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Thermally generated magnetic fields in heavy-fermion superconductors

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We calculate numerically the magnitude of the induced thermomagnetic field due to particle-hole asymmetry in heavy-fermion superconductors. Close to the transition temperature and for a phase shift of the order of $\delta_N = 0.9\pi/2$, this field can be as high as 10^{-2} G for pure samples. The experimental detection of these induced fields and their orientation dependence can be of great help in identifying the internal structure of the order parameter in these exotic superconductors.

Thermoelectric effects in superconductors constitute a valuable tool in studying the nature of quasiparticle scattering mechanisms and in probing the detailed structure of the Fermi surface,[1] the reason being that thermoelectric effects only arise as a result of particle-hole asymmetry in the relaxation properties of excitations. These differences in scattering rates of a particlelike and a holelike excitations will generate a net current in the system, the symmetry of which will depend crucially on the symmetry of the order parameter. Thus for an anisotropic order parameter we should expect an anisotropic thermoelectric coefficient which, as was pointed out by Ginzburg,[2] will give rise to an induced magnetic field. In the usual type of superconductors such a magnetic field is purely due to crystal anisotropy and its magnitude was estimated to be much less than 10^{-6} G, a value still not very easily detectable experimentally. The smallness of this magnetic field is mainly due to the abrupt reduction of the thermoelectric coefficient in the superconducting phase, which is usually of the order of $(\sigma_N/e)(T_c/T_F)$, where σ_N is the normal-state electric conductivity, e is the electronic charge; T_c and T_F are, respectively, the superconducting and Fermi temperatures. Hence, any enhancement of the thermoelectric coefficient will be directly reflected in an enhancement of the induced magnetic field.

In our previous studies on transport properties in heavy-fermion superconductors,[3] we have pointed out that scattering processes in anisotropic superconductors have some unexpected asymmetries when the normal-state phase shift is neither small nor resonant. Most importantly for our purpose is the fact that under such circumstances the scattering rates are not symmetric about the Fermi surface and will give rise to an enhanced thermoelectric effect, generally by a factor of T_F/T_c compared to usual superconductors.

It is widely accepted by now[4] that most heavy-fermion transport properties in the superconducting state can be explained as being due to scattering off nonmagnetic impurities with phase shift close to $\pi/2$. The fact that the phase shift is close to $\pi/2$ was evidenced by a more quantitative fit of the low-temperature data on the specific heat of UBe_{13} by Ott *et al.*[5] Following the work of Hirschfeld *et al.*[4] on the effects of pair breaking on the specific heat, they could fit their experimental data using a phase shift $\delta_N = 0.9\pi/2$. A similar analysis[6] was done on the low-temperature behavior of the nuclear spin relaxation time of ^9Be in UBe_{13}, and the best fit to the low-temperature experimental data was obtained for a phase shift close to $0.9\pi/2$. Thus it seems to be of practical interest to pursue the analysis of all possible consequences on transport and relaxation properties of heavy-fermion superconductors when the phase shift δ_N has the experimentally suggested value of $0.9\pi/2$.

It is the purpose of this paper to give a more thorough analysis of particle-hole asymmetry induced magnetic field due to the fact that the phase shift is different from $\pi/2$. The basic idea is the same as that due to Ginzburg, that is an anisotropic thermoelectric coefficient will result in the appearance of a persistent current and an associated magnetic field in the superconducting phase. But, in our case the anisotropy of the thermoelectric effect is due to the anisotropy of the gap and not to the crystal anisotropy.

To calculate the induced magnetic field we closely follow the treatment of Kresin and Litovchenko.[7] We consider the geometry shown in Fig. 1, where we take our slab of thickness d to be parallel to the XZ plane and the temperature gradient (∇T) is applied along the Y direction, where XYZ is the laboratory reference frame. For simplicity, we consider only axially symmetric superconducting states; the symmetry axis of the gap is denoted by $\hat{\mathbf{l}}$ and lies in the YZ plane, making an angle of θ with the Z axis. The basis for the solution of the problem is Maxwell's equation coupled with the superconducting and normal current equations:

$$\nabla \times \mathbf{H} = 4\pi/c(\mathbf{J}^s + \mathbf{J}^n) , \tag{1}$$

$$\mathbf{J}^n = -\mathsf{L}\cdot\nabla T , \tag{2}$$

$$\mathbf{J}^s = -\frac{c}{4\pi}\mathsf{K}(q)\cdot\mathbf{A}(q) , \tag{3}$$

where $\mathbf{J}^s$ and $\mathbf{J}^n$ are the supercurrent and normal current, respectively, and $\mathbf{A}(q)$ is the Fourier transform of the vector potential. The quantities L and $\mathsf{K}(q)$ are the thermoelectric and electromagnetic tensors, respectively. T stands for temperature, $\mathbf{H}$ for the magnetic field and c for

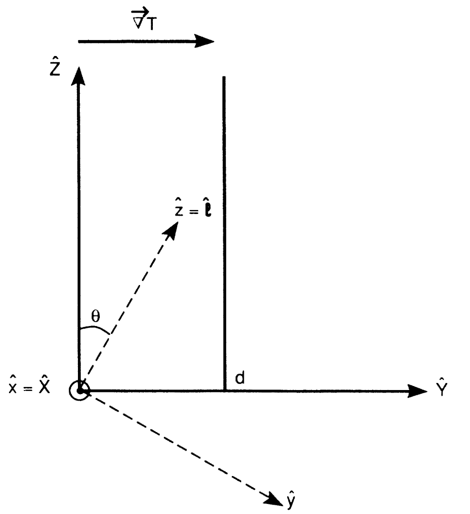

FIG. 1. Geometry of our sample of thickness d, XYZ is the laboratory reference frame, xyz has the z axis along symmetry axis $\hat{l}$ of the gap, and θ is the angle between the $\hat{l}=\hat{\mathbf{z}}$ axis and the Z axis.

the speed of light. First, we notice from these equations that if L is not proportional to the unit matrix then the Meissner-Oschenfeld effect will be incomplete and an induced magnetic field will be present in the sample, this was actually the main idea in Ginzburg's work.[2] Our purpose here is to evaluate such a magnetic field by solving the coupled equations (1)–(3). The analytical expressions of the thermoelectric tensor L have been obtained before[3] on the basis of a linearized Boltzmann equation approach. This thermoelectric tensor was found to be diagonal in the reference frame in which the gap is axially symmetric, but not proportional to the unit matrix, for the polar p-wave state and one representative d-wave state having a line of nodes at the equator. For the Anderson-Brinkman-Morel (ABM) p-wave state, it was found to have a nonvanishing off-diagonal matrix elements which will give rise to an extra component of the magnetic field. The electromagnetic kernel, on the other hand, can be calculated either from a microscopic approach[8] or by use of a simple argument band on gauge invariance as is done in the Appendix.

It is just a simple algebraic exercise to solve the system of equations (1)–(3), for our simple geometry we found for the nonvanishing components of the vector potential the following expressions:

$$A_Z(Y)=\frac{4\pi}{c}\int dq \frac{J^n(q)}{q^2+K(q)}e^{iqY} , \tag{4}$$

$$A_X(Y)=\frac{4\pi}{c}\int dq \frac{J_X^n(q)}{q^2+K_{XX}(q)}e^{iqY} , \tag{5}$$

where

$$J^n(q)=J_Z^n-K_{ZY}(q)K_{YY}^{-1}(q)J_Y^n , \tag{6}$$

$$K(q)=K_{ZZ}(q)-K_{ZY}^2(q)K_{YY}^{-1}(q) , \tag{7}$$

Now since $J^n(q)$ varies on the scale of $q^{-1}\gg\xi_0$, λ_0, where ξ_0 is the zero-temperature coherence length and λ_0 is the zero-temperature London penetration depth, the main contribution to the vector potential components (4)–(5) will come from small q values so that our magnetic-field components read

$$H_X=\frac{4\pi}{c}\frac{\partial}{\partial Y}[K^{-1}(T(Y))J^n(Y)] , \tag{8}$$

$$H_Z=\frac{4\pi}{c}\frac{\partial}{\partial Y}[K_{XX}^{-1}(T(Y))J_X^n(Y)] . \tag{9}$$

Here we need to stress the fact that while the electromagnetic kernel and the thermoelectric tensor are simply expressed in coordinate axes xyz, where $\hat{\mathbf{z}}$ is along $\hat{\mathbf{l}}$, the symmetry axis of the gap, the field components H_X, and H_Z are naturally expressed in the XYZ reference frame. The reason is that one needs to keep a simple form for the angular part of the gap function, and thus we choose our system of coordinates so that the orbital part of the gap looks simple, i.e., $|\Delta_p|$, the magnitude of the gap, is a function of θ' only, the angle between the $\hat{\mathbf{z}}$ axis and the momentum direction $\hat{\mathbf{p}}$. The two systems can be transformed one into the other by use of a simple rotation matrix U defined for our simple geometry (Fig. 1) by

$$U=\begin{bmatrix}1 & 0 & 0\\ 0 & \cos\theta & \sin\theta\\ 0 & -\sin\theta & \cos\theta\end{bmatrix} \tag{10}$$

such that $X_i=U_{ij}x_j$, where $\mathbf{X}$ refers to a vector in the XYZ coordinates and $\mathbf{x}$ refers to a vector in the xyz coordinates. After some algebra one finds for the two components of the induced magnetic field

$$H_X=-\tfrac{1}{2}H_0\sin 2\theta\frac{\partial}{\partial t}\left[\frac{L(t)}{R_{yz}(t)}\right] , \tag{11}$$

$$H_Z=H_0\cos\theta\frac{\partial}{\partial t}\left[\frac{L_{xy}(t)}{R_x(t)}\right] , \tag{12}$$

where H_0 is a constant number that sets the scale of the induced magnetic field and is given by

$$H_0=\frac{4\pi}{c}\frac{\lambda_0^2}{3}\frac{\sigma_N}{e}\frac{k_B}{T_c}(\nabla_Y T)^2 . \tag{13}$$

The quantities $R_i(t)$ and $R_{yz}(t)$ are evaluated in the xyz reference frame and are defined by

$$R_i(T)=\tfrac{1}{3}-2\int_0^\infty dE\left[-\frac{\partial n}{\partial E}\right]\langle\hat{\mathbf{p}}_i^2\rangle , \tag{14}$$

$$R_{yz}(t)=\frac{R_y(t)R_z(t)}{\cos^2\theta R_y(t)+\sin^2\theta R_z(t)} , \tag{15}$$

where the anomalous average $\langle\cdots\rangle$ stands for the following:

$$\langle\cdots\rangle=\int\frac{d\Omega}{4\pi}\frac{E}{(E^2-|\Delta_p|^2)^{1/2}}\cdots . \tag{16}$$

The quantity $E/(E^2-|\Delta_p|^2)^{1/2}$ is the density of quasiparticle states per unit energy in the direction $\hat{\mathbf{p}}$, normalized to its normal-state value, σ_N is the normal-state conductivity, e is the electronic charge, k_B is the Boltzmann constant, T_c is the critical temperature and $t=T/T_c$ is the reduced temperature. The Fermi function is defined by $n(x)=1/(\exp\beta x+1)$, where β is the inverse temperature. The quantities L_{xy} and L are defined in terms of the dimensionless thermoelectric coefficients (or equivalently in units of σ_N/e), L_{xy} is just the off-diagonal element of the tensor L_{ij}, which is nonzero only for the axial p-wave state, and $L(t)=L_{zz}(t)-L_{yy}(t)$. The superconducting states we shall consider in this paper are the axial p-wave state (also called Anderson-Brinkman-Morel or ABM state) defined by its order parameter

$$\Delta(\hat{\mathbf{p}})=\Delta(T)\mathbf{d}\sin\theta\exp i\phi \ , \tag{17}$$

where $\Delta(T)$ is the maximum value of the gap, (θ,ϕ) are the angular coordinates of $\hat{\mathbf{p}}$, and $\mathbf{d}$ is a fixed unit vector in spin space. The second state we shall consider is a d-wave type of state defined by

$$\Delta(\hat{\mathbf{p}})=2\Delta(T)\sin\theta\cos\theta\exp i\phi \ . \tag{18}$$

The full matrix structure of the order parameter reads $\Delta_p=i\sigma_2\boldsymbol{\sigma}\cdot\Delta(\hat{\mathbf{p}})$ for the axial state and $\Delta_p=\sigma_2\Delta(\hat{\mathbf{p}})$ for the d-wave states, where $\boldsymbol{\sigma}$ stands for all three components of Pauli matrices. The thermoelectric coefficients for the above-mentioned states have been calculated before[3] and are given in that reference in units of σ_N/e by formulas (102)–(104), and (107) and (108), for the axial and d-wave states, respectively. In order to calculate the temperature dependence of the magnetic-field components (11) and (12) we need an expression for the magnitude of the gap as a function of temperature. We use the following form:[9]

$$\Delta(T)=\Delta(0)\tanh\left\{\frac{\pi T_c}{\Delta(0)}\left[\frac{2}{3f}\left[\frac{\Delta C}{C}\right]\frac{T_c-T}{T}\right]^{1/2}\right\} , \tag{19}$$

which tends to $\Delta(0)$ as $T\to 0$, and its behavior close to T_c is such that the specific-heat jump at T_c calculated from it is equal to $\Delta C/C$, C being the specific heat and ΔC the specific-heat jump at T_c. The constant f is equal to $\frac{2}{3}$ for the axial state, and $\frac{8}{15}$ for the d-wave state. For $\Delta(0)$ we adopted the weak-coupling values $\Delta(0)=2.02k_BT_c$ (axial), and $\Delta(0)=2.10k_BT_c$ (d wave). Also we need to evaluate H_0, which set the scale of the induced magnetic field in (11) and (12), but before doing that a few remarks are in order. First, from our formula (13) for H_0 we see that the magnitude of this field is enhanced by a factor of T_F/T_c compared to its usual value.[7,10] The reason is that the thermoelectric coefficient itself is enhanced by such a factor due to particle-hole asymmetry inherent to the scattering amplitude in the superconducting state.[3] Second, as explained by Varma *et al.*[11] on theoretical ground and supported by experiment,[12] the square of the London penetration depth in heavy-fermion superconductors is also enhanced by an effective-mass factor m_d/m_e [m_d being the dynamical effective mass defined by $m_d=m^*/(1+F_1^S/3)$ and m_e is the bare electronic mass], due to the difference between the dynamical effective mass and the bare mass unlike one-component translationally invariant Fermi liquids. Consequently, we are talking about an overall enhancement factor of $(T_F/T_c)(m_d/m_e)$ in the induced magnetic field compared to its usual value if the numerical factors coming from the temperature dependence are comparable, here we neglect the difference between m^* and m_d since $F_1^S=O(1)$ in these systems.[11] But this results in an overestimate of the induced field. In fact, numerical calculations show that near T_c (but not too close to it) we have $H_i(t)\simeq\text{const}\Delta(t)^{-3}$ $(i=x,z)$, whereas in the usual type of isotropic superconductors one finds[7] close to T_c, $H_X\simeq\text{const}\Delta(t)^{-4}$; thus close to the transition temperature and for a sample of comparable purity, the induced magnetic field is enhanced by a factor of

$$E=\frac{T_F}{T_c}\frac{m_d}{m_e}\sqrt{1-t} \tag{20}$$

compared to its value in conventional superconductors.

The numerics for the induced magnetic field will be done for UPt_3, which seem to be the cleanest of all heavy-fermion superconductors and for which a Fermi-liquidlike picture is applicable,[3] the validity of which is necessary since we have used the Boltzmann equation approach in calculating the thermoelectric coefficients $L_{ij}(t)$. Other heavy-fermion superconductors such as UBe_{13}, $CeCu_2Si_1$ and URh_2Si_2 have extremely short mean free paths as deduced from their resistivity measurements. The reason for this is that the inelastic contribution to the residual resistivity is substantial in these systems while it is much smaller in UPt_3. Bearing in mind that only elastic processes have been included in our calculation of the transport coefficient L_{ij}, we see that UPt_3 is the most likely candidate to exhibit the thermomagnetic effects of the type discussed here. For the experimental data on UPt_3 we take the Fermi temperature to be $T_F=275$ K, the transition temperature $T_c=0.5$ K and the zero-temperature London penetration depth $\lambda_0=3600$ Å from the measurements of Palstra *et al.*[13] and de Visser's thesis.[13] From de Haas–van Alphen experiments of Taillefer and Lonzarich[14] we take the dynamical mass enhancement factor $\gamma=m_d/m_e$ to be close to 25 and the average Fermi velocity to be $v_F=6\times 10^5$cm/sec, which is close to the value found experimentally for all pieces of the Fermi surface. The residual resistivity in the normal state is taken from the data of Sulpice *et al.*[15] $\rho_N\simeq 0.46$ $\mu\Omega$ cm, from which we can estimate the mean free path to be $1\simeq 2300$ Å. This value of the mean free path is close to the one inferred by Taillefer and Lonzarich from their de Haas–van Alphen experiments. The temperature gradient is taken to have its usual experimental value $|\nabla T|\simeq 0.1$ K/cm. Using these experimental data we found $H_0=10^{-8}$ G, if we use a hypothetical sample of higher purity we can reach values as high as 10^{-5} G for a mean free path of the order of 10^5 Å. To get an idea about the order of magnitude of the induced magnetic field near T_c, we evaluate it at $t=0.99$, the enhancement factor Eq. (20) for UPt_3 at this temperature is calculated to be $E \simeq 1.4\times 10^3$, so that the induced magnetic field becomes of the order of $H_i \simeq 1.4\times 10^5$ G for $l=2300$ Å and $H_i \simeq 1.4\times 10^{-2}$ G for $l=10^5$ Å ($i=X,Z$). We should point out that the highly desired UPt_3 samples with mean free paths of the order of 10^5 Å have not been obtained yet, but their experimental achievement should not constitute a major obstacle.

In making the numerical estimates we adopted the value $\Delta C/C=0.86$ which was extracted by Sulpice *et al.*[15] from their experimental data on UPt_3. As I have explained it before we take for the value of the phase shift the experimentally suggested value $\delta_N=0.9\pi/2$. Now, due to the fact that the value of the induced magnetic field is much larger close to the transition temperature, we thought it would be more beneficial to normalize it by $(\Delta/k_B T_c)^3$ so as to have $H_i \simeq$const close to T_c. In this way, we can see the behavior of H_i at low temperatures. In Fig. 2 we show the H_X component of the magnetic field for the axial (ABM) state, which was evaluated for an angle $\theta=\pi/4$ (the angle between the symmetry axis of the gap, $\hat{l}$, and the $\hat{Z}$ axis). In the range of temperatures between $t=0.8$ and $t=0.98$ we can to a very good accuracy approximate this component by $H_X \simeq 0.5 H_0 (k_B T_c/\Delta)^3$, while at very low temperatures it can reach values around $60 H_0$. Very close to the transition temperature we see an abrupt oscillatory behavior that might have some interesting physical consequences, but due to the delicacy of the critical region (which is not our main concern here) we will not pay too much attention to this phenomena. Similarly in Fig. 3 we show the maximum value of the H_Z component of the magnetic field for the same state, the existence of this component is purely due to the off-diagonal nature of the thermoelectric tensor L_{ij} which in its turn is due to the phase variation and the odd parity of the order parameter. While the magnitude of this component is very small at low temperatures compared to the H_X component, it has comparable magnitude near T_c. Finally, in Fig. 4 we show the H_X component of the magnetic field for the *d*-wave state considered and for an

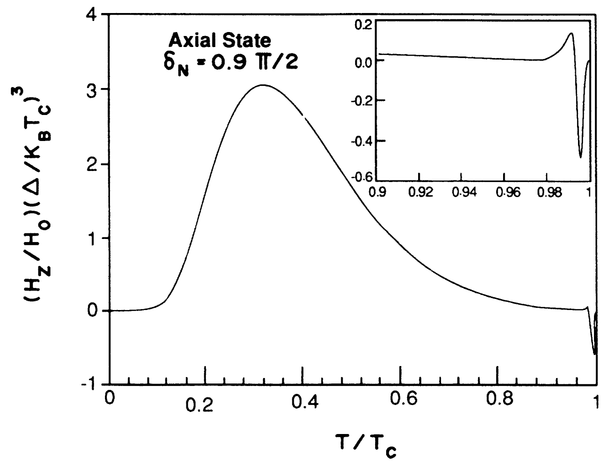

FIG. 3. Plot of the maximum value of the H_Z component of the magnetic field in units of H_0 renormalized by $(\Delta/k_B T_c)^3$ for the axial state. The inset shows the behavior very close to T_c.

angle $\theta=\pi/4$, similar observations to those made for the corresponding component of the axial state hold in this case too.

In conclusion, we think that the experimental detection of such a thermally induced magnetic field and its orientation dependence in heavy-fermion superconductors would be of great help in identifying the correct internal structure of the order parameter. Recently Ginzburg[16] stressed the importance of thermoelectric phenomena in heavy-fermion and high-T_c superconductors, and using a phenomenological approach he estimated the thermopower in these compounds to be at least 2 orders of magnitude larger than in usual type of superconductors. Our study shows that the magnitude of the induced magnetic field in UPt_3 can be enhanced by factors as high as 10^4 compared to their usual values. Hence the possibility of observing such effects in UPt_3 is very great indeed. Finally, we should mention that even though we have predict-

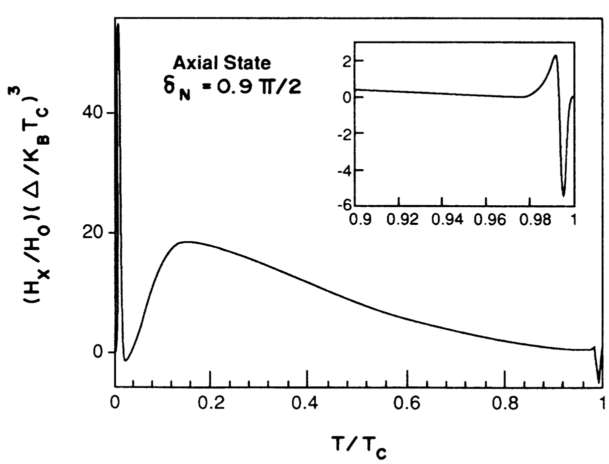

FIG. 2. Plot the H_X component of the magnetic field in units of H_0 and renormalized by $(\Delta/k_B T_c)^3$ for the axial state. The inset show the behavior very close to T_c.

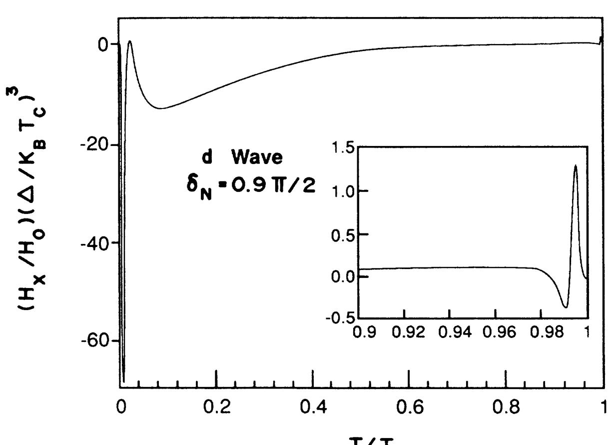

FIG. 4. Plot the H_X component of magnetic field in units of H_0 renormalized by $(\Delta/k_B T_c)^3$ for the *d*-wave state. The inset shows the behavior very close to T_c.

ed a relatively large value of the induced field at very low temperatures, this should not be taken very seriously because impurity renormalization effects become very important in this region and might result in some quantitative changes in our low-temperature results.

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APPENDIX

In this appendix we will calculate the electromagnetic kernel $K(q)$. For that we need to maintain gauge invariance to avoid spurious effects.[17] Since we are interested in the static Meissner effect the local charge conservation reads

$$\mathbf{q}\cdot\mathbf{j}(q)=0 . \tag{A1}$$

It is known that local charge conservation is equivalent to gauge invariance,[18] thus in making sure that our electromagnetic kernel satisfies (A1), our results will automatically be gauge invariant. The exact way to solve this problem is to calculate the renormalized vertex, which amounts to solving an integral equation for the vertex.[17] Another way to handle this question is to calculate the simplest kernel, that is using the unrenormalized vertex, which we call $K_{ij}^0(q)$, then in the last stage we do a gauge transformation

$$\mathbf{A}(q)\rightarrow \mathbf{A}(q)+i\mathbf{q}\Lambda(q) , \tag{A2}$$

where $\Lambda(q)$ is an arbitrary function to be chosen so that local charge conservation (A1) is restored. The calculation of K_{ij}^0 is straightforward and we obtained in the long-wavelength limit

$$K_{ij}^0(q)=\frac{3}{\lambda_0^2}\int\frac{d\Omega_p}{4\pi}\hat{\mathbf{p}}_i\hat{\mathbf{p}}_j R(\hat{\mathbf{p}}) , \tag{A3}$$

where

$$R(\hat{\mathbf{p}})=1-2\int_0^{\infty}dE\left[-\frac{\partial n}{\partial E}\right]\langle 1\rangle \tag{A4}$$

and $\langle\cdots\rangle$ is defined by Eq. (16) in the main text. Now, we do a gauge transformation according to (A2) and require the physical current, which is defined by

$$J_i(q)=-\frac{c}{4\pi}K_{ij}^0(q)[A_j(q)+iq_j\Lambda(q)] , \tag{A5}$$

to satisfy the local charge conservation equation (A1). Solving for the function $\Lambda(q)$ we find

$$\Lambda(q)=\frac{i}{q}\frac{\langle R(\hat{\mathbf{p}})(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})(\hat{\mathbf{p}}\cdot\mathbf{A})\rangle_p}{\langle R(\hat{\mathbf{p}})(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})^2\rangle_p} , \tag{A6}$$

where $\langle\cdots\rangle_p$ denotes the angular average over the directions of $\hat{\mathbf{p}}$, to be distinguished from the anomalous average $\langle\cdots\rangle$ defined by Eq. (16) in the main text, and is defined by

$$\langle\cdots\rangle_p=\int\frac{d\Omega_p}{4\pi}\cdots . \tag{A7}$$

Putting (A6) back in the current (A5) we find that the physical kernal of interest to us is given by

$$K_{ij}(q)=\frac{3}{\lambda_0^2}\left\langle R(\hat{\mathbf{p}})\hat{\mathbf{p}}_i\left[\hat{\mathbf{p}}_j-(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\frac{\langle R(\hat{\mathbf{p}})(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\hat{\mathbf{p}}_j\rangle_p}{\langle R(\hat{\mathbf{p}})(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})^2\rangle_p}\right]\right\rangle_p . \tag{A8}$$

This is exactly the expression derived by Millis[8] on a microscopic basis. To evaluate this kernel (A8) we notice that it is easier first to evaluate the kernel K_{ij} $(i,j=x,y,z)$ in the reference frame having the symmetry axis of the gap $\hat{\mathbf{l}}$ along the $\hat{\mathbf{z}}$ direction, then using the rotation matrix [Eq. (10)] given in the main text we can evaluate K_{kl} $(k,l=X,Y,Z)$ in the laboratory reference frame, which are the quantities needed in calculating the induced magnetic fields.

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