

## Conductivity sum rule: Comparison of coherent and incoherent $c$ -axis coupling

Wonkee Kim and J. P. Carbotte

*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1*

(Received 21 January 2000)

We calculate the  $c$ -axis kinetic-energy difference between normal and superconducting state for coherent and for incoherent interlayer coupling between  $\text{CuO}_2$  planes. For coherent coupling the ratio of the missing conductivity spectral weight to the superfluid density is equal to one and there is no violation of the conventional sum rule, but for the incoherent case we find it is always greater than one whatever the nature of the impurity potential may be. To model more explicitly  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  around optimum doping, which is found to obey the sum rule, we consider a plane-chain model and show that the sum rule still applies. A violation of the sum rule of either sign is found even for coherent coupling when the in-plane density of electronic states depends on energy on a scale of the order of the gap.

It has been proposed that the interlayer coupling along the  $c$  axis of a high transition temperature ( $T_c$ ) superconductor is incoherent, and the electronic kinetic energy along the  $c$  axis changes when the system enters the superconducting state.<sup>1-4</sup> Recently, Basov *et al.*<sup>5</sup> have reported that there is a significant discrepancy between the superfluid density  $\rho_s$  and the spectral weight missing from the real part of the  $c$ -axis conductivity  $N_n - N_s = 8 \int_0^{\omega_c} d\omega [\sigma_{1c}^n(\omega) - \sigma_{1c}^s(\omega)]$ , where  $\omega_c$  is a cutoff frequency of the order of a bandwidth, in several high- $T_c$  cuprate superconductors such as optimally doped  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}$  (Tl2201). This implies that the conventional sum rule of Ferrel, Grover, and Tinkham (FGT) (Ref. 6) is violated. However, the spectral discrepancy becomes vanishing for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$  and disappears for the optimally doped  $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$  (YBCO) crystal with  $T_c \approx 93$  K as the  $c$ -axis response become more coherent with increasing oxygen content.<sup>5,7</sup> Basov *et al.* also pointed out that there is no such discrepancy in the in-plane response for any cuprate. Moreover, for overdoped Tl2201, the sum-rule discrepancy vanishes and a Drude-like peak develops in the conductivity for  $T > T_c$ .<sup>8</sup> These observations, therefore, suggest that for coherent interlayer coupling in the cuprate superconductors the conventional sum rule is obeyed.

In this paper, we consider both coherent and incoherent  $c$ -axis coupling between  $\text{CuO}_2$  planes. For the coherent case we find that the superfluid density remains equal to the missing optical spectral weight; in other words, it does not violate the FGT sum rule. The  $c$ -axis kinetic energies in the normal and superconducting state have the same value. For incoherent  $c$ -axis coupling the ratio of the missing area to the superfluid density is always larger than one in disagreement with some recent experiments. In YBCO the  $\text{CuO}$  chains play an important role in the electrodynamics and at the optimal doping a plane-chain model<sup>9,10</sup> is needed to be complete. Here we use this model to investigate the  $c$ -axis conductivity sum rule. An algebraic calculation of the electronic kinetic energies is complicated and a numerical calculation is required although it can be reduced a lot in a special case, in which only the leading order in perturbation theory is kept. This case is particularly interesting because it has been shown to exhibit a pseudogap in the  $c$ -axis conductivity.<sup>10</sup> Finally, we

discuss the possibility that the FGT sum rule is violated in the plane-plane case when the in-plane density of states depends on energy even for coherent case.

The Hamiltonian  $H$  for a cuprate superconductor with coherent  $c$ -axis coupling is  $H = H_0 + H_c$ , where  $H_0$  describes a  $d$ -wave superconductor in a plane and  $H_c = \sum_{i\sigma} t_{\perp} [c_{i1\sigma}^+ c_{i2\sigma} + c_{i2\sigma}^+ c_{i1\sigma}]$  is a coherent interlayer coupling due to the overlap of electronic wave functions which is represented by  $t_{\perp}$ ; therefore, by coherent coupling we mean a tight-binding-like coupling along the  $c$  axis. It will not be necessary to treat  $t_{\perp}$  as a constant in what follows. It can depend on an angle in the plane. For incoherent coupling the Hamiltonian is  $H'_c = \sum_{i\sigma} V_i [c_{i1\sigma}^+ c_{i2\sigma} + c_{i2\sigma}^+ c_{i1\sigma}]$ , where  $V_i$  is an impurity scattering potential, so that impurity scattering mediates the  $c$ -axis hopping and an impurity average is implied.<sup>11,12</sup>

In the presence of an external vector potential  $A_z$ ,  $H_c$  is modified to  $H_c(A_z)$  by the phase factor  $\exp(-ieA_z)$  for  $c_{i1\sigma}^+ c_{i2\sigma}$  and  $\exp(ieA_z)$  for  $c_{i2\sigma}^+ c_{i1\sigma}$ . For the response to an external field,  $H_c(A_z)$  is expanded up to the second order of  $A_z$  to obtain the current  $j_c = -\delta H_c(A_z)/\delta A_z = j_p + j_d$ , where  $j_p = -ied \sum_{i\sigma} t_{\perp} [c_{i1\sigma}^+ c_{i2\sigma} - c_{i2\sigma}^+ c_{i1\sigma}]$  and  $j_d = e^2 d^2 H_c A_z$  with  $d$  the interlayer spacing. In linear-response theory,  $\langle j_c \rangle = [-\Pi + e^2 d^2 \langle H_c \rangle] A_z$ , where  $\Pi$  is the current-current correlation function associated with  $j_p$  and  $\langle H_c \rangle$  is the perturbation of  $j_d$  due to  $H_c$ . The conductivity  $\sigma_c(\mathbf{q}, \omega)$  is given by

$$\sigma_c(\mathbf{q}, \omega) = \frac{i}{\omega} [\Pi(\mathbf{q}, \omega) - e^2 d^2 \langle H_c \rangle]. \quad (1)$$

In the Matsubara formalism,

$$\begin{aligned} \Pi(\mathbf{q}, \omega) = & 2(ed)^2 T \sum_{\omega'} \sum_{\mathbf{k}} t_{\perp}^2 \\ & \times \text{Tr}[\hat{\tau}_0 \hat{G}(\mathbf{k}, \omega') \hat{\tau}_0 \hat{G}(\mathbf{k}, \omega' + \omega)], \end{aligned} \quad (2)$$

and

$$\langle H_c \rangle = 2T \sum_{\omega} \sum_{\mathbf{k}} t_{\perp}^2 \text{Tr}[\hat{\tau}_3 \hat{G}(\mathbf{k}, \omega) \hat{\tau}_3 \hat{G}(\mathbf{k}, \omega)], \quad (3)$$

where  $\hat{\tau}_i$  is the Pauli matrix in the spin space, and  $\hat{G}(\mathbf{k}, \omega)$  is the Green's function in Nambu representation, namely,  $\hat{G}(\mathbf{k}, \omega) = -(i\omega\hat{\tau}_0 + \xi_{\mathbf{k}}\hat{\tau}_3 - \Delta_{\mathbf{k}}\tau_1)/(\omega^2 + \xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)$  with  $\xi_{\mathbf{k}}$  the in-plane energy and  $\Delta_{\mathbf{k}}$  the gap which has  $d_{x^2-y^2}$  symmetry in the cuprates.

The  $c$ -axis conductivity sum rule<sup>4,13,14</sup> of the system is

$$\frac{2}{\pi} \int_0^{\omega_c} d\omega \sigma_{1c}(\omega) = -e^2 d^2 \langle H_c \rangle. \quad (4)$$

We use the unit such that  $\hbar = c = k_B = 1$  and set the volume of the system to be unity. From the sum rule, the superfluid density  $\rho_s$  can be written as

$$\rho_s = 8 \int_0^{\omega_c} d\omega [\sigma_{1c}^n(\omega) - \sigma_{1c}^s(\omega)] - 4\pi e^2 d^2 [\langle H_c \rangle^s - \langle H_c \rangle^n], \quad (5)$$

where  $\omega_c$  is the cutoff frequency for interband transitions that  $H_c$  does not account for.

Since the difference between the superfluid density and the missing spectral weight is proportional to the kinetic-energy difference between normal and superconducting state as seen in Eq. (5), it is necessary to calculate  $\langle H_c \rangle^s - \langle H_c \rangle^n$  to see if the FGT sum rule is violated by coherent  $c$ -axis coupling. For the normal state,

$$\langle H_c \rangle^n = 4T \sum_{\omega} \sum_{\mathbf{k}} t_{\perp}^2 G_0(\mathbf{k}, \omega)^2, \quad (6)$$

where  $G_0(\mathbf{k}, \omega)$  is a normal-state Green's function and  $t_{\perp}$  may depend on  $k_z$  and  $\phi = \tan^{-1}(k_y/k_x)$ . We assume a cylindrical Fermi surface with  $\xi = k^2/2m - \mu$ , where  $\mu$  is a chemical potential in the plane, and a  $d$ -wave gap  $\Delta_{\mathbf{k}} = \Delta(T) \cos 2\phi_{\mathbf{k}}$ . Then, we obtain

$$\begin{aligned} \langle H_c \rangle^n &= 4 \sum_{k_z} \int \frac{d\phi}{2\pi} t_{\perp}^2 \int_{-\omega_c}^{\omega_c} d\xi N(\xi) \frac{\partial f(\xi)}{\partial \xi} \\ &= -4N(0) \sum_{k_z} \int \frac{d\phi}{2\pi} t_{\perp}^2 \tanh\left(\frac{\omega_c}{2T}\right), \end{aligned} \quad (7)$$

where the integration range is limited by  $\omega_c$ , and the density of states,  $N(\xi)$ , is approximated by a constant value  $N(0)$  around the Fermi energy. Later, we will discuss the effect of  $N(\xi)$  on  $\langle H_c \rangle$  and will note the possibility that the FGT sum rule may be violated even for coherent  $c$ -axis coupling. Since  $\partial f(\xi)/\partial \xi = -\delta(\xi)$  at zero temperature ( $T=0$ ),  $\langle H_c \rangle^n$  turns out to be  $-4N(0) \sum_{k_z} \int d\phi/(2\pi) t_{\perp}^2$ . For a superconducting state with superconducting Green's functions  $G(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \omega)$ ,

$$\begin{aligned} \langle H_c \rangle^s &= 4T \sum_{\omega} \sum_{\mathbf{k}} t_{\perp}^2 [G(\mathbf{k}, \omega)^2 - F(\mathbf{k}, \omega)^2] \\ &= -4T \sum_{\omega} \sum_{k_z} \int \frac{d\phi}{2\pi} t_{\perp}^2 \int_{-\omega_c}^{\omega_c} d\xi N(\xi) \frac{\omega^2 - \xi^2 + \Delta_{\mathbf{k}}^2}{(\omega^2 + \xi^2 + \Delta_{\mathbf{k}}^2)^2} \\ &= -4N(0) \sum_{k_z} \int \frac{d\phi}{2\pi} t_{\perp}^2 \frac{\omega_c}{\sqrt{\omega_c^2 + \Delta_{\mathbf{k}}^2}} \tanh\left(\frac{\sqrt{\omega_c^2 + \Delta_{\mathbf{k}}^2}}{2T}\right). \end{aligned} \quad (8)$$

The difference between  $\langle H_c \rangle^s$  and  $\langle H_c \rangle^n$  is of the order of  $(\Delta(T)/\omega_c)^2$ ; therefore, coherent  $c$ -axis coupling does not violate the FGT sum rule as long as  $\omega_c \gg \Delta(0)$  even if  $t_{\perp}$  depends on  $\phi$ . Note that the difference is largest at  $T=0$  and vanishes as  $T \rightarrow T_c$ .

The calculations for incoherent (impurity mediated)  $c$ -axis coupling proceed in the same way as before. Note that in this case  $j_p = -ied \sum_{i\sigma} V_i [c_{i1\sigma}^+ c_{i2\sigma} - c_{i2\sigma}^+ c_{i1\sigma}]$  and  $j_d = e^2 d^2 H_c' A_z$ , and an impurity configuration average is required. We derive the normalized missing spectral weight  $(N_n - N_s)/\rho_s$  under assumption of a constant density of states and show that it is greater than one.

The penetration depth  $\lambda_c$  can be calculated in two ways. Based on the Kramers-Kronig relation for the conductivity, we obtain  $\lambda_c$ , namely,  $1/4\pi\lambda_c^2 = \lim_{\omega \rightarrow 0} [\omega \text{Im} \sigma_c(0, \omega)]$ . Alternatively, using Eq. (5) we can also calculate  $\lambda_c (= 1/\sqrt{\rho_s})$ . Equate these two expressions of  $\lambda_c$ , then after integration over energy we arrive the formula as follows:

$$\frac{(N_n - N_s)}{\rho_s} = \frac{1}{2} + \frac{1}{2} \frac{\sum_{\omega} \int d\phi_k d\phi_p |V(\phi_k, \phi_p)|^2 \left[ 1 - \frac{\omega^2}{\sqrt{\omega^2 + \Delta_k^2} \sqrt{\omega^2 + \Delta_p^2}} \right]}{\sum_{\omega} \int d\phi_k d\phi_p |V(\phi_k, \phi_p)|^2 \frac{\Delta_k}{\sqrt{\omega^2 + \Delta_k^2}} \frac{\Delta_p}{\sqrt{\omega^2 + \Delta_p^2}}}. \quad (9)$$

The second term in Eq. (9) can easily be shown to be bigger than one half whatever the angular dependence of the impurity potential  $V(\phi_k, \phi_p)$  may be.<sup>15</sup> Thus the normalized missing spectral weight is always greater than one. In a simple model of impurity scattering,<sup>2,11</sup> for which  $|V(\phi_k, \phi_p)|^2 = |V_0|^2 + |V_1|^2 \cos 2\phi_p \cos 2\phi_k$ , we found that  $(N_n - N_s)/\rho_s \geq 1.58$ . This incoherent coupling model, therefore, does not agree with recent findings. The sum rule is one for YBCO around optimum doping indicating coherent

$c$ -axis coupling and less than one for the underdoped case. To treat YBCO around optimum doping more realistically we need to include the complications introduced by existence of the chains along the  $b$  axis.

Penetration depth ( $\lambda_{a(b)}$ ) experiments<sup>16</sup> in YBCO have shown that both  $\lambda_a$  and  $\lambda_b$  are linear  $T$  at a low temperature and that a considerable amount of the condensate resides on the chains. To treat this case we need to consider a plane-chain coupling model.<sup>9,10</sup> We assume the hybridization of

Fermi surfaces between plane and chain arising through coherent coupling. For simplicity we also assume the gap in the chain has a  $d$ -wave symmetry and its magnitude is of the order of that in the plane. The Hamiltonian for a coupled plane-chain system is  $H = \sum_{\mathbf{k}} \hat{C}_{\mathbf{k}}^+ \hat{h}_{\mathbf{k}} \hat{C}_{\mathbf{k}}$ , where  $\hat{C}_{\mathbf{k}}^+ = (C_{1\mathbf{k}\uparrow}^+, C_{1-\mathbf{k}\downarrow}^+, C_{2\mathbf{k}\uparrow}^+, C_{2-\mathbf{k}\downarrow}^+)$  and

$$\hat{h}_{\mathbf{k}} = \begin{pmatrix} \xi_{1\mathbf{k}} & -\Delta_{1\mathbf{k}} & t(k_z) & 0 \\ -\Delta_{1\mathbf{k}} & -\xi_{1\mathbf{k}} & 0 & -t(k_z) \\ t(k_z) & 0 & \xi_{2\mathbf{k}} & -\Delta_{2\mathbf{k}} \\ 0 & -t(k_z) & -\Delta_{2\mathbf{k}} & -\xi_{2\mathbf{k}} \end{pmatrix}, \quad (10)$$

where  $t(k_z) = -t_0 \cos(k_z d/2)$  for coherent coupling between plane and chain,  $\xi_{1(2)}$  is the energy dispersion in the plane (chain), and  $\Delta_{1(2)}$  is a gap of the plane (chain). We point out here that the conclusion we make later does not depend on the simple form of  $t(k_z)$ , and that  $\Delta_{1(2)}$  and  $\xi_{1(2)}$  depend only on  $k_x$  and  $k_y$ .

The Hamiltonian of the plane-chain coupling model is also decomposed into two parts,  $H = H_0 + H_c$ .  $H_0$  is for the superconductivity in the plane-chain coupling system and its eigenvalues can be reduced to  $\pm E_{\pm} = \pm \sqrt{\epsilon_{\pm}^2 + \Delta_{\mathbf{k}}^2}$ , where  $\epsilon_{\pm}$  are normal-state energy dispersions  $\epsilon_{\pm} = (\xi_1 + \xi_2)/2 \pm \sqrt{(\xi_1 - \xi_2)^2/4 + t(k_z)^2}$  with  $\Delta_{1\mathbf{k}} = \Delta_{2\mathbf{k}} = \Delta_{\mathbf{k}}$  for simplicity. Extensive work on this Hamiltonian can be found in Ref. 9.

In order to calculate the linear response of the system to the external electromagnetic field, we modify  $H_c$  with the phase factor mentioned before and follow the same procedure to derive the current  $j_c = j_p + j_d$ . Then, we obtain

$$j_p = \frac{edt_0}{2} \sum_{\mathbf{k}} \sin(k_z d/2) \hat{C}_{\mathbf{k}}^+ \hat{\sigma}_1 \otimes \hat{\tau}_0 \hat{C}_{\mathbf{k}}, \quad (11)$$

where  $d/2$  is the distance between a plane and a chain and  $\hat{\sigma}_1$  is a Pauli matrix in the plane-chain space, and  $j_d = e^2 (d/2)^2 H_c A_z$ , where  $H_c = \sum_{\mathbf{k}} t(k_z) \hat{C}_{\mathbf{k}}^+ \hat{\sigma}_1 \otimes \hat{\tau}_3 \hat{C}_{\mathbf{k}}$ . The  $c$ -axis conductivity for  $\mathbf{q} = 0$ ,  $\sigma_c(0, \omega)$ , of the system is also derived to be  $\sigma_c(0, \omega) = (i/\omega) [\Pi(0, \omega) - e^2 (d/2)^2 \langle H_c \rangle]$ , where

$$\begin{aligned} \Pi(0, \omega) &= (edt_0)^2 T \sum_{\omega'} \sum_{\mathbf{k}} \sin^2(k_z d/2) \\ &\times \text{Tr}[\hat{\sigma}_1 \otimes \hat{\tau}_0 \hat{G}(\mathbf{k}, \omega') \hat{\sigma}_1 \otimes \hat{\tau}_0 \hat{G}(\mathbf{k}, \omega' + \omega)], \end{aligned} \quad (12)$$

and

$$\begin{aligned} \langle H_c \rangle &= t_0^2 T \sum_{\omega} \sum_{\mathbf{k}} \cos^2(k_z d/2) \text{Tr}[\hat{\sigma}_1 \otimes \hat{\tau}_3 \hat{G}(\mathbf{k}, \omega) \hat{\sigma}_1 \\ &\otimes \hat{\tau}_3 \hat{G}(\mathbf{k}, \omega)], \end{aligned} \quad (13)$$

with  $\hat{G}(\mathbf{k}, \tau) = -\langle \mathcal{T} \hat{C}_{\mathbf{k}}(\tau) \hat{C}_{\mathbf{k}}^+(0) \rangle$ , which is a  $(4 \times 4)$  matrix. The Green's function  $\hat{G}(\mathbf{k}, \omega)$  is given by  $\hat{G}(\mathbf{k}, \omega) = (i\omega - \hat{h}_{\mathbf{k}})^{-1}$ . We emphasize that the Hamiltonian in this model is quite different from the usual macroscopic tunneling Hamiltonian,<sup>17</sup> for which, for example,  $\hat{G}_{13}(\mathbf{k}, \tau) = -\langle \mathcal{T} [C_{1\mathbf{k}\uparrow}(\tau) C_{2\mathbf{k}\uparrow}^+(0)] \rangle$  is not allowed because each layer

is independent (as is the case for the previous coupling model); however, it is possible in the present model because of the hybridization through the chain between the two Fermi surfaces of plane and chain. Introducing a unitary matrix  $U$  which diagonalizes  $\hat{h}_{\mathbf{k}}$ , one can show  $\hat{G}_{ij}(\mathbf{k}, \omega) = \sum_{m=1}^4 U_{im} U_{mj}^+ / (i\omega - E_m)$ , where  $E_m = \pm E_{\pm}$  if  $\Delta_{1\mathbf{k}} = \Delta_{2\mathbf{k}}$ .

$\langle H_c \rangle$  becomes complicated and the energy dispersion in the chain is quite different from that in the plane so that a numerical calculation is required to see if the difference between  $\langle H_c \rangle^s$  and  $\langle H_c \rangle^n$  is negligible. However, since  $t_0$  in Eq. (13) is assumed small we may expand  $\langle H_c \rangle$  in terms of  $t_0$  and keep only the leading order, which is  $t_0^2$ . This case includes only interband Hamiltonian but is still very interesting as it can exhibit a  $c$ -axis pseudogap.<sup>10</sup> In this approximation with  $\Delta_{1\mathbf{k}} = \Delta_{2\mathbf{k}} = \Delta_{\mathbf{k}}$  and for  $\mu' = \mu$  as a special case,  $\langle H_c \rangle^s$  becomes

$$\langle H_c \rangle^s = -4T \sum_{\omega} \sum_{\mathbf{k}} t(k_z)^2 \frac{\omega^2 - \xi_1 \xi_2 + \Delta_{\mathbf{k}}^2}{(\omega^2 + \xi_1^2 + \Delta_{\mathbf{k}}^2)(\omega^2 + \xi_2^2 + \Delta_{\mathbf{k}}^2)}. \quad (14)$$

Note that  $\langle H_c \rangle^s$  in Eq. (14) is almost same as  $\langle H_c \rangle^s$  in Eq. (8) for the simple coherent coupling case except that now  $\xi_1 \neq \xi_2$  and  $d/2$  appears rather than  $d$  in  $t(k_z)$ . One, therefore, may expect that  $\delta \langle H_c \rangle$  will vanish to order  $(\Delta(T)/\omega_c)^2$ . It is obvious that  $\delta \langle H_c \rangle$  is identically zero along the nodal lines, and  $\delta \langle H_c \rangle$  is largest along the antinodal directions. Since  $\xi_1 = k^2/2m - \mu$  and  $\xi_2 = k_y^2/2m - \mu$ , we introduce  $\xi = \xi_1$ , then  $\xi_2 = \xi \sin(\phi)^2 - \mu \cos(\phi)^2$ . If  $\phi = \pi/2$ , then  $\xi_2 = \xi$ ; therefore, it can be seen that  $\delta \langle H_c \rangle_{\phi=\pi/2}$  is of the order of  $(\Delta/\omega_c)^2$ . For  $\phi = 0$ ,  $\xi_2 = -\mu$  and it can be shown that

$$\begin{aligned} \langle H_c \rangle_{\phi=0}^s &\approx 2N(0) \sum_{k_z} t_1^2 \int_{-\omega_c}^{\omega_c} d\xi \left[ \frac{\mu}{\xi^2 - \mu^2} \tanh\left(\frac{\mu}{2T}\right) \right. \\ &\left. - \frac{\xi^2}{(\xi^2 - \mu^2) \sqrt{\xi^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\xi^2 + \Delta^2}}{2T}\right) \right]. \end{aligned} \quad (15)$$

Now, the leading order of  $\delta \langle H_c \rangle_{\phi=0}$  changes to  $(\Delta/\mu)^2$ . It is possible to show that for an arbitrary  $\phi$ , as long as  $\mu$  and  $\omega_c \gg \Delta$ ,  $\delta \langle H_c \rangle_{\phi}$  is negligible, and consequently, the FGT sum rule is not violated in the plane-chain coupling model.

In a numerical calculation for the general case without the above simplification, we have computed  $\delta \langle H_c \rangle / \langle H_c \rangle^s$ , which is the fractional change in kinetic energy. We have taken  $\xi_2 = k_y^2/2m - \mu'$  for the chain energy dispersion, where  $\mu'$  is a chemical potential in the chain. For simplicity, we also assume  $\mu' = \mu$ . It has been shown that  $\mu' - \mu (\ll \mu)$  may correspond to the pseudogap seen in the  $c$ -axis response of overdoped YBCO,<sup>10</sup> however, it makes no difference in the numerical evaluation of  $\delta \langle H_c \rangle / \langle H_c \rangle^s$ . We choose  $T = 12$  K,  $\Delta(T) = 20$  meV,  $t_0 = 2$  meV,  $\mu = 500$  meV and  $\omega_c = 400$  meV. We found that  $\delta \langle H_c \rangle / \langle H_c \rangle^s$  becomes more negligible as we increase the summation range of the Matsubara frequency  $\omega$ . For  $|\omega| \leq 200\pi T$ ,  $\delta \langle H_c \rangle / \langle H_c \rangle^s \approx 8.8 \times 10^{-3}$ , and for  $|\omega| \leq 2000\pi T$ ,  $\delta \langle H_c \rangle / \langle H_c \rangle^s \approx 5.4 \times 10^{-3}$ .

One may consider a plane-plane coupling through a chain. In order to investigate the  $c$ -axis kinetic energy for

such a coupling, one needs to replace  $\xi_2$  and  $\Delta_2$  with  $\xi_1$  and  $\Delta_1$ , respectively. For the hopping amplitude,  $t(k_z)$  can be simply changed to  $t(k_z)^2$  because the plane-chain and chain-plane distances are the same and equal to  $d/2$ . Then, one can algebraically show that  $\delta\langle H_c \rangle$  is as negligible as before. It is also possible to see that  $\delta\langle H_c \rangle$  has a symmetry with respect to  $\xi_1 \leftrightarrow \xi_2$  and  $\Delta_1 \leftrightarrow \Delta_2$ ; in other words,  $\delta\langle H_c \rangle$  for the *chain-plane* coupling is the same as that for the *plane-chain* coupling. Therefore, it implies that  $\delta\langle H_c \rangle$  along the  $c$  axis is conserved for coherent coupling.

So far we have taken the density of states as a constant:  $N(\xi) = N(0)$  ( $-\omega_c \leq \xi \leq \omega_c$ ) and concluded that the difference of the  $c$ -axis electronic kinetic energies between normal and superconducting state is negligible. Now we would like to consider the effect of  $N(\xi)$  on the sum rule when it is a function of  $\xi$  to illustrate possible changes. If it varies strongly with  $\xi$ , it clearly cannot be approximated by  $N(0)$ . We Taylor expand  $N(\xi)$  up to  $\xi^2$  near  $\xi=0$ . Then,  $N(\xi) = N(0) + \xi \partial N(\xi)/\partial \xi|_0 + (\xi/2)^2 \partial^2 N(\xi)/\partial \xi^2|_0$ . At  $T=0$ ,  $\langle H_c \rangle^n$  of Eq. (7) does not change; however, Eq. (8) for  $\langle H_c \rangle^s$  changes due to  $(\xi/2)^2 N''(0)$ , where  $N''(0) = \partial^2 N(\xi)/\partial \xi^2|_0$ . Assuming  $t_\perp$  in Eqs. (7) and (8) does not depend on  $\phi$ , we obtain

$$\delta\langle H_c \rangle / \langle H_c \rangle^n \approx [8N(0)]^{-1} N''(0) \Delta(0)^2 \ln[\omega_c / \Delta(0)]. \quad (16)$$

Note that this correction can have either sign depending on the sign of the second derivative. For  $N''(0)/N(0) \sim 1/\omega_c^2$ ,  $\delta\langle H_c \rangle / \langle H_c \rangle^n \sim x^{-1.65}$ , where  $x = \omega_c / \Delta(0)$ , because  $\ln(x)/x^2 \approx x^{-1.65}$  when  $x \gg 1$ . If  $N''(0)/N(0) \sim 1/(\Delta(0)\omega_c)$ , then  $\delta\langle H_c \rangle / \langle H_c \rangle^n \sim x^{-0.65}$ ; thus,  $\delta\langle H_c \rangle$  is considerable. For this to be the case  $N''(0)$  needs to exhibit variation on an energy scale of order  $\Delta$  rather than  $\omega_c$ . In a realistic model a Taylor expansion about  $\xi=0$  may not be accurate but our calculations serve to illustrate the main point. Violation of the FGT sum rule of either sign can result

from an energy dependence in the in-plane electronic density of states  $N(\xi)$ . The exact amount depends on details and cannot be known without a specific knowledge of the band structure involved. In-plane dynamics gets reflected in  $c$ -axis properties.

For coherent interlayer coupling between  $\text{CuO}_2$  planes the superfluid density is equal to the missing optical weight; the FGT sum rule is satisfied. This applies even in more realistic model for YBCO around optimum doping such as the plane-chain model with two atoms per unit cell. On the other hand incoherent  $c$ -axis coupling mediated through impurity scattering gives a sum rule which is always larger than one and is in disagreement with experiment. To get the sum rule to be less than one as is observed in underdoped YBCO and other systems such as optimally doped Tl2201, it may be necessary to go to more exotic non-Fermi liquid pseudogap model for the in-plane motion as discussed recently by Ioffe and Millis.<sup>18</sup> Their arguments, however, do not apply to optimally doped Tl2201 because this system does not show a pseudogap. Their pseudogap argument that leads to the cancellation of  $G(\mathbf{k}, \omega)$  and  $G_0(\mathbf{k}, \omega)$  contribution to the ratio of missing area to superfluid density making it one half instead of one for the preformed pair model was made for coherent  $c$ -axis coupling, but we find it also applies to the incoherent case.<sup>15</sup> Another interesting model for the in-plane dynamics is the “mode” model of Norman *et al.*<sup>19</sup> introduced from consideration of ARPES data. In more conventional models a sum rule violation of either sign can also be obtained if there is a strong energy dependence to the density of states near the Fermi surface on the scale of a few times the gap.

W.K. is grateful to N. D. Whelan and C. Kallin for useful discussions, and J.P.C. to D. Basov for discussions. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) and by the Canadian Institute for Advanced Research (CIAR).

<sup>1</sup>P. W. Anderson, *The Theory of Superconductivity in the High- $T_c$  Cuprates* (Princeton Univ. Press, Princeton, NJ, 1997); P. W. Anderson, *Science* **279**, 1196 (1998).  
<sup>2</sup>E. H. Kim, *Phys. Rev. B* **58**, 2452 (1997).  
<sup>3</sup>S. Chakravarty, *Eur. Phys. J. B* **5**, 337 (1998).  
<sup>4</sup>J. E. Hirsh, *Physica C* **199**, 305 (1992); **201**, 347 (1992).  
<sup>5</sup>D. N. Basov *et al.*, *Science* **283**, 49 (1999).  
<sup>6</sup>R. A. Ferrel and R. E. Glover, *Phys. Rev.* **109**, 1398 (1958); M. Tinkham and R. A. Ferrel, *Phys. Rev. Lett.* **2**, 331 (1959).  
<sup>7</sup>D. N. Basov (unpublished).  
<sup>8</sup>A. S. Katz *et al.*, *Phys. Rev. B* **61**, 5930 (2000).  
<sup>9</sup>W. A. Atkinson and J. P. Carbotte, *Phys. Rev. B* **52**, 10 601 (1995); **55**, 3230 (1997); **55**, 12 748 (1997).  
<sup>10</sup>W. C. Wu, W. A. Atkinson, and J. P. Carbotte, *J. Supercond.* **11**, 305 (1998).  
<sup>11</sup>P. J. Hirschfeld, S. M. Quinlan, and D. J. Scalapino, *Phys. Rev. B* **55**, 12 742 (1997).

<sup>12</sup>R. J. Radtke, V. N. Kostur, and K. Levin, *Phys. Rev. B* **53**, R522 (1996).  
<sup>13</sup>M. V. Klein and G. Blumberg, *Science* **283**, 42 (1999).  
<sup>14</sup>S. Chakravarty, H. -Y. Kee, and E. Abrahams, *Phys. Rev. Lett.* **82**, 2366 (1999).  
<sup>15</sup>We assume the infinite band approximation ( $\omega_c \rightarrow \infty$ ) for simplicity. However, it is generally true even for a finite  $\omega_c$ . Note that  $|V(\phi_k, \phi_p)|^2$  is positive definite. For more details see W. Kim, N. D. Whelan, and J. P. Carbotte (unpublished).  
<sup>16</sup>K. Zhang *et al.*, *Phys. Rev. Lett.* **73**, 2484 (1994); D. N. Basov *et al.*, *ibid.* **74**, 598 (1995).  
<sup>17</sup>See, for example, G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1990).  
<sup>18</sup>L. B. Ioffe and A. J. Millis, *Science* **285**, 1241 (1999).  
<sup>19</sup>M. R. Norman *et al.*, cond-mat/9912043, *Phys. Rev. B* (to be published).