)$$

Thus the total increase in free energy is

$$\delta F = \delta F_a + \delta F_b = \frac{1}{2} \sum_{i,j} \varphi_i K_{ij} \varphi_j - m_{\text{st}} \sum_j (\xi^x \cos \varphi_j + \xi_j \sin \varphi_j). \quad (5.30)$$

Now the  $\varphi_j$  follow from the stationarity of  $\delta F$ , which leads (for small  $\varphi_j$ ) to the linear equations

$$\sum_i K_{ji} \varphi_i + m_{\text{st}} \xi^x \varphi_j = \xi_j m_{\text{st}}. \quad (5.31)$$

Due to the translational invariance of  $K_{ij}$  one finds that (5.2) and (5.5) do indeed form a solution with  $A$  and  $\xi$  related by

$$(K(\mathbf{q}) + m_{\text{st}} \xi^x) A = m_{\text{st}} \xi \quad (5.32)$$

where  $K(\mathbf{q})$  follows from (5.27):

$$K(\mathbf{q}) = \mathbf{q} \cdot \bar{\rho}_s \cdot \mathbf{q} \quad \mathbf{q} \rightarrow 0. \quad (5.33)$$

Now we can safely let  $\xi^x \rightarrow 0$  and one sees that (5.10), (5.32) and (5.33) lead to

$$(N^y(\mathbf{q}), N^y(\mathbf{q})) = \frac{M_{\text{st}}^2}{\beta N \mathbf{q} \cdot \bar{\rho}_s \cdot \mathbf{q}} \quad \mathbf{q} \rightarrow 0 \quad (5.34)$$

which is a slight generalization of (3.14) to systems with a symmetry lower than the cubic symmetry. Since the same  $\bar{\rho}_s$  as in the previous section does indeed appear, we have demonstrated the equivalence of the thermodynamic and hydrodynamic definitions of the spin stiffness.

## 6. The response to a gauge field

A third aspect of  $\rho_s$ , which is unusual in the context of antiferromagnetic order, is its role in the response to a gauge field. This role is familiar in superconductivity, where the presence of  $\rho_s$  leads to special electromagnetic behaviour in a symmetry-broken state: the Meissner effect. In a lattice system the electromagnetic field is introduced by the so-called Peierls substitution [11]. It amounts to the replacement

$$c_{j\sigma} \rightarrow c_{j\sigma} \exp \left[ -ie \int_0^{r_j} d\mathbf{r} \cdot \mathbf{A}(\mathbf{r})/\hbar \right] \quad (6.1)$$

where  $e$  is the electric charge and  $\mathbf{A}(\mathbf{r})$  the vector potential. Executing this replacement in the Hubbard Hamiltonian changes it into

$$\mathcal{H}_A = -t \sum_{j,\delta,\sigma} c_{j+\delta,\sigma}^\dagger c_{j\sigma} e^{ie\mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta/\hbar} + U \sum_j n_{j\uparrow} n_{j\downarrow}. \quad (6.2)$$

We have introduced the abbreviation

$$\int_{r_j}^{r_{j+\delta}} d\mathbf{r} \cdot \mathbf{A}(\mathbf{r}) = \mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta \quad (6.3)$$

such that in the lattice version the vector potential  $\mathbf{A}_{j+\delta/2}$  is associated with the link between the sites  $j$  and  $j + \delta$ . By introducing the vector potential in this way one has to change the expression for the electric current concomitantly. The current  $\mathbf{J}_{j+\delta/2}$  is also associated with the link  $[j, j + \delta]$  and it should obey the lattice version of charge conservation

$$\frac{\partial \rho_j}{\partial t} + \sum_\delta \mathbf{J}_{j+\delta/2} \cdot \mathbf{r}_\delta = 0 \quad (6.4)$$

with the charge density given by

$$\rho_j = e \sum_\sigma n_{j\sigma}. \quad (6.5)$$

Using the equation of motion for  $\rho_j$  one finds

$$\mathbf{J}_{j+\delta/2} = \frac{iet}{\hbar} \mathbf{r}_\delta \sum_\sigma \left\{ c_{j+\delta,\sigma}^\dagger c_{j\sigma} e^{ie\mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta/\hbar} - c_{j\sigma}^\dagger c_{j+\delta,\sigma} e^{-ie\mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta/\hbar} \right\}. \quad (6.6)$$

When the system becomes superconducting the electric current  $\mathbf{J}$  becomes proportional to  $\mathbf{A}$  (the London equation):

$$\mathbf{J} = - \left( \frac{n_s e^2}{m} \right) \mathbf{A} \quad (6.7)$$

where  $n_s$  is the density of the superconducting carriers and  $m$  is their mass. Superconductivity occurs in the negative- $U$  Hubbard model and it is the counterpart of

the antiferromagnetism in the positive- $U$  Hubbard model that we have been considering so far. The two can be related to each other by the transformation (see, e.g., [8])

$$c'_{j\uparrow} = c_{j\uparrow} \quad c'_{j\downarrow} = (-1)^j c_{j\downarrow}^\dagger. \quad (6.8)$$

The transformation (6.8) transforms the charge density

$$\rho'_j = e \sum_{\sigma} n'_{j\sigma} = e \sum_{\sigma} \sigma n_{j\sigma} = 2e s_j^z \quad (6.9)$$

into the  $z$ -component of the magnetization. The Hamiltonian  $\mathcal{H}_A$  from (6.2) is transformed into

$$\mathcal{H}'_A = -t \sum_{j,\delta,\sigma} c_{j+\delta,\sigma}^\dagger c_{j\sigma} e^{ieA_{j+\delta/2} \cdot \mathbf{r}_\delta \sigma / \hbar} + U \sum_j n_{j\uparrow} n_{j\downarrow}. \quad (6.10)$$

Note the appearance of a factor  $\sigma$  in the phase factor. Comparing this expression with (5.21), we see that they are equivalent for

$$\mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta = (\varphi_{j+\delta} - \varphi_j) \frac{\hbar}{2e}. \quad (6.11)$$

The charge conservation law transforms into a conservation law for the  $z$ -component of the magnetization

$$\frac{\partial s_j^z}{\partial t} + \sum_{\delta} \mathbf{J}_{j+\delta/2}^z \cdot \mathbf{r}_\delta = 0 \quad (6.12)$$

with the current  $\mathbf{J}_{j+\delta/2}^z$  given by

$$\mathbf{J}_{j+\delta/2}^z = \frac{it}{2\hbar} \mathbf{r}_\delta \sum_{\sigma} \left\{ c_{j+\delta,\sigma}^\dagger c_{j\sigma} e^{ieA_{j+\delta/2} \cdot \mathbf{r}_\delta \sigma / \hbar} - c_{j\sigma}^\dagger c_{j+\delta,\sigma} e^{-ieA_{j+\delta/2} \cdot \mathbf{r}_\delta \sigma / \hbar} \right\}. \quad (6.13)$$

The equivalent of the London equation is the response of  $\mathbf{J}^z$  to  $\mathbf{A}$ . We have two contributions: one because  $\mathbf{J}^z$  depends on  $\mathbf{A}$  and one because the Hamiltonian (6.10) depends on  $\mathbf{A}$ . Expansion of  $\mathbf{J}^z$  gives:

$$\mathbf{J}_{j+\delta/2}^z = \mathbf{J}_{j+\delta/2}^0 + \frac{2e}{\hbar} \overline{\overline{\mathbf{J}}^1}_{j+\delta/2} \cdot \mathbf{A}_{j+\delta/2} + \dots \quad (6.14)$$

with

$$\mathbf{J}_{j+\delta/2}^0 = \frac{it}{2\hbar} \mathbf{r}_\delta \sum_{\sigma} \left( c_{j+\delta,\sigma}^\dagger c_{j\sigma} - c_{j\sigma}^\dagger c_{j+\delta,\sigma} \right) \sigma \quad (6.15)$$

$$\overline{\overline{\mathbf{J}}^1}_{j+\delta/2} = -\frac{t}{4\hbar} \mathbf{r}_\delta \mathbf{r}_\delta \sum_{\sigma} \left( c_{j+\delta,\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{j+\delta,\sigma} \right). \quad (6.16)$$

Secondly, we have a contribution which results from the expansion (6.10) for small  $\mathbf{A}$ :

$$\delta \mathcal{H}_A = -\frac{iet}{\hbar} \sum_{j,\delta,\sigma} c_{j+\delta,\sigma}^\dagger c_{j\sigma} \mathbf{r}_\delta \sigma \cdot \mathbf{A}_{j+\delta/2}. \quad (6.17)$$

We note that  $\vec{\mathcal{H}}_1$  and  $\overline{\overline{\mathcal{H}}}_2$  as found in (4.15) and (4.16) are related to  $\mathbf{J}^0$  and  $\overline{\overline{\mathbf{J}}^1}$  (note that the two terms in the sum over  $\sigma$  in (6.15) and (6.16) contribute equally):

$$\vec{\mathcal{H}}_1 = -\frac{\hbar}{2i} \sum_{j,\delta} \mathbf{J}_{j+\delta/2}^0 \quad (6.18)$$

$$\overline{\overline{\mathcal{H}}}_2 = \frac{\hbar}{2} \sum_{j,\delta} \overline{\overline{\mathbf{J}}^1}_{j+\delta/2}. \quad (6.19)$$

The London equation (6.7) only holds for sufficiently slowly varying  $\mathbf{A}_{j+\delta/2}$ , i.e. the spatial variations must be small over a coherence length. So we may take  $\mathbf{A}$  constant and we then also have

$$\delta\mathcal{H}_A = \frac{2ie}{\hbar} \vec{\mathcal{H}}_1 \cdot \mathbf{A}. \quad (6.20)$$

The total magnetization current is defined as

$$\mathbf{J}^z = \frac{1}{2N} \sum_{j,\delta} \mathbf{J}_{j+\delta/2}^z. \quad (6.21)$$

From linear response theory we obtain for homogeneous  $\mathbf{A}$  (cf. (2.8))

$$\langle \mathbf{J}^z \rangle_{\mathcal{H}+\delta\mathcal{H}} = \frac{1}{2N} \left\{ \sum_{j,\delta} \frac{2e}{\hbar} \langle \overline{\overline{\mathbf{J}}}_{j+\delta/2}^1 \rangle \cdot \mathbf{A} - \beta \left( \delta\mathcal{H}_A, \sum_{j,\delta} \mathbf{J}_{j+\delta/2}^0 \right) \right\} \quad (6.22)$$

that is,

$$\langle \mathbf{J}^z \rangle_{\mathcal{H}+\delta\mathcal{H}} = \frac{2e}{N\hbar^2} \left\{ \langle \overline{\overline{\mathcal{H}}}_2 \rangle + \beta \left( \vec{\mathcal{H}}_1, \vec{\mathcal{H}}_1 \right) \right\} \cdot \mathbf{A}. \quad (6.23)$$

Comparing this with the expression (4.18) for  $\overline{\overline{\rho}}_s$ , we may write

$$\langle \mathbf{J}^z \rangle_{\mathcal{H}+\delta\mathcal{H}} = -\frac{2e}{\hbar^2} \overline{\overline{\rho}}_s \cdot \mathbf{A}. \quad (6.24)$$

Therefore the same  $\overline{\overline{\rho}}_s$  as before does indeed appear and we see that the superconducting weight in the response to a gauge field is also equivalent to the spin stiffness associated with a twist in the order parameter. Very recently, a discussion of the effect of a spin-dependent gauge field, as used in this section, was given in [12] in the framework of Fermi liquid theory.

## 7. Alternative forms for $\rho_s$

In this section, we discuss some formal manipulations with the expression for  $\rho_s$ . These are included because they involve some subtleties due to the symmetry breaking. The manipulations lead to expressions which are more general or easier to interpret. The formula (4.18) for  $\rho_s$  together with the definitions (4.15) and (4.16) refer explicitly to the Hubbard model. We can obtain a more general expression by expanding  $\mathcal{U}$ , as given by (4.5), in powers of  $i\mathbf{q}$ :

$$\mathcal{U} = e^{i\mathbf{q} \cdot \vartheta^z} = 1 + i\mathbf{q} \cdot \vartheta^z + \dots \quad (7.1)$$

with  $\vartheta^z$  given by

$$\vartheta^z = \sum_j \mathbf{r}_j s_j^z. \quad (7.2)$$

Inserting (7.1) into the definition of  $\mathcal{H}'$  yields an expansion similar to (4.14) with

$$\vec{\mathcal{H}}_1 = [\vartheta^z, \mathcal{H}_h] \quad \overline{\overline{\mathcal{H}}}_2 = [\vartheta^z, [\vartheta^z, \mathcal{H}_h]]. \quad (7.3)$$

Using this in the expression (4.18) gives

$$\overline{\overline{\rho}}_s = -\frac{1}{N} \left\{ \langle [\vartheta^z, [\vartheta^z, \mathcal{H}_h]] \rangle^x + \beta \left( [\vartheta^z, \mathcal{H}_h], [\vartheta^z, \mathcal{H}_h] \right)^x \right\}. \quad (7.4)$$

This expression makes no reference to the Hubbard model and is therefore generally valid for lattice Hamiltonians. We have augmented the average and the inner product with a

superscript  $x$  to reflect the fact that the averages are taken in a system where the order parameter points in the  $x$ -direction. Such a warning signal is not superfluous as the following ‘derivation’ may show. Suppose that we use the relation

$$\dot{\vartheta}^z = \frac{i}{\hbar} [\mathcal{H}, \vartheta^z] \quad (7.5)$$

to write for the second term in (7.4)

$$([\vartheta^z, \mathcal{H}], [\vartheta^z, \mathcal{H}]) = -\frac{\hbar}{i} ([\vartheta^z, \mathcal{H}], \dot{\vartheta}^z) \quad (7.6)$$

and use the relation (2.12) to transform it into

$$([\vartheta^z, \mathcal{H}], [\vartheta^z, \mathcal{H}]) = -\frac{1}{\beta} \langle [\vartheta^z, [\vartheta^z, \mathcal{H}]] \rangle. \quad (7.7)$$

Then we would discover that the two contributions in (7.4) exactly compensate each other! The error in this reasoning is that we have ignored the fact that the averages have to be taken in a symmetry-broken state. However, relation (2.12) is based on a cyclic rotation of the operators in a trace, which is only permitted when the trace is taken over the whole Hilbert space.

We can elucidate this point further by implementing the constraint on the order parameter by including a symmetry-breaking term in the Hamiltonian as in (5.3). Then we would have for (7.5)

$$[\vartheta^z, \mathcal{H}_h] = [\vartheta^z, \mathcal{H}] + \xi^x [\vartheta^z, N^x] = -\frac{\hbar}{i} \dot{\vartheta}^z + i\xi^x \sum_j (-1)^j r_j s_j^y. \quad (7.8)$$

The extra term looks innocent, because  $\xi^x$  is vanishingly small, but it is not, as we shall see. Using (7.8) gives for the second term in (7.4)

$$([\vartheta^z, \mathcal{H}_h], [\vartheta^z, \mathcal{H}_h])^x = -\frac{1}{\beta} \langle [\vartheta^z, [\vartheta^z, \mathcal{H}_h]] \rangle^x + i\xi^x \left( [\vartheta^z, \mathcal{H}_h], \sum_j (-1)^j r_j s_j^y \right)^x. \quad (7.9)$$

Using (7.8) again in the first entry of the second term of (7.9), we obtain two contributions, one proportional to  $\xi^x$  and one to  $(\xi^x)^2$ . The former reads with the use of (2.12)

$$i\xi^x \frac{i}{\hbar} \left( \dot{\vartheta}^z, \sum_j (-1)^j r_j s_j^y \right)^x = \frac{\xi^x}{\beta \hbar^2} \left( \sum_j r_j r_j \right)_{m_{st}}. \quad (7.10)$$

The lattice sum can take arbitrarily large values and thus one cannot rely on the smallness of  $\xi^x$  to ignore its contribution. The term proportional to  $(\xi^x)^2$  is equally difficult to interpret.

We may, however, use these types of operation to give the expression for  $\rho_s$  in yet another form, and thereby bring this subtle point into focus. First, we relate the second part of (7.4) to a current–current inner product:

$$([\vartheta^z, \mathcal{H}_h], [\vartheta^z, \mathcal{H}_h])^x = \hbar^2 N^2 (\mathbf{J}_h^z, \mathbf{J}_h^z)^x \quad (7.11)$$

with  $\mathbf{J}_h^z$  defined in (4.15). Next, we use the identity,

$$[\vartheta^z, [\vartheta^z, \mathcal{H}_h]] = [\vartheta^x, [\vartheta^x, \mathcal{H}_h]] \quad (7.12)$$

which is a direct consequence of the magnetic isotropy and which is easily proven for the Hubbard model by direct evaluation. Now for the right-hand side of (7.12) we can apply the train of arguments (7.5)–(7.7) everywhere replacing  $z$  by  $x$ , since  $\vartheta^x$  commutes with the symmetry-breaking term. So (7.7) holds for the  $x$ -component. This permits us to write the expression for  $\rho_s$  in the form

$$\bar{\rho}_s = \beta \hbar^2 N \left\{ (\mathbf{J}_h^{\parallel}, \mathbf{J}_h^{\parallel}) - (\mathbf{J}_h^{\perp}, \mathbf{J}_h^{\perp}) \right\} \quad (7.13)$$

where we have used the coordinate-free notation: parallel and perpendicular are to be understood with respect to the orientation of the order parameter. This expression most clearly shows that  $\rho_s$  is induced by symmetry breaking: without symmetry breaking the distinction between parallel and perpendicular disappears and  $\rho_s$  vanishes. In a mean-field (or BCS) approximation one finds at  $T = 0$  only the parallel contribution. For increasing  $T$  a gradual compensation occurs between the two terms, which becomes complete at  $T = T_c$ .

Since (7.12) relies on the magnetic isotropy of the model, the expression (7.13) is no longer valid when the isotropy is broken by an external magnetic field in the  $z$ -direction. Then (7.4) still holds and also the Halperin–Hohenberg relation (3.18) remains valid. Of course both  $\rho_s$  and  $\chi_\perp$  are affected by the presence of such a magnetic field, as can, for example, be seen from a mean-field treatment of these quantities [8, 13].

As a final comment on this genre of expressions we discuss the Bogoliubov inequality which is sometimes used to make (3.14) plausible [1]. The general form reads

$$(\mathcal{A}, \mathcal{A})(\mathcal{B}, \mathcal{B}) \geq |(\mathcal{A}, \mathcal{B})|^2. \quad (7.14)$$

Take  $\mathcal{A} = N^y(\mathbf{k})$  and  $\mathcal{B} = \dot{M}^z(\mathbf{k})$  such that  $(\mathcal{A}, \mathcal{A})$  is the desired inner product. The right-hand side of (7.14) is then given by (3.9). One might think that  $(\mathcal{B}, \mathcal{B})$  is associated with the inner product  $(\mathbf{J}^z, \mathbf{J}^z)$ , since for small  $\mathbf{k}$  one has

$$\dot{M}^z(\mathbf{k}) \simeq \frac{\mathbf{k}}{\hbar} \cdot [\vartheta^z, \mathcal{H}] = iN\mathbf{k} \cdot \mathbf{J}^z. \quad (7.15)$$

This is not correct as a more precise analysis shows. First we use (2.12) to write

$$(\dot{M}^z(\mathbf{k}), \dot{M}^z(\mathbf{k})) = \frac{i}{\beta\hbar} \langle [\dot{M}^z(-\mathbf{k}), M^z(\mathbf{k})] \rangle. \quad (7.16)$$

Then we expand the first entry as in (7.15), but taking the symmetry-breaking term explicitly into account

$$\dot{M}^z(-\mathbf{k}) \simeq -\frac{\mathbf{k}}{\hbar} \cdot [\vartheta^z, \mathcal{H}_h] - \frac{\xi^x}{\hbar} (N^y(-\mathbf{k}) - N^y). \quad (7.17)$$

The small symmetry-breaking term gives

$$-\frac{i\xi^x}{\beta\hbar^2} \langle [N^y(-\mathbf{k}) - N^y, M^z(\mathbf{k})] \rangle = \frac{\xi^x M_{\text{st}}}{\beta\hbar^2}. \quad (7.18)$$

Then we obtain for small  $\mathbf{k}$  for (7.16)

$$(\dot{M}^z(\mathbf{k}), \dot{M}^z(\mathbf{k})) = \frac{1}{\beta\hbar^2} \{ -\mathbf{k} \cdot \langle [\vartheta^z, [\vartheta^z, \mathcal{H}_h]] \rangle \cdot \mathbf{k} + \xi^x M_{\text{st}} \}. \quad (7.19)$$

Substituting all of this in (7.14) we have

$$(N^y(\mathbf{k}), N^y(\mathbf{k})) \geq \frac{M_{\text{st}}^2}{\beta (-\mathbf{k} \cdot \langle [\vartheta^z, [\vartheta^z, \mathcal{H}_h]] \rangle \cdot \mathbf{k} + \xi^x M_{\text{st}})}. \quad (7.20)$$

This result should be compared to (5.34); substituting for  $\bar{\rho}_s$  the expression (4.18), with (7.3) for  $\vec{\mathcal{H}}_1$  and  $\vec{\mathcal{H}}_2$ , one sees that the Bogoliubov inequality above only involves the double commutator, or, equivalently, the inner product of parallel currents, and not the inner product of perpendicular currents. Note that (7.15) seems to suggest that the inner product of perpendicular currents would be involved. This is not the case and generally we are indeed faced with an *inequality* (the symmetry-breaking term is innocent in this respect).

## 8. Discussion

In the foregoing sections we have discussed the role of  $\rho_s$ :

- as a parameter in the hydrodynamic (spin-wave) equations;
- as the parameter determining the increase in the free energy due to long-wavelength variations in the phase of the order parameter;
- as the proportionality parameter between a perturbing gauge field and the induced current.

By explicit calculation we have shown that it is the same  $\rho_s$  entering in all these aspects. We have placed the discussion in the context of the Hubbard model which allows us to use more explicit expressions. As we have indicated, the expressions can easily be extended to more general lattice models.

In the case of magnetic isotropy we can write  $\rho_s$  as the difference of two current–current inner products containing the spin currents parallel and perpendicular to the order parameter. The Bogoliubov inequality only involves the parallel current. In the BCS approximation it becomes an equality only at  $T = 0$ .

A final comment that we want to make concerns the issue of gauge invariance. The London equation (6.7) can be extended to the frequency wavevector domain as

$$\langle \mathbf{J}(\mathbf{k}, \omega) \rangle = \overline{\overline{\chi}}(\mathbf{k}, \omega) \cdot \mathbf{A}(\mathbf{k}, \omega) \quad (8.1)$$

where  $\mathbf{A}(\mathbf{k}, \omega)$  is the double Fourier transform of  $\mathbf{A}(\mathbf{r}, t)$  with respect to space and time and  $\overline{\overline{\chi}}(\mathbf{k}, \omega)$  is a generalized susceptibility (which has the role  $\rho_s$  had before). The limit of slow variations in space and time is delicate [2]. In the limit of first  $\mathbf{k} \rightarrow 0$  and then  $\omega \rightarrow 0$  one has an electric response and  $\overline{\overline{\chi}}$  leads to the Drude weight. In the opposite order, first  $\omega \rightarrow 0$  and then  $\mathbf{k} \rightarrow 0$ , one has a magnetic response leading to a non-vanishing superconducting weight, which is considered here. Electromagnetic gauge invariance requires that a purely longitudinal  $\mathbf{A}(\mathbf{k}, \omega) = \mathbf{k}a(\mathbf{k}, \omega)$  has no response, since it can be gauged away. Thus

$$\overline{\overline{\chi}}(\mathbf{k}, \omega) \cdot \mathbf{k} = 0. \quad (8.2)$$

We have been considering a static response throughout, so we have taken the limit  $\omega \rightarrow 0$  first and we have not been concerned with the  $\mathbf{k}$ -dependence of the spin stiffness  $\overline{\overline{\rho}}_s$ . Thus the expressions given for  $\overline{\overline{\rho}}_s$  do not obey the condition (8.2). The origin of this paradox is not to be traced to shortcomings of, e.g., the BCS approximation, as is sometimes done with the idea that vertex corrections will restore gauge invariance [2]. The answer comes from the change in gauge invariance in the symmetry-broken state. In section 6, we saw that gauge fields are similar to imposed twists on the phase of the order parameter. The theory is required to be invariant under the combined gauge transformation

$$\mathbf{A}'_{j+\delta/2} \cdot \mathbf{r}_\delta = \mathbf{A}_{j+\delta/2} \cdot \mathbf{r}_\delta + \chi_{j+\delta} - \chi_j \quad (8.3)$$

$$\phi'_j = \phi_j + \frac{2e}{\hbar} \chi_j \quad (8.4)$$

where  $\phi_j$  is the phase of the order parameter and  $\chi_j$  an arbitrary function. Correspondingly the London equation (6.24) should be formulated in a gauge-invariant way as

$$\langle \mathbf{J} \rangle_{\mathcal{H}+\delta\mathcal{H}} = -\frac{2e}{\hbar^2} \overline{\overline{\rho}}_s \cdot \left( \mathbf{A} - \frac{\hbar}{2e} \nabla \phi \right). \quad (8.5)$$

Then the requirement of gauge invariance is automatically fulfilled and it imposes no further requirements on  $\overline{\overline{\rho}}_s$ .



## Appendix

In this appendix we derive expressions for the change in the average of an operator  $\mathcal{J}$  and the change in free energy upon perturbing the Hamiltonian  $\mathcal{H}$  by adding an operator  $\delta\mathcal{H}$ . These expressions, up to first and second order in  $\delta\mathcal{H}$ , respectively, are given in equations (2.8) and (2.9) in terms of the inner product defined by (2.7) and are repeated here:

$$\delta\langle\mathcal{J}\rangle \equiv \langle\mathcal{J}\rangle_{\mathcal{H}+\delta\mathcal{H}} - \langle\mathcal{J}\rangle = -\beta (\delta\mathcal{H}^\dagger, \mathcal{J}) \quad (\text{A.1})$$

$$\delta F \equiv -\frac{1}{\beta} [\ln \text{tr} e^{-\beta(\mathcal{H}+\delta\mathcal{H})} - \ln \text{tr} e^{-\beta\mathcal{H}}] = \langle\delta\mathcal{H}\rangle - \frac{\beta}{2} (\delta\mathcal{H}^\dagger, \delta\mathcal{H}). \quad (\text{A.2})$$

Unless explicitly indicated averages are taken with respect to the operator  $e^{-\beta\mathcal{H}}$  (see (2.6)).

The derivation of both equations proceeds by way of the operator identity

$$e^{-\beta(\mathcal{H}+\delta\mathcal{H})} = e^{-\beta\mathcal{H}} - \int_0^\beta d\lambda e^{-(\beta-\lambda)\mathcal{H}} \delta\mathcal{H} e^{-\lambda(\mathcal{H}+\delta\mathcal{H})} \quad (\text{A.3})$$

which is proven by noting that the left- and right-hand sides are equal for  $\beta = 0$  and have identical derivatives with respect to  $\beta$ .

Equation (A.1) is now derived by inserting (A.3) into

$$\langle\mathcal{J}\rangle_{\mathcal{H}+\delta\mathcal{H}} = \frac{\text{tr} e^{-\beta(\mathcal{H}+\delta\mathcal{H})} \mathcal{J}}{\text{tr} e^{-\beta(\mathcal{H}+\delta\mathcal{H})}} \quad (\text{A.4})$$

and then expanding to first order in  $\delta\mathcal{H}$  and using the following result (which is easily proved via cyclic permutation in the trace):

$$\int_0^\beta d\lambda \langle\delta\mathcal{H}(\lambda)\rangle \equiv \int_0^\beta d\lambda \langle e^{\lambda\mathcal{H}} \delta\mathcal{H} e^{-\lambda\mathcal{H}} \rangle = \beta\langle\delta\mathcal{H}\rangle. \quad (\text{A.5})$$

To derive (A.2), we start by iterating (A.3) once and expanding to second order in  $\delta\mathcal{H}$ :

$$\text{tr} e^{-\beta(\mathcal{H}+\delta\mathcal{H})} = \text{tr} e^{-\beta\mathcal{H}} \left( 1 - \int_0^\beta d\lambda \langle\delta\mathcal{H}(\lambda)\rangle + \int_0^\beta d\lambda \int_0^\lambda d\lambda' \langle\delta\mathcal{H}(\lambda) \delta\mathcal{H}(\lambda')\rangle + \dots \right). \quad (\text{A.6})$$

Before taking the logarithm in order to compute  $\delta F$  it is useful to prove the identity

$$\int_0^\beta d\lambda \int_0^\lambda d\lambda' \langle\delta\mathcal{H}(\lambda) \delta\mathcal{H}(\lambda')\rangle = \frac{\beta}{2} \int_0^\beta d\lambda \langle\delta\mathcal{H}(\lambda) \delta\mathcal{H}\rangle. \quad (\text{A.7})$$

The proof proceeds by a sequence of changes of variable in the integral, introducing the notation

$$f(\tau) = \langle\delta\mathcal{H}(\tau) \delta\mathcal{H}\rangle \quad (\text{A.8})$$

and using

$$f(\beta - \tau) = f(\tau). \quad (\text{A.9})$$

Equation (A.9) is again proved by cyclical permutations in the trace. Explicitly:

$$\begin{aligned} & \int_0^\beta d\lambda \int_0^\lambda d\lambda' \langle\delta\mathcal{H}(\lambda) \delta\mathcal{H}(\lambda')\rangle \\ &= \int_0^\beta d\lambda \int_0^\lambda d\lambda' \langle\delta\mathcal{H}(\lambda - \lambda') \delta\mathcal{H}\rangle \\ &= \int_0^\beta d\lambda \int_0^\lambda d\tau f(\tau) \end{aligned}$$

$$\begin{aligned}
&= \int_0^\beta d\tau \int_\tau^\beta d\lambda f(\tau) \\
&= \int_0^\beta d\tau (\beta - \tau) f(\tau) \\
&= \int_0^\beta d\tau \tau f(\beta - \tau) \\
&= \frac{1}{2} \int_0^\beta d\tau (\beta - \tau + \tau) f(\tau) \\
&= \frac{\beta}{2} \int_0^\beta d\tau \langle \delta\mathcal{H}(\tau) \delta\mathcal{H} \rangle.
\end{aligned} \tag{A.10}$$

Now equation (A.2) is easily derived by inserting (A.7) and (A.5) into (A.6), taking the logarithm, expanding to second order in  $\delta\mathcal{H}$ , and recognizing in the final result the inner product (2.7).

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