Holes are not like electrons \([1,2]\). This fundamental fact continues to be ignored in contemporary solid state science \([3]\). By holes and electrons we mean the charge carriers in energy bands in a metal when the Fermi level is near the top and near the bottom of the band respectively.

The physical difference between electron and hole carriers is not captured by Hamiltonians commonly used to study many-body phenomena in solids such as the Hubbard model. Thus, new Hamiltonians need to be considered that contain the fundamental charge asymmetry of condensed matter. The generalized Hubbard model with correlated hopping \([4]\) contains part of the essential physics of electron-hole asymmetry. The other part is incorporated by Hamiltonians that describe also high energy degrees of freedom, which may be generically termed electron-hole asymmetric polaron models \([5,6]\). These models can be formulated with only electronic degrees of freedom \([5]\) (more than one band is needed) or with coupled electronic and bosonic degrees of freedom \([7,8]\). The generalized Hubbard model with correlated hopping is near the top and near the bottom of the band respectively.

We argue that the transport of electricity is fundamentally different when the carriers in the metal are electrons and when they are holes. Holes cause a large disruption in their electronic environment when they propagate, while electrons cause little or no disruption. As a consequence, holes are heavy and electrons are light, and hole transport is largely incoherent. The qualitative difference in the frequency dependent conductivity of electrons and holes is depicted in Figure 1. As the number of physical electrons in a nearly empty band is increased, electrons turn gradually into holes, and become heavier and more incoherent. This is because they become increasingly 'dressed', due to electron-electron interactions, as depicted schematically in figure 2. Conversely, as the number of physical electrons in a nearly full band is decreased, holes turn gradually into electrons, and become lighter and more coherent as they gradually undress. The other way that hole carriers can turn into electrons is by pairing, thereby mimicking locally a situation where the band is less full. As a consequence, superconductivity will be characterized by the carriers becoming lighter and more coherent in the superconducting than in the normal state, and kinetic energy will be lowered \([8,9]\). Since pairing of electron carriers would instead lead to carriers becoming heavier and more incoherent in the superconducting state, and increased kinetic energy, pairing of electron carriers cannot drive superconductivity.

A single electron in an empty band is a non-interacting particle, with spectral function given by

\[
A(k, \omega) = \delta(\omega - \epsilon_k)
\]

with \(\epsilon_k\) the band energy. The single particle spectral function in a many-body system, for momentum \(k\) close to the Fermi surface, is of the form

\[
A(k, \omega) = z\delta(\omega - \epsilon_k) + A'(k, \omega)
\]

where \(z\) is the quasiparticle weight, and \(A'\) is the incoherent part of the spectral function (we have neglected possible dependence of \(z\) on \(k\)). One has in general \(z < 1\), and only for non-interacting particles is \(z = 1\). The normalization condition \(\int A(k, \omega) d\omega = 1\) ensures that \(A'\) will be nonzero whenever \(z < 1\). A single hole in a full band has \(z < 1\) and \(A' \neq 0\), thus is qualitatively different.
from a single electron in an empty band (Eq. (1)) for which \( z = 1 \) and \( A' = 0 \).

The difference between a single electron in an empty band and a single hole in a full band is simplest to understand in a tight binding formulation. Consider as the simplest case the band formed by overlap of 1s orbitals in a lattice of hydrogen-like ions, with nuclear charge \( Z \). The process of creating an electron in the empty 1s orbital (figure 3a)

\[
| \uparrow \rangle = \varphi_{1s}(r) = Ce^{-Zr/a_0}
\]

\((a_0 = \text{Bohr radius})\) does not affect any other degree of freedom. Hence the single particle spectral function is given by

\[
A_0(\omega) = \delta(\omega - \epsilon_{1s})
\]

(with \( \epsilon_{1s} = -13.6 eV \)). Consider instead the process of creating an electron of spin \( \uparrow \) when an electron of spin \( \downarrow \) already exists in the 1s orbital (figure 3b). If the second electron is created in the 1s orbital also, a state of very high energy will result, due to the large Coulomb repulsion between two electrons in that orbital \((17ZeV)\). Instead, consider the ground state of the two-electron ion in the Hartree approximation

\[
| \uparrow \downarrow \rangle = \tilde{\varphi}_{1s}(r_1)\varphi_{1s}(r_2)
\]

\[
\tilde{\varphi}_{1s}(r) = Ce^{-Zr/a_0}
\]

\[
\tilde{Z} = Z - 5/16
\]

To obtain the lowest energy state we want to create the second electron in the expanded orbital \( \tilde{\varphi}_{1s} \), with creation operator \( \tilde{c}_1^\dagger \). We have then

\[
\tilde{c}_1^\dagger| \downarrow \rangle = | \uparrow \downarrow \rangle < \uparrow | \tilde{c}_1^\dagger | \downarrow \rangle + \sum_{l \neq 0} | \uparrow \downarrow \rangle < \uparrow | c_l^\dagger | \downarrow \rangle
\]

\((6)\)

where \(| \uparrow \downarrow \rangle\) are a complete set of excited states of the doubly occupied ion, with energies \( \epsilon_{1s}^{(l)} \). The single particle spectral function for this process is

\[
A_1(\omega) = z_h \delta(\omega - (\epsilon_{1s}^{(0)} - \epsilon_{1s})) + A'_1(\omega)
\]

\(z_h = | < \uparrow | \tilde{c}_1^\dagger | \downarrow \rangle |^2
\]

\(A'_1(\omega) = \sum_{l \neq 0} < \uparrow | c_l^\dagger | \downarrow \rangle |^2 \delta(\omega - (\epsilon_{1s}^{(l)} - \epsilon_{1s}))
\]

\((7c)\)

\(A_2(\omega) = z_h \delta(\omega - (\epsilon_{1s} - \epsilon_{1s}^{(0)})) + A'_2(\omega)
\]

\((8a)\)

\[
A'_2(\omega) = \sum_{l \neq 0} < \uparrow | c_l^\dagger | \downarrow \rangle |^2 \delta(\omega - (\epsilon_{1s}^{(l)} - \epsilon_{1s}))
\]

\((8b)\)

Eqs. (4) and (7), (8) show the fundamental difference between the spectral functions for creating electrons in empty bands and creating or destroying holes in full bands. The qualitative structure does not depend on the Hartree approximation, and illustrates the general fact that the hole spectral function will have a large incoherent contribution and a small quasiparticle weight, as shown schematically in Figure 4. This is due to the physical fact that the spacing between atomic energy levels is smaller than the Coulomb repulsion between electrons in a level, thus when an electron is created in an already occupied level the wavefunctions will expand into other atomic levels. This physics cannot be captured with a single orbital per site \([1]\). This effect then leads to the fundamental difference in the transport properties when the band is almost empty and when it is almost full. For electrons in nearly empty bands the hopping between atoms \( t \) is unrenormalized, while for holes in a full band it is reduced by the quasiparticle weight

\[
t_h = z_h t
\]

\((9)\)

due to the disruption caused in the other electron in the orbital during the hopping process, as depicted schematically in figure 5. This leads to an enhanced effective mass for holes, hence a larger dc resistivity, and to a large incoherent contribution to the frequency dependent conductivity from hopping processes where the electrons end up in excited states.

We can find the quasiparticle weight for the hole explicitly in this Hartree approximation

\[
z_h = | < \varphi_{1s} | \tilde{\varphi}_{1s} > |^2 = \frac{(1 - \frac{5Z}{16})^3}{(1 - \frac{5Z}{32})^6}
\]

\((10)\)

which approaches unity as the nuclear charge \( Z \) increases, and becomes small as \( Z \to 0.3125 \). Even though obtained in the Hartree approximation, the qualitative effect will be generally true (and even larger when one goes beyond the Hartree approximation \([2]\)). When the effective nuclear charge \( Z \) is large \( z_h \to 1 \), hence hole quasiparticles become coherent and light, and resemble electron quasiparticles. Instead, when the effective nuclear charge is small, \( z_h \to 0 \) and holes become very heavy and incoherent. This is the regime most favorable for high temperature superconductivity. Note how this is in qualitative
agreement with the situation in cuprates, where the relevant ions, $O^\infty$, are highly negatively charged, corresponding to a small $Z$. Moreover the entire $CuO$ planes are highly negatively charged, giving rise to highly "floppy" orbitals thus creating the most favorable environment for hole pairing. This also provides a rationale for the advantage of the two-dimensional structure. Since the negative charge needs to be compensated for charge neutrality, one way to do it is to arrange the excess negative charge in the conducting two-dimensional planes where the pairing occurs and the compensating positive charge outside the main conducting structures. It is possible that highly negatively charged conducting substructures could also be created in three-dimensional structures, which would be even more advantageous for high temperature superconductivity since, everything else being equal, higher coordination strongly enhances superconductivity in this model \[13\].

Superconductivity occurs in this theory from the enhanced hopping amplitude when two hole carriers pair. In that case the hopping is $t'_h = \sqrt{\epsilon n_i}$ and the difference $\Delta t = t'_h - t_h$ drives the transition to superconductivity, as discussed in detail elsewhere \[13\]. The superconducting condensation energy is kinetic \[10\], and the quasiparticle weight is larger in the superconducting than in the normal state \[3\].

To study quantitatively the physics described above requires information on excitation energies and matrix elements of electronic states in multi-electron atoms, and is a difficult many-body problem. It is useful to first understand throughly the novel physical phenomena that emerge, for which we can use a variety of model Hamiltonians that contain the essential physics \[6–9\]. As perhaps the simplest realization, consider the site Hamiltonian

$$H_i = \omega_0 a_i^\dagger a_i + g \omega_0 (a_i^\dagger + a_i) n_i^\dagger n_i$$  \hspace{1cm} (11)$$

where $a_i$ is a local boson operator and $n_i,\sigma$ is an electron number operator. This is a special case of the generalized Holstein model discussed in Ref. \[9\], with fully non-linear coupling. Using a generalized Lang-Firsov transformation the following relation between electron particle ($c_i^\dagger$) and quasiparticle ($\tilde{c}_i$) operators results \[3\]:

$$c_i^\dagger = e^{g(a_i^\dagger - a_i)} \tilde{n}_i, - \sigma \tilde{c}_i$$  \hspace{1cm} (12)$$

so that for an empty site, creating an electron particle is the same as creating a quasiparticle

$$c_i^\dagger = c_i^\dagger$$  \hspace{1cm} (13a)$$

and the quasiparticle weight is 1, while instead if the site is already occupied by an electron of opposite spin,

$$c_i^\dagger = e^{g(a_i^\dagger - a_i)} c_i^\dagger$$  \hspace{1cm} (13b)$$

Taking the ground state expectation value of the exponential in Eq. (12) yields

$$< e^{g(a_i^\dagger - a_i) \tilde{n}_i, - \sigma} > = e^{-(g^2/2) \tilde{n}_i, - \sigma}$$  \hspace{1cm} (14)$$

so that the hole quasiparticle spectral weight is

$$z_h = e^{-g^2}$$  \hspace{1cm} (15)$$

and holes become heavily dressed if $g$ is large, while electrons remain undressed. The quasiparticle weight for general electronic band filling $n$ is given by

$$z(n) = \left[ 1 + \frac{n}{2} (e^{-g^2/2} - 1)^2 \right]$$  \hspace{1cm} (16)$$

which interpolates between 1 and $z_h$ and quantifies the magnitude of coherent response of the system for given band filling. The relation Eq. (12) can be written as

$$c_i^\dagger = [1 + (e^{-g^2/2} - 1) n_{i, - \sigma} ] c_i^\dagger + \tilde{n}_{i, - \sigma} \times \text{incoherent part}$$  \hspace{1cm} (17)$$

where the 'incoherent part' describes the processes where bosons are created when the electron is created at the site. This represents the second term in Eq. (6), where the ion ends up in an excited state when the second electron is created. The full Hamiltonian to be studied is then

$$H = \sum_i H_i - \sum_{<ij>} t_{ij} (c_i^\dagger c_j + h.c.) + \sum_{<ij>} V_{ij} n_i n_j$$  \hspace{1cm} (18)$$

with $H_i$ given by Eq. (11). The low energy effective Hamiltonian for quasiparticles that results, using Eq. (14), is

$$H_{eff} = - \sum_{<ij>} t_{ij}^\sigma (c_i^\dagger \tilde{c}_j + h.c.) + \sum_{<ij>} V_{ij} \tilde{n}_i \tilde{n}_j$$  \hspace{1cm} (19a)$$

$$t_{ij}^\sigma = t_{ij} [1 - (1 - \sqrt{\epsilon n}) (\tilde{n}_{i, - \sigma} + \tilde{n}_{j, - \sigma}) + (1 - \sqrt{\epsilon n})^2 \tilde{n}_{i, - \sigma} \tilde{n}_{j, - \sigma}]$$  \hspace{1cm} (19b)$$

which in particular describes the superconducting state \[13\]. However to understand the fundamental processes of spectral weight transfer that occur it is necessary to use the full Hamiltonian Eq. (17) \[13\]. This Hamiltonian predicts that spectral weight will be transferred from the high energy scale determined by $\omega_0$, which represents an electronic excitation energy scale of the multielectron atom, down to low (intraband) energies, both when the system goes superconducting and when it is doped with holes, both in the one-particle spectral function (photomission \[14\]) and in the two-particle spectral function (optical conductivity \[13\]).

We believe that the physics described by these models represents a new paradigm in many-body physics. When the system goes superconducting, hole quasiparticles ‘undress’ and become more like bare particles. In the conventional Fermi liquid approach quasiparticles are fixed objects, that interact weakly with one another and
develop special correlations when a transition to a collective state occurs, but do not change their intrinsic nature. Here instead quasiparticles change their most fundamental properties, their weight and their effective mass, as the ordered state develops. The energy that drives the transition to superconductivity originates in the very large energy renormalization that is involved in going from a description based on bare, strongly interacting particles, to one based on dressed, weakly interacting quasiparticles. The theory of hole superconductivity proposes that holes, by undressing and turning into electrons, manage to take advantage of this rich source of untapped energy.

What are measurable consequences of the fundamental charge asymmetry on which this theory is based? We have shown that it leads to universal asymmetry in NIS tunneling [1], with larger conductance predicted for a negatively biased sample, and to the prediction of positive thermoelectric power for NIS and SIS tunnel junctions [7]. There exists some experimental evidence for the former, while the latter has not been experimentally tested. Furthermore, we have recently proposed that it should lead to negatively charged vortices in the mixed state of type II superconductors, and more generally to a tendency for superconductors to expel negative charge from the bulk [15], leading to higher negative charge density and superfluid density near the surface, as shown schematically in figure 6. Because the principles on which the theory is based are very general, we expect that if the theory is valid it should apply to all superconducting materials [19].

FIG. 1. Qualitative difference between frequency-dependent conductivity when the conduction band is almost empty (electron carriers) and when it is almost full (hole carriers) (schematic). Holes have a large effective mass, resulting in a small value of $\sigma_1(\omega = 0)$, and give rise to a large incoherent contribution to $\sigma_1(\omega)$ extending to frequencies well beyond the band energies. Electrons give rise to Drude-like conductivity with large $\sigma_1(\omega = 0)$ due to their small effective mass.

FIG. 2. When the Fermi level is near the bottom of a band, carriers are undressed, light, coherent, and electron-like. As electrons are added to the band and the Fermi level rises, carriers become increasingly dressed, heavier, incoherent, and hole-like. The thickness of the $\epsilon$ versus $k$ line indicates qualitatively the strength of the quasiparticle weight.

FIG. 3. An electron created in the empty 1s orbital of the ion (a) produces no disruption in another degree of freedom; an electron created in the orbital that is already occupied by another electron (b) will create a disruption of that degree of freedom, and the resulting state can be any of the excited states of the doubly occupied ion. Similarly a hole created in the doubly occupied ion (an electron destroyed) will leave the remaining electron in any of the possible excited states of the singly occupied ion.

FIG. 4. Qualitative difference of single particle spectral functions for particles near the Fermi level for a nearly empty band (electrons) and a nearly full band (holes). For the nearly full band the quasiparticle spectral weight is small and a large incoherent contribution exists. For the nearly empty band the spectral function is entirely coherent.

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FIG. 5. Hopping processes giving rise to conduction when the band is almost empty (a) and when it is almost full (b). In (b) the 'diagonal hopping processes', where the ions make ground state to ground state transitions, involve a rearrangement of the electrons that are not hopping. In addition, the hopping process may lead to the ion making a transition to an excited state.

FIG. 6. Schematic picture of a spherical superconducting body. Negative charge is expelled from the bulk to the surface.
Figure 1

Figure 2

electronic energy band

carriers

Figure 3

(a)  

(b)
A(k, ω)

_atz_ = 1

\text{single electron spectral function}

A(k, ω)

\_zh_ < 1 \_1-zh_

\text{single hole spectral function}

Figure 4

\text{(a) single electron hopping}

\text{(b) single hole hopping}

Figure 5

Figure 6