Strong Correlation Transport and Coherence

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ABSTRACT: We discuss the notion of fermi liquid coherence in the different regimes of the Anderson lattice. For finite doping heavy fermion (HF) behaviour results when the kondo exchange energy $J_K$ is smaller than the oxygen oxygen overlap $t_{pp}$. High temperature superconductors (HTS) are in the opposite regime ($J_K \gg t_{pp}$). Doping the charge transfer insulator state introduces Zhang Rice singlet like states in the gap. These states, at zero temperature, continuously evolve into Kondo resonances as $t_{pp}$ is increased. The mechanism for destruction of coherence, at finite temperatures, is qualitatively different in the HF and the HTS regime. We study the temperature dependence of the transport coefficients when the charge transfer gap is large, in the temperature regime $T \gg T_{coh}$. We discuss our results in connection with the anomalous properties of the copper oxides.

I. INTRODUCTION

A review of the experimental properties of the high $T_c$ materials reveals several features that need to be reconciled by a fundamental theory of these materials:

1) Angular resolved photoemission and positron annihilation experiments are consistent with a relatively sharp fermi surface. Its shape is predicted correctly by density functional calculations. This is a Luttinger fermi surface enclosing $1 + \delta$ holes per copper plane; $\delta$ is the nominal doping away from half filling since $\delta$ is small, ranging between .15 in 214 $La_{0.65}Sr_{0.35}CuO_4$, .2 in 2212 $Bi_2Sr_2CaCu_2O_8$, and .3 -.5 in 123$YBa_2Cu_3O_6$, the fermi surface has a large area.

2) Several transport measurements, however, suggest a low density of carriers. The Hall number at room temperature, $n_H \equiv \nu_e / (\rho_H e)$, ($\rho_H$ is the Hall resistivity and $\nu_e$ is the volume containing one copper), reveals that $n_H$ is a small number of the order of $2 \cdot \delta$. In the 214 compound $n_H \approx .3$, in Bi 2214 $n_H \approx .3$. From measurement of the optical conductivity or the zero temperature penetration depth, one extracts the ratio $\frac{\mu_m}{\mu_e} \approx \frac{c}{4\pi\varepsilon_0\lambda}$. This ratio, normalized to its band structure value, is equal to .05 in 214, .2 in 123, and .1 in 2212.

3) Optical and d.c. conductivity measurements indicate that the carriers are strongly scattered, giving rise to an inverse carrier lifetime or order $T$ rather than
$T^2$ as in conventional fermi liquid theory. 

In this talk I would like to present an attempt to reconcile these aspects of the experimental data starting from a microscopic model, the infinite U Anderson lattice treated by means of the large N expansion. 

In the first part I will discuss the different parameters of the infinite U Anderson lattice hamiltonian. Since this model hamiltonian describes the physical properties of the heavy fermions, this analysis elucidates the important differences between these materials and the high temperature superconductors.

The heavy electron problem illustrates the idea that strongly correlated fermi systems form fermi liquids below certain characteristic temperature, the coherence temperature, $T_{coh}$. In the heavy fermion problem one can loosely think of $T_{coh}$ as the binding energy, $T_b$, of a localized spin and a conduction electron, and is of the same magnitude as the Kondo temperature. Recently K. Levin and collaborators have discussed the notion of the coherence temperature in the heavy fermions and high temperature superconductors and presented the similarities of large body of experimental data in both systems. In this talk we will emphasize the differences between the two systems, and the need for new techniques in describing the normal state of the high temperature superconductors.

In the second part of the talk we use an effective lagrangian to describe the very low energy physics in the incoherent regime of a doped Mott or Charge Transfer insulator.

**II. THE HTS AND THE HF REGIMES OF THE ANDERSON LATTICE.**

We investigate the Anderson lattice hamiltonian:

\[
H = \varepsilon_d \sum_i d_i^+ d_i + \varepsilon_p \sum_{j,a} p_{j,a}^+ p_{j,a} + i \sum_i \lambda_i (d_i^+ d_i + b_i^+ b_i - \frac{N}{2}) + \frac{V}{N} \sum_{i,\sigma} d_i^+ d_i \sum_{\sigma',a} (p_{i,\sigma'a}^+ p_{i,\sigma'a} + p_{i,\sigma'a}^+ p_{i,\sigma'a}) + \frac{J}{N} \sum_{i,\sigma,\sigma'} \sum_{\sigma',\sigma''} d_i^+ d_i \sigma \sigma' \sigma'' d_i^+ d_i \sigma' \sigma'' \\
\quad \quad - \frac{t_{pd}}{\sqrt{N}} \sum_{i,\sigma} (p_{i,\sigma}^+ - p_{i,\sigma=-x}^+ + p_{i,\sigma-y}^+ - p_{i,\sigma-y}^+) d_i^+ b_i^+ + c.c + \frac{t_{pp}}{N} \sum_{i,\sigma} p_{i,\sigma}^+ (p_{i,\sigma-y} - p_{i,\sigma-y} + p_{i,\sigma-y} - p_{i,\sigma-y}) + c.c
\]

It describes the hybridization of local moments on the copper $d_{\sigma\sigma'}$ orbitals with
two $p_\sigma$ orbitals on the oxygen sites. $t_{pp}$ is a direct oxygen oxygen overlap, V is the direct nearest neighbour repulsion introduced by Varma Schmitt Rink and Abrahams. The on site repulsion on the copper is assumed to be infinite and this is taken into account using a slave boson, $b$, to label the empty site and a lagrange multiplier, $\lambda$, to enforce the single occupancy constraint, $J$ is the direct copper copper superexchange.

This hamiltonian is known to describe the basic physics of the heavy fermion compounds. The analogy with the heavy fermions and the high temperature superconductors is useful in that it illustrates how a system of local moments and conduction electrons can behave as a Fermi liquid with a Luttinger (i.e containing $1+\delta$ electrons) Fermi surface, below a characteristic coherence temperature $T_{\text{coh}}$.

In the slave boson formalism this temperature appears as the condensation temperature of the slave bosons $b$.

Consider first the model at half filling. When $t_{pp}$ and $V$ are set equal to zero the model undergoes a metal charge transfer insulator transition (MCTIT) when the ratio $\frac{t_{pp}}{\epsilon_p - \epsilon_d}$ is decrease below a critical value. This transition has many similarities with the Brinkman Rice transition in the Hubbard model. The minimal value of $t_{pp}$ which is necessary to sustain a metallic state is increased by $t_{pp}$ and by $V$. $V$ renormalizes the charge transfer gap $E_g = \epsilon_p - \epsilon_d + (1 - \delta)V$. The oxygen oxygen overlap makes the conduction electron wavefunctions stiffer decreasing the energy gained by hybridization and making the system more insulating.

Upon doping, new states are introduced inside the charge transfer gap, given by $\epsilon_d = \epsilon_p - \epsilon_d$. These states form a band centered around the renormalized level $c_d \approx \epsilon_p - \alpha_1 J_K$ as shown in fig 1. Their bandwidth is given approximately by $\alpha_1 \delta J_K + \alpha_2 J^{19}$. $\alpha_1$ and $\alpha_2$ are numbers of order unity. We can think of the states that appear inside the charge transfer gap, in terms of a $\delta$ holes or in terms of $1+\delta$ particles. Taking the first point of view we have a large N version of the Zhang Rice (ZR) singlet construction. The second point of view shows that the $1+\delta$ particles form a fermi liquid of mixed copper and oxygen character with a Luttinger fermi surface.

So far we have assumed that $t_{pp}$ is smaller than the Kondo exchange coupling $J_K = t_{pp}^4/(4\epsilon_p - \epsilon_d)$. Then the renormalized level is clearly outside the p band. As $t_{pp}$ increases the renormalized d level moves into the p band, and the renormalized band structure assumes the standard heavy fermion form (see fig 1b).
FIG. 1. Bare (dotted lines) and renormalized (solid lines) band structure of the Anderson Lattice in the HTS (left) and HF (right) regimes.

Notice that the gap between the bands and the inverse density of states around the fermi level, in the HF regime, are exponentially small and proportional to the Kondo temperature, $T_K$.

$$T_K \simeq 4\delta_{PP}^{\gamma P} e^{-\frac{\beta}{\hbar \rho_d}}$$

(2)

In this limit the Zhang Rice bound states have turned into Kondo resonances. This transition between the HTS regime and the HF regime as one increases the oxygen oxygen overlap is a smooth crossover. The ZR singlet is the bound state which is form as we pull the Kondo resonance out of the oxygen continuum.
There are essential differences between the copper oxides and the high temperature superconductors. In the heavy fermions the doping is large and \( tpp \gg J_0 \).

The high \( T_c \) materials are closer to the opposite limit. In the heavy fermion materials the magnetic interaction between the moments is comparable with the Kondo temperature, \( J \leq T_{coh} \), as a result the heavy fermions obey Curie law above the coherence temperature. The opposite behaviour occurs in the high \( T_c \) materials, the coherence temperature is much smaller than the exchange, and the susceptibility is Pauli like. There are no free magnetic moments above \( T_{coh} \).

Heavy fermion masses, are the result of the free moment entropy which is transferred to the fermi liquid below the coherence temperature \(^{21}\). In the HTS, there is never a free moment as long as \( T \leq J \) and the mass renormalizations are not large.

The physics above the coherence temperature is very different in the two materials. In the heavy fermion systems the scale of the coherence temperature is set by the Kondo temperature \(^{22}\), eq. (2). This is the binding energy of the spin conduction electron compensation that forms the Kondo resonance. The formula for the binding energy is reminiscent of the transition temperature of a BCS superconductor.

In the HTS limit the binding energy of the singlet is of the order of \( J_K \), a much larger than the coherence temperature which is only a fraction of \( \delta J_K \). In the superfluid analogy, the ZR limit is close to the Bose Condensation of tightly bound pairs of molecules in which the condensation temperature is determined by the excitations of collective modes and is much smaller than the binding energy. In the regime \( T_{coh} \ll T \ll J \) the transport is dominated by incoherent holes but the spins are locked by the superexchange interaction and the susceptibility is weakly temperature dependent.

The similarities and the differences between the high temperature superconductors and the high \( T_c \) materials are summarized schematically in table 1 below.

There are several theoretical and experimental indications that the high temperature superconductors are very close to (but on the Mott insulating side of) the MCTIT boundary. A large part of the charge transfer gap is due to the nearest neighbor repulsion \( V \). This view is consistent with: a) the rapid destruction of magnetism by doping b) the small jump in the chemical potential seen in photoemission experiments \(^{23}\) and c) the sensitivity of the optically measured charge transfer gap to substitutions. \(^{24}\) Also, evaluation of the effective interactions between the quasiparticles (\( \frac{1}{N} \) corrections) results in attraction in the s wave channel only when \( V \) is comparable with \( t_{pd} \). \(^{25,26}\)
### TABLE I. High Tc Superconductors and Heavy Fermions: Differences and Similarities

<table>
<thead>
<tr>
<th>Similarities</th>
<th>High Tc Superconductors</th>
<th>Heavy Fermions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Similarities</td>
<td>system of local moments</td>
<td>+ conduction electrons</td>
</tr>
<tr>
<td>Similarities</td>
<td>Luttinger fermi surface</td>
<td>contains 1 + $\delta$ holes</td>
</tr>
<tr>
<td>Energy scales</td>
<td>$J \gg T_{coh}$</td>
<td>$J \leq T_{coh}$</td>
</tr>
<tr>
<td></td>
<td>$t_{pp} \leq J_K$</td>
<td>$t_{pp} \gg J_K$</td>
</tr>
<tr>
<td></td>
<td>$\epsilon_p - \epsilon_d \geq t_{pd}$</td>
<td>$\epsilon_p - \epsilon_d \gg t_{pd}$</td>
</tr>
<tr>
<td>Magnetic Susceptibility</td>
<td>$\chi \approx \text{const}$</td>
<td>$\chi \approx \frac{1}{T}$</td>
</tr>
<tr>
<td>Resistivity</td>
<td>$\rho \approx T$</td>
<td>$\rho \approx \text{const} - \log T$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T \gg T_{coh}$</td>
</tr>
<tr>
<td>Binding Energy</td>
<td>$\frac{t_{pd}^2}{\epsilon_p - \epsilon_d}$</td>
<td>$T_K \approx \frac{46}{\epsilon_p - \epsilon_d}$</td>
</tr>
<tr>
<td>Coherence temperature</td>
<td>$T_{coh} &lt; \delta \frac{t_{pd}^2}{\epsilon_p - \epsilon_d}$</td>
<td>$T_{coh} \approx T_K$</td>
</tr>
<tr>
<td>Superfluid analogy</td>
<td>bose condensation of molecules</td>
<td>BCS limit</td>
</tr>
</tbody>
</table>

### III. TRANSPORT ABOVE $T_{COH}$

In the heavy fermion problem one describes the incoherent regime by expanding the hamiltonian in eq. (1) around a zero expectation value of the bose field. This is a reasonable approximation since both the binding energy and the coherence are negligible above the Kondo temperature. The starting point is then free moments interacting weakly with conduction electrons. This starting point is not valid in the HTS regime. The holes lose coherence at temperatures which are much smaller than the Kondo exchange and the copper copper superexchange. The $p^3d$ complexes are strongly bound but incoherent. This situation is not described by a simple expansion around zero bose field because, locally, the magnitude of the bose field is large. It is the strong fluctuations of the phase of the bose field which results in the absence of Bose condensation.

To simplify the treatment of the regime where the coherence temperature is much smaller than the binding energy of the ZR singlets we will assume that the charge transfer gap is much larger than other scales in the problem. This assumption is qualitative valid at very low energies, as long as we are on the insulating side of the MCTIT, and we will therefore only discuss d.c. transport.

Well above the MCTIT the effective interactions and the propagators of model (2) reduce to the corresponding vertices of the t-J model:
\[ H = -\frac{t}{N} \sum_{ij} C^+_{i\sigma} b_{j\sigma} C_{j\sigma} + \frac{J}{N} \sum_{ij} C^+_{i\sigma} C_{i\sigma} C^+_{j\sigma} C_{j\sigma} \] (3)

For sufficiently large dopings and at low energies is described by the effective lagrangian of the uniform resonating valence bond state \(^{27,29,30}\)

\[ H = -\frac{1}{2m_F} C^+ C + \frac{1}{2m_B} b^+ [(\nabla - i\alpha)]^2 b + i\lambda (b^+ b + C^+ C - 1) \] (4)

The fermion \( C^+ \) denotes a creation operator for the lowest quasiparticle band in fig. (1). \( m_F \) and \( m_B \) are parameters of the low energy theory. Their values can be evaluated in the \( 1/N \) expansion. \(^{30}\) Integrating out the fermion and the bosons one obtains an effective action for the gauge field \(^{28}\)

\[ \mathcal{L} = a^\mu(q, \omega) [\Pi_B^{\mu\nu}(q, \omega) + \Pi_F^{\mu\nu}(q, \omega)] a^\nu(q, \omega) \] (5)

\( \Pi_F^{\mu\nu} \) and \( \Pi_B^{\mu\nu} \) are the current current correlation functions of the Bose and Fermi system. The retarded transverse part of this correlation is given by \( \Pi_F^{\mu\nu}(q, \omega) = \chi_{F,B} q^2 - i \omega \Gamma_{F,B} \), \( \chi_F \sim \frac{1}{m_F^2} \) and \( \chi_B \sim \frac{\xi}{m_B} \) are the fermi and bose diamagnetic susceptibilities. \( \Gamma \approx 1/qa \), \( \Gamma_B \approx \sqrt{\beta/(qa)} \) are the landau damping coefficients and \( \alpha \) is the lattice spacing. The gauge field, \( a^\mu \), plays a dual role. It screens the external fields, deciding dynamically which part of the external field is felt by the fermi or the bose subsystem, and it scatters the fermions and the bosons. This effective lagrangian has been recently applied to the calculation of transport coefficients by Nagaosa and Lee \(^{31}\) and Ioffe and Kotliar \(^{32}\). We will follow the kinetic equation approach of the latter authors. This method separates neatly the screening from the scattering aspects of the problem. The starting point is a kinetic equation for the deviations away from equilibrium of the distribution functions of the fermions bosons and gauge fields \( \delta n_f, \delta n_b \) and \( \delta n_a \) respectively. Then one proves that \( \delta n_a = 0 \), that is, there is no "photon drag". The physical reason for this is that the fermions and the bosons are pulled in different directions by their effective fields, and the photons do not follow any of them. In this circumstance the kinetic equations decouple in two separate equations for the bosons and the fermions. In steady state they have the following form:

\[ v_{b\alpha} \nabla \delta n_b + (E_B - \nabla \mu_b) \delta n_b = C_b(\delta n_b) \]
\[ v_{F\alpha} \nabla \delta n_F + (E_F - \nabla \mu_F) \delta n_F = C_F(\delta n_F) \] (6)

The fields in this equation are the effective fields which are felt by the fermi and bose subsystem (this is the external field which are screened by the gauge field).
The collision operators describe the scattering mechanism between the fermion and bose subsystem and the effective field.

The solution to the kinetic equation proceeds in several steps:

First one computes the eigenvalues corresponding to different deviations from equilibrium in the fermi and bose subsystem. \( C(\delta n_\lambda) = \frac{1}{\tau_\lambda} \delta n_\lambda \). The results are summarized in table 2.

<table>
<thead>
<tr>
<th>Eigenvector</th>
<th>( \delta n \propto \cos \theta )</th>
<th>( \delta n \propto \epsilon_p - \mu )</th>
<th>( \delta n \propto \cos \theta(\epsilon_p - \mu) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fermion</td>
<td>( \frac{1}{\tau} \sim T^{4/3}m_F^{1/3} )</td>
<td>( \frac{1}{\tau} \sim T^{2/3}m_F^{-1/3} )</td>
<td>( \frac{1}{\tau} \sim m_F^{-1/3}T^{2/3} )</td>
</tr>
<tr>
<td>Boson</td>
<td>( \frac{1}{\tau} \sim \frac{T}{m_B(x_F+x_B)} )</td>
<td>( \frac{1}{\tau} \sim \frac{T^{3/3}}{(x_F+x_B)m_B^{1/3}} )</td>
<td>( \frac{1}{\tau} \sim \frac{T}{m_B(x_F+x_B)} )</td>
</tr>
</tbody>
</table>

Second having computed \( \tau_F, \tau_B \) one computes the transport coefficients of the fermi and bose subsystem:

\[
R_B = \frac{T}{4\pi \delta(\chi_B + \chi_F)}
\]

\[
\kappa_B = \delta(\chi_F + \chi_B)
\]

\[
R_F \sim (Tm_F)^{4/3}
\]

\[
\kappa_F \sim T^{1/3}m_F^{-2/3}
\]

(7)

3) Given \( E, \nabla \mu, B, \nabla T \) compute the effective fields felt by the fermi and bose subsystem (this is where the screening aspects of the gauge field come into play).

For example, from the condition that the effective fields acting on the bosons and the fermions add up to give the external field \( E_F + E_B = E \) and the condition that the fermion current and minus the bose current describe the same physical electric current \( 0 = J_F + J_B = \sigma_F E_F + \sigma_B E_B \) one determines the effective fields felt by the bose and the fermi subsystem.

\[
E_F = \frac{\sigma_B E}{\sigma_F + \sigma_B}, \quad E_B = -\frac{\sigma_F E}{\sigma_F + \sigma_B}
\]

(8)

4) One then computes the physical currents. The electrical current is given by

\[
J = J_F = -J_B
\]

(9)

while the heat current is given by the sum of the Fermi and Bose contributions.

\[
U = U_B + U_F
\]

(10)
This allows us to express the transport coefficients of the electrons in terms of the transport coefficients of the fermi and the bose subsystem. Combining the previous equations one obtains the following results: The electric resistivity is given by Ioffe Larkin \[28\] formulae

\[
\rho = \rho_F + \rho_B \sim \rho_B = \frac{T}{\delta (\chi_F + \chi_B)}
\]  

(11)

The resistivity is linear as long as \( \chi_B \ll \chi_F \), i.e. \( \frac{\mu_B}{\mu_F} \ll 1 \) The thermopower is constant in temperature with logarithmic corrections.

\[ Q \sim 2 + \log\left(\frac{T}{\delta m_B}\right) \]  

(12)

The thermal resistivity is given by

\[
\kappa = 8\delta (\chi_F + \chi_B) + T^{1/3} m_F^{-2/3}
\]  

(13)

Since \( T \ll m_F^{-1} \) there is a regime where the wiedeman Franz law is well obeyed, deviations from this law occur when \( T \gg \frac{\delta}{m_F} \) but they are very weak since the second term in eq. 13 is a very weak function of temperature.

The effects of screening are very pronounced in the response to an external magnetic field. Minimizing the free energy \( F = \chi_B B_B^2 + \chi_F B_F^2 \) subject to the external field constraint \( B_F + B_B = B \) one determines the effective magnetic fields felt by the fermi and bose subsystem.

\[
B_B = \frac{-\chi_F}{\chi_F + \chi_B} B, \quad B_F = \frac{\chi_B}{\chi_F + \chi_B} B
\]  

(14)

combining this expression with the composition law for the off diagonal resistivity \( \rho_{xy} = \rho_{xy}^F + \rho_{xy}^B \) one obtains the electronic Hall coefficient.

\[
\frac{1}{n_H} = \frac{B_F}{B} \left( \frac{\rho_{xy}^F}{\rho_{xy}} \right) + \frac{B_B}{B} \left( \frac{\rho_{xy}^B}{\rho_{xy}} \right) \sim \frac{1}{\delta}
\]  

(15)
IV. CONCLUSIONS

In this talk we reviewed the heavy fermion and HTS regime of the Anderson lattice. We discussed first the nature of the carriers as we dope the insulating state. We argue that the mechanisms that are responsible for the destruction of fermi liquid coherence in the high Tc regime are very different, even though, at zero temperature the Zhang Rice singlets and the Kondo resonance evolve continuously into each other as the oxygen oxygen overlap is increased. This is analogous to the crossover between bose condensation of tightly bound pairs and the usual BCS limit. At zero temperature it possible to interpolate smoothly between these two limits. At finite temperatures, superconductivity is destroyed by very different mechanisms in the two limits. Hence, the incoherent state of the high temperature superconductors is not simply related to the finite temperature state of the heavy fermion systems.

The copper oxides seem to be above the MCTI transition however they are very close to it and a large part of it is due to the next nearest neighbor repulsion term. To treat the regime above $T_{coh}$ we presented results based on the Ioffe Larkin effective lagrangian. It is possible to derive this effective lagrangian in the limit of very large charge transfer gap. We assume it is valid at very low energies as long as the charge transfer gap is above the critical value necessary to have a charge transfer insulator. If the parameter $m_F \ll m_B$ it is possible to account for the temperature dependence of the resistivity, the thermopower and the thermal conductivity which are observed experimentally.

The large $N$ approach maintains a (large) Luttiger fermi surface. The transport properties are those of a small number of holes.

Intermediate energy experiments like the optical properties in the infrared are outside the scope of the effective lagrangian Eq. 4. To understand finite frequencies experiments and the effective interaction between the quasiparticles one has to go back to three band hamiltonian starting point.

V. ACKNOWLEDGMENT

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5J. Orenstein, G Thomas, A. Millis, S. Cooper, D. Rapkine and T. Timusk Preprint.


8W. Pickett, Rev. Mod. Phys. 61, 433 (1989).


19The exchange J in the bandwidth enters the quasiparticle or specific heat mass. It
cancels in the optical mass which enters the plasma frequency. This cancellation is discussed in M. Grilli and G. Kotliar, Phys Rev. Lett. 64, 1170 (1990).


22 While the kondo temperature sets the scale of the coherence temperature, \( T_{\text{coh}} \), it can be lower than \( T_K \) by a system dependent numerical factor.


30 To study this regime one introduces a kinetic energy term expressed in terms of Hubbard operators \( T = \frac{1}{N} \sum_{\sigma} \sum_{\sigma} X_{\sigma}^{\dagger} X_{\sigma} \) where \( \sigma \) runs over \( N \) fermionic generators and \( \sigma' \) over \( \frac{N}{2} \) bosonic generators. In terms of slave bosons the kinetic energy reads \( T = \frac{1}{N} \sum_{\sigma} \sum_{\sigma} b_{\sigma}^{\dagger} b_{\sigma} b_{\sigma'}^{\dagger} f_{\sigma} \sigma = 1 \cdots N, \sigma' = 1 \cdots N/2 \). Adding the usual large \( N \) generalization of the magnetic exchange term one obtains a Hamiltonian which at \( N = \infty \) reduces at wavelengths to the Ioffe–Larkin effective Hamiltonian.

