Optical Excitations From a Flux Phase

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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 $T \to 0$.

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 resisitivity that is proportional to temperature (T), even as $T \to 0$.

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 **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 **A** the spinless fermion kinetic energy is specified by a nearest-neighbor tight binding Hamiltonian with hopping integral t. In the presence of **A**, the hopping integral is modified according to

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

where j and ℓ are neighboring lattice points. For the present problem the effect of **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

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

where a^{+}_{j}, a_j and b^{+}_{ℓ}, b_ℓ 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→∞) 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 x 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 $\sqrt{2}$ x $\sqrt{2}$ situation considered here.

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

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

where the wavevectors k lie in the first Brillouin zone of the doubled unit cell. This spectrum has been obtained by Baskaran, Tosatti and Yu[3] 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, α^{+}_{k}, α_k and β^{+}_{k}, β_k, for the positive and negative energy states, respectively, the diagonalized Hamiltonian is

$$H = \sum_{k} E_{k} (\alpha_k^{+} \alpha_k - \beta_k^{+} \beta_k) \qquad (3)$$

The remarkable property of this fermion system is that its Fermi surface consists of two points, namely, (0, (π/2a)) and (0,-(π/2a)), where the first component refers to k_x. Let us denote these points by k_s, where s=±1 refers to the sign of k_y. In their region, the band energies are, from Eq. (2), $\epsilon_{k,s} = \pm \hbar v \mid k - k_s \mid$, where v is the characteristic velocity v=(2ta/$\hbar$). Thus, in the region of the "Fermi energy," the fermions exhibit the dispersion relation of a massless Dirac cone and a density of states $\rho(E) = (a^2 / \pi \hbar^2 v^2) \mid E \mid$ 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.

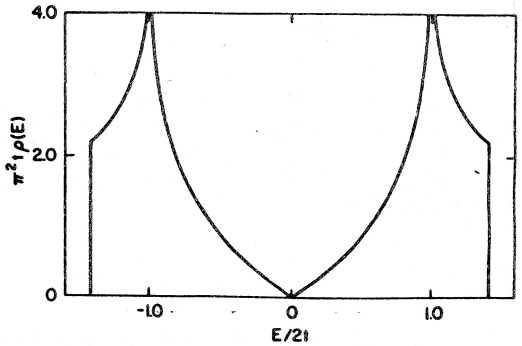

Fig. 1. Density of states of the flux phase. The chemical potential lies at the center of the band.

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

$$\sigma_1(\omega) = (\pi e^2 v^2 / Ad) \sum_k \cos^2(k_x a) \left\{ 2\sin^2(\Phi_k)(-\partial n_k / \partial E_k)\delta(\omega) \right. \tag{4}$$

$$\left. + \cos^2(\Phi_k) \tanh(\beta E_k / 2)\omega^{-1}\delta(2E_k - \omega) \right\}$$

$$\sigma_2(\omega) = (v^2 e^2 / A\,d) \sum_k \cos^2(k_x a) \left\{ 2\sin^2(\Phi_k)(-\partial n_k / \partial E_k)\omega^{-1} \right. \tag{5}$$

$$\left. - \cos^2(\Phi_k)(\omega / E_k)(4E_k^2 - \omega^2)^{-1} \tanh(\beta E_k / 2) \right\}$$

In these expressions $\tan\Phi_k = \sin(k_x a)/\cos(k_y a)$ and $n_k = 1/(\exp(\beta E_k)+1)$ 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 *intraband* 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 *interband* 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 $\sigma_2(\omega)$; $\delta(\omega) \to \tau / (1 + \omega^2 \tau^2)$, $\omega^{-1} \to \omega\tau^2 / (1 + \omega^2 \tau^2)$, where τ denotes a phenomenological relaxation time which in general may depend on the fermion energy E_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

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

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 $\hbar\omega << 4k_BT$ it is proportional to $(\hbar\omega/k_BT)$, while for $\hbar\omega >\sim 4k_BT$ 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 $(e^2/2dt)=2$, $(k_BT/2t)=0.03$, 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 $(k_BT/2t) = 0.015$ and $(k_BT/2t) = 0.03$.

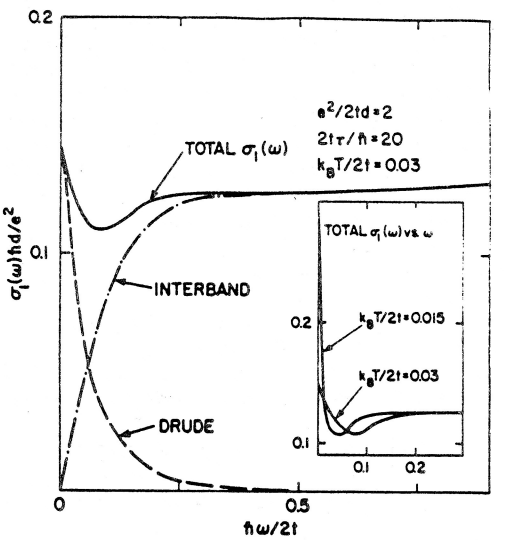

Fig. 2. $\sigma_1(\omega)$ versus ω. The Drude-like and interband components are indicated. The panel compares the frequency dependences of $\sigma_1(\omega)$ for the two different temperatures indicated.

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

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

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 the sound velocity, and M a mean ionic mass. Making use of the Fermi rule to estimate a scattering time, we find an energy-dependent quasi-elastic relaxation time

$$(1/\tau_k) \sim (\pi C^2 a^2 k_B T \rho(E_k)/2M\hbar s^2) \qquad (9)$$

Provided that v>>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 $\hbar\omega_p = \hbar s2k \sim 4k_BT(s/v)$ typically. In an ordinary metal $\hbar\omega_p \sim \hbar s2k_F$, where k_F is the Fermi wavevector. Eq. (9) shows that $\tau_k \alpha (1/k_BT E_k)$. Thus, in view of Eqs. (6) and (7) this leads to a resistivity proportional to T, even in the limit T→0.

The theoretical results obtained in this paper bear an interesting resemblance to the observed[8] normal state optical conductivity of $YBa_2Cu_3O_{7-\delta}$ 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 $YBa_2Cu_3O_{7-\delta}$. 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 ($\sigma_{dc} \alpha T^{-1}$) 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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