

Optical Excitations From a Flux Phase

M.J. Rice and Y.R. Wang

Materials Research Laboratory, Xerox, Webster Research Center, Webster, NY 14580, USA
and

E.J. Mele

Department of Physics, University of Pennsylvania, Philadelphia, PA 19104, USA

We calculate the optical conductivity $\sigma(\omega)$ of a model "flux phase," i.e., a condensed many-fermion state on a two-dimensional lattice characterized by nonvanishing orbital currents of the underlying fermions. In addition to a Drude-like term, it is found that there is a temperature (T) independent broad band absorption corresponding to vertical interband excitations near a point Fermi surface. Scattering of the quasi-particle excitations by acoustic phonons leads to a resistivity that is proportional to T , even as $T \rightarrow 0$.

A number of recent theoretical studies have been suggesting that a novel form of quantum dynamics can occur in the ground state of a strongly correlated fermion system on a two dimensional (2D) lattice. The discussions of references 1-7 have examined the possibility of the stabilization of a "flux phase," namely, a condensed many body state characterized by nonvanishing orbital currents of the underlying fermions. These phases are condensed "spin liquid" states, which nonetheless exhibit ordering of a superlattice of orbital currents around the elementary plaquettes of the underlying Bravais lattice. A number of workers have suggested that states of this form provide an appropriate description of the dynamics of a resonating-valence-bond (RVB) state near the half filled band, and, in a recent communication,⁷ one of us noted that a simple construction for a class of Gutzwiller projected singlet spin liquid states naturally leads to states of this form for general band filling in the 2D problem.

A unique feature common to all (or nearly all) of the treatments of these orbitally ordered flux phases is the appearance of singular points in k -space for the quasiparticle dispersion relations. The Fermi surface for the effective fermions of the theories of references 1-7 are shrunk to a pair of fermi points, and locally exhibit the dispersion relation of a massless Dirac cone. The resulting quasiparticle dispersion relation and spectral density exhibit the form expected for a prototypical two dimensional semimetal, with a spectral density vanishing linearly in E near the effective Fermi energy. In the theory of reference 7, applied off of the half filled band, the single particle excitations around this cone are *charged* excitations and can be excited optically. In this paper we pursue this idea and investigate the temperature and frequency dependence of the resulting optical excitation spectrum for such a system. The excitation spectrum that we obtain is unusual and quite interesting, consisting of a low frequency intraband part, and a higher frequency interband contribution. The first of these may be regarded as a strongly temperature dependent free particle absorption, roughly analogous to the Drude absorption expected for a simple metal, and results from the thermally excited free carrier density around the effective Fermi energy. The second piece is a relatively structureless, temperature *independent* broad band excitation spectrum resulting from vertical interband excitations near the point Fermi surfaces. We also find that scattering of the quasi-particle excitations by acoustic phonons leads to a resistivity that is proportional to temperature (T), even as $T \rightarrow 0$.

We carry out calculations on the simplest flux phase model exhibiting the point fermi surfaces. In this model the ordering of the orbital currents around the

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elementary plaquettes of a square lattice assumes the form of a $\sqrt{2} \times \sqrt{2}$ superlattice. In this case, the fermions move in an effective vector potential \mathbf{A} which generates one-half of a flux quantum (ϕ_0) of circulation in each plaquette, there being one fermion per two lattice points. We will assume that in the absence of \mathbf{A} the spinless fermion kinetic energy is specified by a nearest-neighbor tight binding Hamiltonian with hopping integral t . In the presence of \mathbf{A} , the hopping integral is modified according to

$$t_{\ell,j} = t \exp\left((2\pi i/\phi_0) \int_{\ell}^j d\ell \cdot \mathbf{A}\right)$$

where j and ℓ are neighboring lattice points. For the present problem the effect of \mathbf{A} can be conveniently treated by alternating the *sign* of t along rows of atoms, say those along the x -axis. In this arrangement the phase of the sign alternation of successive rows has to be staggered by one bond distance, a . The Hamiltonian describing our problem is therefore

$$H = -t \sum a_j^+ (b_{j+\tau} - b_{j-\tau} + b_{j+\sigma} + b_{j-\sigma}) \quad (1)$$

where a_j^+ , a_j and b_j^+ , b_j are fermion operators which create or destroy fermions at "a" and "b" sites, respectively. An a-site has a reversed sign of t to its left, while a b-site has a reversed sign of t to its right. The summation in (1) is over the $(N/2)$ a-sites, labelled by j , where N ($N \rightarrow \infty$) denotes the total number of lattice sites. The quantities $\tau = a\hat{x}$ and $\sigma = a\hat{y}$ denote the nearest neighbor separations along the x and y axes, respectively.

We should point out that the stable flux phases off the half filled band for doping concentration, c , will generally lead to a $n \times m$ flux superlattice where $mn=q$ and where $(1-c)/2=p/q$, p and q being integers.⁷ We expect that the features associated with the Dirac cone in these generalized flux phases will be closely analogous to the analytically simpler $\sqrt{2} \times \sqrt{2}$ situation considered here.

The Hamiltonian (1) is readily diagonalized to give the fermion spectrum

$$\varepsilon_{\pm}(\mathbf{k}) = \pm 2t [\sin^2(k_x a) + \cos^2(k_y a)]^{1/2} = \pm E_{\mathbf{k}} \quad (2)$$

where the wavevectors \mathbf{k} lie in the first Brillouin zone of the doubled unit cell. This spectrum has been obtained by Baskaran, Tosatti and Yu³ in a related boson problem where only states at the bottom of the lower band are of interest. In the present fermion problem, however, the lower, negative energy, sub-band is completely filled at $T=0$, while the upper, positive energy, sub-band is completely empty. In terms of the creation and annihilation operators, $\alpha_{\mathbf{k}}^+$, $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}^+$, $\beta_{\mathbf{k}}$, for the positive and negative energy states, respectively, the diagonalized Hamiltonian is

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} (\alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} - \beta_{\mathbf{k}}^+ \beta_{\mathbf{k}}) \quad (3)$$

The remarkable property of this fermion system is that its Fermi surface consists of two points, namely, $(0, (\pi/2a))$ and $(0, -(\pi/2a))$, where the first component refers to k_x . Let us denote these points by k_s , where $s=\pm 1$ refers to the sign of k_x . In their region, the band energies are, from Eq. (2), $\epsilon_{k_s} = \pm \hbar v |k - k_s|$, where v is the characteristic velocity $v=(2ta/\hbar)$. Thus, in the region of the "Fermi energy," the fermion exhibit the dispersion relation of a massless Dirac cone and a density of states $\rho(E) = (a^2 / \pi \hbar^2 v^2) |E|$ vanishing linearly in E . In Fig. 1, we show the total density of states function $\rho(E)$ calculated over the entire band width $W=4\sqrt{2}t$.

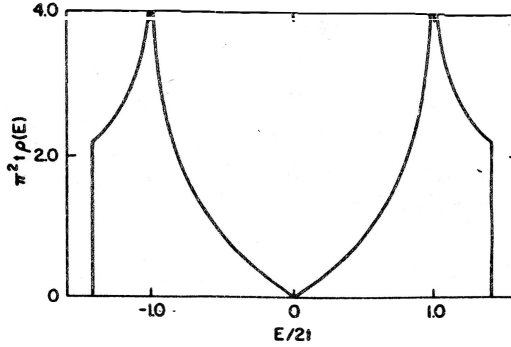


Fig. 1. Density of states of the flux phase. The chemical potential lies at the center of the band.

The complex optical conductivity $\sigma(\omega) = \sigma_1(\omega) + i \sigma_2(\omega)$ is readily obtained from the standard Kubo formula. With $1/d$ parallel layers per unit length along the z -axis we find

$$\sigma_1(\omega) = (\pi e^2 v^2 / A d) \sum_{\mathbf{k}} \cos^2(k_x a) \left\{ 2 \sin^2(\Phi_{\mathbf{k}}) (-\partial n_{\mathbf{k}} / \partial E_{\mathbf{k}}) \delta(\omega) \right. \\ \left. + \cos^2(\Phi_{\mathbf{k}}) \tanh(\beta E_{\mathbf{k}} / 2) \omega^{-1} \delta(2E_{\mathbf{k}} - \omega) \right\} \quad (4)$$

$$\sigma_2(\omega) = (v^2 e^2 / A d) \sum_{\mathbf{k}} \cos^2(k_x a) \left\{ 2 \sin^2(\Phi_{\mathbf{k}}) (-\partial n_{\mathbf{k}} / \partial E_{\mathbf{k}}) \omega^{-1} \right. \\ \left. - \cos^2(\Phi_{\mathbf{k}}) (\omega / E_{\mathbf{k}}) (4E_{\mathbf{k}}^2 - \omega^2)^{-1} \tanh(\beta E_{\mathbf{k}} / 2) \right\} \quad (5)$$

In these expressions $\tan \Phi_{\mathbf{k}} = \sin(k_x a) / \cos(k_y a)$ and $n_{\mathbf{k}} = 1 / (\exp(\beta E_{\mathbf{k}}) + 1)$ is the Fermi-Dirac function (We note that the numerical value of the chemical potential is zero and independent of temperature because of the symmetry of $\rho(E)$ about $E=0$). The first terms in $\sigma_1(\omega)$ and $\sigma_2(\omega)$ are *intra*band contributions arising from fermion and hole quasi-particles thermally excited in the region of the Fermi points. The second terms in Eqs. (4) and (5) correspond to real and virtual *inter*band transitions across the pseudo gap separating the negative energy fermions from the positive energy fermions.. In our subsequent calculations we shall introduce the following replacements in the Drude-like contributions to $\sigma_1(\omega)$ and $\sigma_2(\omega)$; $\delta(\omega) \rightarrow \tau / (1 + \omega^2 \tau^2)$, $\omega^{-1} \rightarrow \omega \tau^2 / (1 + \omega^2 \tau^2)$, where τ denotes a phenomenological relaxation time which in general may depend on the fermion energy $E_{\mathbf{k}}$. Such a replacement would

arise, for example, in a simple Boltzmann transport equation treatment of the thermally excited quasi-particles.

For $\hbar\omega$ small by comparison to the band width $W=4\sqrt{2}t$, Eq. (4) for $\sigma_1(\omega)$ may be evaluated analytically to give

$$\sigma_1(\omega) = (e^2/\hbar\pi d)f(\omega, T) + (e^2/8d\hbar) \tanh(\hbar\omega/4k_B T) \tag{6}$$

where the function f is

$$f(\omega, T) = - \int_{-\infty}^{\infty} (dE |E|/2\hbar) (\partial n/\partial E) \tau(E)/(1 + \omega^2 \tau^2(E)) \tag{7}$$

The Drude term in Eq. (6) is similar to that of a classical gas of charged particles. The second, interband, term in Eq. (6) has a most interesting form: for $\hbar\omega \ll 4k_B T$ it is proportional to $(\hbar\omega/k_B T)$, while for $\hbar\omega \gg 4k_B T$ it is a constant, independent of both temperature and frequency. The frequency dependence predicted by Eq. (6) is shown in Fig. 2, where we have calculated $\sigma_1(\omega)$ for the parameter choices $(e^2/2dt)=2$, $(k_B T/2t)=0.03$, and an energy independent τ of magnitude $\tau=(20\hbar/2t)$. Both the Drude and interband components are separately indicated. The panel in Fig. 2 compares the frequency dependences of $\sigma_1(\omega)$ calculated for the two temperatures $(k_B T/2t) = 0.015$ and $(k_B T/2t) = 0.03$.

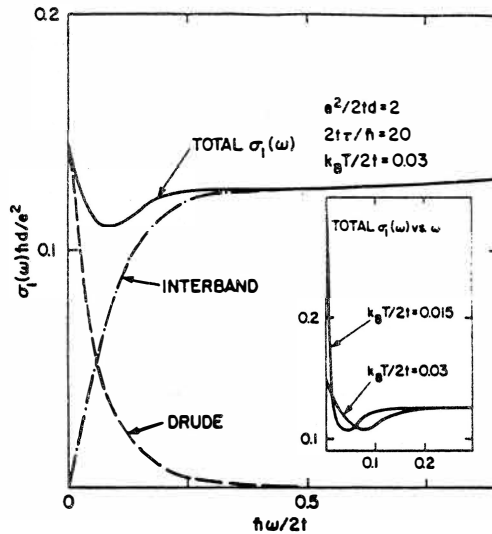


Fig. 2. $\sigma_1(\omega)$ versus ω . The Drude-like and interband components are indicated. The panel compares the frequency dependences of $\sigma_1(\omega)$ for the two different temperatures indicated.

Finally, we derive a qualitative expression for the “Drude” relaxation time τ for a specific model scattering mechanism, namely, the scattering of the fermion quasi-particles by a 2D acoustic phonon field. We assume that the site energies of the a and b sites are modulated by the amounts

$$C \Delta_j = C \sum_q \exp(i\mathbf{q} \cdot \mathbf{R}_j) |q| u_q (d_q + d_{-q}^+) \quad (8)$$

where Δ_j is the dilation and C is a deformation coupling constant. In Eq. (8) $u_q = (\hbar/2MN\omega_q)^{1/2}$ is the zero-point motion contributed by the phonon whose frequency is $\omega_q = sq$, d_q^+ and d_q^- are phonon creation and destruction operators, s is the sound velocity, and M is a mean ionic mass. Making use of the Fermi rule to estimate a scattering time, we find an energy-dependent quasi-elastic relaxation time

$$(1/\tau_k) \sim (\pi C^2 a^2 k_B T \rho(E_k) / 2MAs^2) \quad (9)$$

Provided that $v \gg s$, this result is valid for *arbitrary low temperatures*. The reason for this is that the point Fermi surface limits the largest energy of a phonon exchanged in the scattering to $\hbar\omega_p = \hbar s 2k \sim 4k_B T (s/v)$ typically. In an ordinary metal $\hbar\omega_p \sim \hbar s 2k_F$, where k_F is the Fermi wavevector. Eq. (9) shows that $\tau_k \propto (1/k_B T E_k)$. Thus, in view of Eqs. (6) and (7) this leads to a resistivity proportional to T , even in the limit $T \rightarrow 0$.

The theoretical results obtained in this paper bear an interesting resemblance to the observed⁸ normal state optical conductivity of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and doped La_2CuO_4 . In particular, our theoretical computation of $\sigma_1(\omega)$ presented in Fig. 2 is strikingly similar to the normal state optical conductivity deduced by Timusk et al.⁹ and by Orenstein et al.¹⁰ from Kramers-Kronig transformation of reflectivity measurements on $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. Their data for $\sigma_1(\omega)$ can be described by a low-frequency Drude absorption that tracks the temperature dependence of the d.c. conductivity ($\sigma_{dc} \propto T^{-1}$) and a relatively structureless, temperature independent broad "midinfrared" band. This suggests the intriguing possibility that the normal state of the quasi-2D electron system in the copper oxide superconductors exhibits the correlated behavior of a flux phase. We are currently exploring these ideas.

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References and Footnotes

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