Appearance of "Fragile" Fermi Liquids in Finite-Width Mott Insulators Sandwiched between Metallic Leads

H. Zenia,[1] J. K. Freericks,[1] H. R. Krishnamurthy,[1,2,3] and Th. Pruschke[4]

[1]*Department of Physics, Georgetown University, Washington, District of Columbia, 20057 USA*
[2]*Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India*
[3]*Condensed Matter Theory Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore 560064, India*
[4]*Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany*

(Received 18 September 2008; published 9 September 2009)

Using inhomogeneous dynamical mean-field theory, we show that the normal-metal proximity effect could force any finite number of Mott-insulating "barrier" planes sandwiched between semi-infinite metallic leads to become "fragile" Fermi liquids. They are fully Fermi-liquid-like at $T = 0$, leading to a restoration of lattice periodicity at zero frequency, with a well-defined Fermi surface, and perfect (ballistic) conductivity. However, the Fermi-liquid character can rapidly disappear at finite ω, V, T, disorder, or magnetism, all of which restore the expected quantum tunneling regime, leading to fascinating possibilities for nonlinear response in devices.

DOI: 10.1103/PhysRevLett.103.116402 PACS numbers: 71.27.+a, 71.10.Fd, 73.21.−b, 73.40.−c

In recent years, there has been significant activity in the study of multilayered heterostructures of strongly correlated materials [1–3]. New physical phenomena have been seen to emerge in the heterostructures that are absent in the bulk materials they are composed from, like the appearance of two-dimensional electron gases at the interfaces between band and Mott insulators [1] and their low-temperature superconductivity [2]. Here, we show the possibility of another such quantum emergent phenomenon, namely, that finite width Mott-insulating "barriers" sandwiched between two metallic leads *become "fragile" Fermi liquids*; i.e., at sufficiently low temperatures, they are described by a robust Fermi-liquid fixed point, and display *perfect dc conductance*, but with finite frequency driving fields (ω), bias voltage (V), temperature (T), disorder, or magnetic order, a conventional quantum tunneling regime characteristic of *N-I-N* junctions (where *N* denotes normal metal and *I* insulator) is quickly restored. The fragility generates possibilities for striking nonlinear responses to these perturbations in these structures, with significant device potential. This is especially true because the Fermi liquids become more fragile the deeper into the barrier one goes.

While this possibility sounds counterintuitive, it arises in a natural way within an inhomogeneous dynamical mean-field theory (IDMFT) [4–6] treatment of the sandwich structure, due to a normal-state proximity effect [7]. At sufficiently high temperatures, the Mott insulator develops a thermal excitation induced (one electron) density of states (DOS) within the Mott gap, and the system conducts electricity. As the temperature is lowered, this DOS decreases, but can never become smaller than the DOS induced via tunneling from the metallic leads. The tunneling DOS at zero frequency decreases exponentially with thickness as one moves deeper into the barrier planes, but never vanishes. Consequently, in a pure system, at $T = 0$, the self-energy at each of the Mott-insulating sites (corresponding to the self-consistently embedded quantum impurity problems that arise in IDMFT) vanishes at $\omega = 0$. Hence, a low-temperature Fermi liquid forms, restoring full periodicity, a well-defined Fermi surface, and zero scattering at $T = 0$. The temperature scale that governs the vanishing of the self-energy is the effective Fermi temperature of the innermost barrier plane; hence, this state will be fragile with respect to increasing T, to the passage of finite ω currents, and to the presence of a voltage across the planes, disorder, or magnetic order in the system (we assume a paramagnetic phase in this work). However, for thin enough barriers, where the low-energy scale is not exponentially small, and quantum fluctuations will suppress magnetic order, one can create unique devices with highly nonlinear properties. For example, the system will pass dc current up to some maximal current with ease, but then rapidly make a transition to a tunneling response as the current gets too large (a current limiter); and similarly, if the driving fields change with too rapid a frequency (a low-pass filter), or if the system is in the presence of a high enough T or applied voltage. Our detailed solution of the IDMFT shows that for ultrathin Mott-layers made up of materials with small Mott gaps there is a wide parameter range where one should be able to see this phenomena experimentally.

We take the Mott-insulating barrier layers of our sandwich structure to be described by the single-band Hubbard model and the metallic leads by the noninteracting tight-binding model. The Hamiltonian for the system can then be written as

$$\mathcal{H} = -\sum_{ij\alpha\sigma} t_{ij}^{\parallel} c_{i\alpha\sigma}^{\dagger} c_{j\alpha\sigma} - t\sum_{i\alpha\sigma}[c_{i\alpha\sigma}^{\dagger} c_{i\alpha+1\sigma} + \text{H.c.}] - \mu\sum_{i\alpha\sigma} c_{i\alpha\sigma}^{\dagger} c_{i\alpha\sigma} + \sum_{i\alpha} U_{\alpha}\left(n_{i\alpha\uparrow} - \frac{1}{2}\right)\left(n_{i\alpha\downarrow} - \frac{1}{2}\right). \quad (1)$$

Here, the label α indexes the planes, and the label i indexes

sites of the two-dimensional square-lattice in each plane. The operator $c^{\dagger}_{i\alpha\sigma}$ ($c_{i\alpha\sigma}$) creates (destroys) an electron of spin σ at site i on the plane α. We set the in-plane hopping $t^{\parallel}$ to be nearest neighbor only, and equal to t, the hopping between planes, so that the lattice structure is that of a simple cubic lattice. The interaction term is written in a particle-hole symmetric fashion, with $U_\alpha = U$ for the barrier planes, and zero for the metallic planes. Hence, the chemical potential μ is equal to zero for half filling, both for the half-filled ballistic metal and the half-filled Hubbard system. The system, assumed to be at half filling, is then particle-hole symmetric; so we drop μ hereafter, and also set $t = 1$.

The many-body problem is solved within a self-consistent IDMFT framework, using the method of Potthoff and Nolting [4–6]. That is, we assume that the self-energy is local and the same for all the sites in a barrier plane, but can vary from plane to plane, i.e., depends on the index α. We label the barrier planes with α values from 1 to N. Thus, $\alpha \geq (N+1)$ or $\alpha \leq 0$ correspond to the metallic layers. Furthermore, because DMFT overestimates magnetic ordering, we assume a paramagnetic regime to suppress the order [8] and then, without loss of generality, drop the spin label. The local Green's function at plane α is found by employing the quantum zipper algorithm. The Green's function is expressed in terms of two continued fractions, one from the left, $L_\alpha(\epsilon, \omega)$ and one from the right, $R_\alpha(\epsilon, \omega)$ as

$$G_\alpha(\omega) = \int d\epsilon \rho_{2d}(\epsilon) \frac{1}{L_\alpha(\epsilon,\omega) + R_\alpha(\epsilon,\omega) - Z_\alpha(\omega) + \epsilon}, \tag{2}$$

where $\rho_{2d}(\epsilon)$ is the noninteracting DOS for the square-lattice and $Z_\alpha(\omega) \equiv \omega - \Sigma_\alpha(\omega)$, with $\Sigma_\alpha(\omega)$, the local self-energy for plane α, being nonzero only for the barrier planes ($1 \leq \alpha \leq N$). L_α and R_α are given by

$$L_\alpha(\epsilon,\omega) = Z_\alpha(\omega) - \epsilon - \cfrac{1}{Z_{\alpha-1}(\omega) - \epsilon - \cfrac{1}{Z_{\alpha-2}(\omega) - \epsilon - \ddots \cfrac{}{Z_1 - \epsilon - 1/[(1/2)(\omega-\epsilon) \pm (1/2)\sqrt{(\omega-\epsilon)^2 - 4}]}}} \tag{3}$$

$$R_\alpha(\epsilon,\omega) = Z_\alpha(\omega) - \epsilon - \cfrac{1}{Z_{\alpha+1}(\omega) - \epsilon - \cfrac{1}{Z_{\alpha+2}(\omega) - \epsilon - \ddots \cfrac{}{Z_N - \epsilon - 1/[(1/2)(\omega-\epsilon) \pm (1/2)\sqrt{(\omega-\epsilon)^2 - 4}]}}}. \tag{4}$$

Furthermore, $L_\alpha(\epsilon,\omega) = g^{-1}_{1d}(\omega - \epsilon) = R_{\alpha'}(\epsilon,\omega)$ for $\alpha \leq 0$ (L_α) and $\alpha' \geq (N+1)$ ($R_{\alpha'}$), where $g^{-1}_{1d}(\omega) \equiv \frac{1}{2}\omega \pm \frac{1}{2}\sqrt{\omega^2 - 4}$ is the inverse local Green's function for a 1D tight-binding band. The $\pm$ sign in the above equations has to be chosen so that in the upper half of the complex ω plane, L_α, R_α and g^{-1}_{1d} are analytic, have a positive imaginary part, and go asymptotically as ω for large $|\omega|$. Thus, we get N separate Anderson impurity problems, one for each barrier plane, which need to be solved to obtain $\Sigma_\alpha(\omega)$. The effective medium or bath Green's function $G_{0\alpha}$ for the αth impurity is determined by the inverse Dyson equation $G^{-1}_{0\alpha} = G^{-1}_\alpha + \Sigma_\alpha$. These are coupled via Eqs. (2)–(4) to determine $G_\alpha(\omega)$, and hence the N bath Green's functions. These self-consistent equations are solved iteratively. The details of the algorithm are described elsewhere [5,6]. Note that $G_\alpha(\omega)$ for the metallic planes do not enter the IDMFT recursions and can be calculated at the end for any α. This is then the IDMFT for a finite number of barrier layers sandwiched between *semi-infinite metallic leads*.

As is well known [9], for a homogeneous Hubbard model, the hybridization parameter for the DMFT self-consistent impurity problem, Γ_0 [$\equiv \mathrm{Im}G^{-1}_0(\omega \approx 0)$], iterates to zero for U sufficiently large, leading to a Mott-insulating solution. In striking contrast, we next show that the DOS for each barrier plane is bounded from below by the tunneling result, whence the hybridization parameter $\Gamma_{0\alpha}$ [$\equiv \mathrm{Im}G^{-1}_{0\alpha}(\omega \approx 0)$] at plane α *cannot iterate to zero* via the self-consistent IDMFT algorithm, and is nonzero for all α. Hence, there is an effective Fermi temperature $T_{F\alpha} \gtrsim \exp[-8U/\pi\Gamma_{0\alpha}]$ for each Mott-insulating plane, such that for $T \ll T_{F\alpha}$ that plane will be in a Fermi-liquid state, leading to a vanishing self-energy at $\omega = 0$ and $T = 0$. For a thick barrier, with a large U, these temperature scales are exponentials of exponentially large negative numbers, and are hence exceedingly small, and would never be observed in the laboratory. But for thin barriers, with a small Mott gap, the effective Fermi temperatures could become high enough to be accessible experimentally.

The tunneling DOS, determined by the proximity effect, gets smaller, and hence the self-energy larger, as we move deeper into the barrier. Therefore, if tunneling dominates

$$|\Sigma_{N/2}(\omega \approx 0)| \gg |\Sigma_{N/2\pm1}(\omega \approx 0)| \gg |\Sigma_{N/2\pm2}(\omega \approx 0)| \gg \cdots \gg |\Sigma_{N/2\pm N/2}(\omega \approx 0)|. \tag{5}$$

Hence, we can write

$$L_\alpha(\epsilon,\omega) \approx Z_\alpha(\omega) - \epsilon + \bar{\gamma}^L_\alpha(\epsilon,\omega); \quad (6)$$

$$R_\alpha(\epsilon,\omega) \approx Z_\alpha(\omega) - \epsilon + \bar{\gamma}^R_\alpha(\epsilon,\omega). \quad (7)$$

Here, $\bar{\gamma}^L_\alpha(\epsilon,\omega) = 1/\Sigma_{\alpha-1}(\omega)$ for $\alpha > 1$, and $\bar{\gamma}^L_1(\epsilon,\omega) = -g_{1d}(\omega-\epsilon)$ for $\alpha = 1$. Similarly, $\bar{\gamma}^R_\alpha(\epsilon,\omega) = 1/\Sigma_{\alpha+1}(\omega)$ for $\alpha < N$, and $\bar{\gamma}^R_N(\epsilon,\omega) = -g_{1d}(\omega-\epsilon)$ for $\alpha = N$. Substituting into Eq. (2), using the result $|\Sigma_\alpha(\omega \approx 0)| \gg |\bar{\gamma}^{L,R}_\alpha(\epsilon,\omega)|$, expanding the asymptotic form of the fraction and performing the integration over ϵ yields

$$G_\alpha(\omega \approx 0) \approx -\frac{1}{\Sigma_\alpha(\omega \approx 0)}\left[1 + \frac{\omega + \gamma^L_\alpha + \gamma^R_\alpha}{\Sigma_\alpha(\omega \approx 0)} + \cdots\right], \quad (8)$$

with $\gamma^{L,R}_\alpha = \int d\epsilon \rho_{2d}(\epsilon)\bar{\gamma}^{L,R}_\alpha(\epsilon,\omega \approx 0)$. Furthermore, $\gamma^L_\alpha = 1/\Sigma_{\alpha-1}(\omega \approx 0)$ for $\alpha > 1$, $\gamma^L_1 = 0.525i$, $\gamma^R_\alpha = 1/\Sigma_{\alpha+1}(\omega \approx 0)$ for $\alpha < N$, and $\gamma^R_N = 0.525i$. Using this result, we obtain

$$\Gamma_{0\alpha} = \mathrm{Im}G^{-1}_{0\alpha}(\omega \approx 0) \approx \mathrm{Im}(\gamma^L_\alpha + \gamma^R_\alpha). \quad (9)$$

In general, this result is a *lower bound* for $\Gamma_{0\alpha}$, as the DOS may never become this small as T is lowered from high temperature; this implies that our estimates for $T_{F\alpha}$ will also be lower bounds (sometimes significantly lower than what the numerics predicts).

The *bulk* insulator phase of the Hubbard model at half filling is characterized by a pole in the self-energy that takes the form

$$\Sigma_{\mathrm{bulk}}(\omega \approx 0) = \frac{r(U)}{\omega + i\delta}, \quad (10)$$

where $r(U)$, the residue of the pole, vanishes when the insulating state is no longer stable, i.e., when $U < U_{c1} \approx 11.4$ for the simple cubic lattice solved with DMFT (the metallic phase disappears for $U > U_{c2} \approx 13.1$). For the heterostructure, it is interesting to explore the consequences of an ansatz of the form

$$\Sigma_\alpha(\omega \approx 0) = \frac{r(U)}{\omega + \gamma^L_\alpha + \gamma^R_\alpha}, \quad (11)$$

which arises in an exact solution of the impurity problem for the Falicov-Kimball model in the insulating phase, and in the Hubbard III approximation for the Hubbard model with the $\Gamma_{0\alpha}$ in Eq. (9). In this case, the imaginary part of the denominator never vanishes and instead is forced to be nonzero due to the normal-state proximity effect. Using this result and the definitions of the γ coefficients, we obtain, for odd N,

$$\Gamma_{0\alpha}(\omega \approx 0) \gtrsim \begin{cases} 0.525/[r(U)]^{\alpha-1} & 1 \le \alpha \le \frac{N-1}{2} \\ 1.05/[r(U)]^{N-1/2} & \alpha = \frac{N+1}{2} \\ 0.525/[r(U)]^{N-\alpha} & \frac{N+3}{2} \le \alpha \le N \end{cases}. \quad (12)$$

Note that this behavior corresponds to an exponential decay of the tunneling DOS at $\omega = 0$, with a correlation length given by $1/\ln r(U)$. In the Falicov-Kimball model on a simple cubic lattice, one has $r(U) = (U^2 - 24)/4$ [10]; for $U = 6$, just slightly above the critical U for the Mott transition at $U_c = 2\sqrt{6}$, the correlation length is 0.62 [6] and the analytic approach predicts it to be 0.92. For the Hubbard model on a simple cubic lattice, a *fit obtained from numerics* (see below) gives $r(U) \simeq (U^2 - U^2_{c1})/4 - 0.13(U - U_{c1}) + 13.4\sqrt{U - U_{c1}} - 52.3\ln(U/U_{c1})$.

The above considerations suggest that at $T = 0$, each barrier plane of the metal-Mott-insulator-metal structure will become a Fermi liquid, leading thereby to a half-filled, simple cubic lattice Fermi surface and perfect (ballistic) conductivity (but a finite conductance due to a finite number of conducting channels). Below, we confirm this by solving the impurity problem on each interacting plane with the numerical renormalization group (NRG) [11], which is the best available impurity solver. We choose the discretization parameter $\Lambda = 2$, and we keep 1200 states at each NRG iteration, and calculate the local DOS or one particle spectral function on different planes, given by $A_\alpha(\omega) = -\mathrm{Im}G_\alpha(\omega)/\pi$.

Figure 1 shows our results for the DOS at the barrier plane for the single-plane barrier ($N = 1$) multilayer, for $T = 0.01$ (about 30 K for a 4 eV bandwidth) and different values of U. Note how one can clearly see the Fermi-liquid coherence peak forming for all values of U, but the coherence is not complete for the larger U values because the effective Fermi temperature of the central plane falls below $T = 0.01$ for those U values; in addition, note how the Fermi peak is narrower for larger U values.

Figure 2 shows our results for a five-plane ($N = 5$) device at three different temperatures for $U = 16$. We see that as the temperature is lowered, the spectral functions on all the layers tend to the noninteracting simple cubic DOS value at $\omega = 0$, but the temperature at which the Fermi peak develops is lower for the deeper planes, and

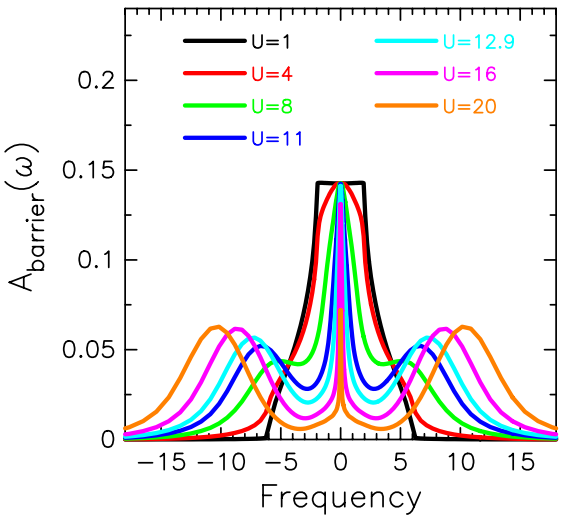

FIG. 1 (color online). Local spectral function at the barrier plane for a single-barrier-plane multilayer, for $T = 0.01$, and a range of U's (increasing from top to bottom near zero frequency).

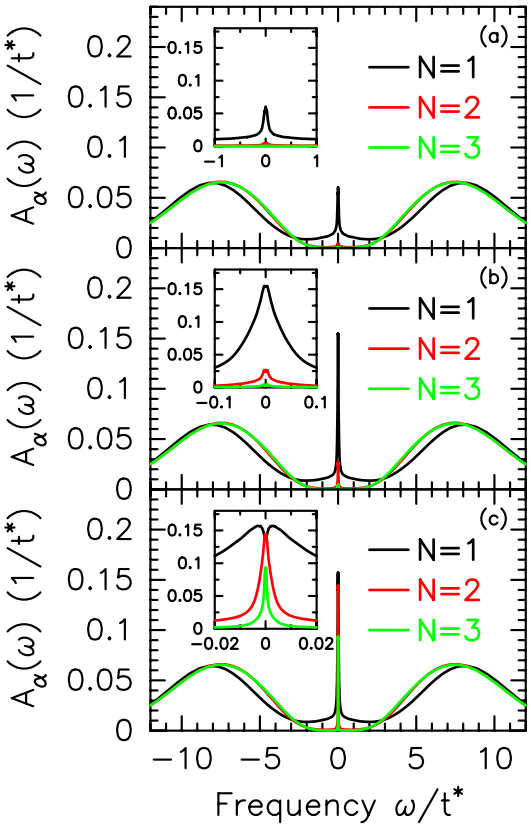

FIG. 2 (color online). Local spectral function of the five-barrier-plane multilayer for $U = 16$, and three different temperatures: (a) $T = 0.01$, (b) $T = 0.001$, and (c) $T = 0.0001$. We show the three inequivalent barrier planes ($N = 1$ is next to the interface, $N = 3$ is at the center). The insets show blowups of the low frequency region.

the width is significantly narrower. We estimate the Fermi temperatures for the different planes to be $T_{F1} \approx 0.015$, $T_{F2} \approx 0.0009$, and $T_{F3} \approx 0.00025$. The high energy features in the DOS remain unchanged as T is lowered.

Insofar as transport is concerned, because of the small coherence scales involved, our numerical techniques are not yet reliable enough to determine the conductance of these devices with a Kubo formula. Nevertheless, we conjecture that decreasing the temperature is tantamount to decreasing the length of the barrier as each insulating layer becomes metallic in turn. This would result in a strong nonlinear dependence of the dc conductance on temperature, which will be tunneling like, but with sharp increases as T is lowered below the effective Fermi temperature of each symmetric pair of planes. Finally, when T becomes much smaller than the Fermi temperature of the central planes, the system will become a perfect dc conductor. We also expect a very narrow Drude peak at low temperatures, which should be observable in optical conductivity. However, in order to be able to see the metallic regime and access the nonlinear responses in real samples, thin layers of materials with small Mott-Hubbard gaps, and frustrated magnetic correlations would need to be used, and the disorder present in any real device, would need to be minimized.

In summary, we argued that Mott-insulating barrier layers sandwiched between metallic leads transform into "fragile" Fermi liquids, and the system *develops a perfectly conducting channel* at sufficiently low temperatures even for large interaction U, as long as the barrier thickness is finite. This striking result is similar to the zero-bias anomaly in quantum dots coupled to metallic leads in the Kondo regime [12]. The particle-hole symmetric system (with the same hopping for all planes and directions) we are considering here has the special feature that at zero temperature and zero frequency it becomes translational invariant and equivalent to the noninteracting problem. The hierarchical fragility of the Fermi liquid is likely to lead to striking nonlinear response of the system to perturbations, with significant device potential.

H. Z. and J. K. F. acknowledge support from the National Science Foundation under Grant No. DMR-0705266. H. R. K. is supported under ARO Grant No. W911NF0710576 with funds from the DARPA OLE Program, and from the Department of Science and Technology, India. Th. P. acknowledges support from the collaborative research center (SFB) 602.

[1] A. Ohtomo and H. Y. Hwang, Nature (London) **427**, 423 (2004).
[2] S. Thiel *et al.*, Science **313**, 1942 (2006).
[3] R. W. Helmes, T. A. Costi, and A. Rosch, Phys. Rev. Lett. **101**, 066802 (2008).
[4] M. Potthoff and W. Nolting, Phys. Rev. B **59**, 2549 (1999).
[5] J. K. Freericks, Phys. Rev. B **70**, 195342 (2004).
[6] J. K. Freericks, *Transport in Multilayered Nanostructures: the Dynamical Mean-field Theory Approach* (Imperial College Press, London, 2006).
[7] Notions of such an effect can be inferred from the results shown in Ref. [3] where Mott layers are studied in proximity to a normal metal in an interface geometry.
[8] This is standard practice in DMFT [9] and is done with the expectation that the regime with enforced paramagnetism correctly captures some features of the low-temperature regimes in contexts where magnetism is suppressed due to frustration effects or fluctuation effects.
[9] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[10] D. O. Demchenko, A. V. Joura, and J. K. Freericks, Phys. Rev. Lett. **92**, 216401 (2004).
[11] R. Bulla, T. A. Costi, and Th. Pruschke, Rev. Mod. Phys. **80**, 395 (2008), and references therein.
[12] The one-dimensional analog of the $N = 1$ case considered above corresponds to a tight-binding chain with a nonzero U only at one central site (the Wolff model). H. R. Krishnamurthy, K. G. Wilson, and J. W. Wilkins, Phys. Rev. B **21**, 1003 (1980) show it is in the universality class of the Anderson impurity model. At $T = 0$, it has a Kondo resonance (local Fermi liquid), no matter how large U is, which again translates into ballistic dc conductance.