Possible Cooper instabilities in pair Green functions of the two-dimensional Hubbard model.

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Abstract

In analogy with ordinary BCS superconductivity, we identify possible pairing instabilities with poles in a certain class of Green functions of the two-dimensional repulsive Hubbard model, which normally signify bound states. Relating the gap to the location of these poles, we find that these instabilities exist in the range of hole doping between 0 and 0.24. The magnitude of the gap can be calculated without introducing an explicit cut-off, and for reasonably large coupling $U$, the maximum gap is on the order of 0.01 in units of the hopping parameter $t$. 
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References
I. INTRODUCTION

The microscopic physics underlying high $T_c$ superconductivity in the cuprates is believed to be purely electronic in origin, in contrast to ordinary superconductors where the attractive mechanism is due to phonons. Strongly correlated electron models such as the two-dimensional Hubbard model have been proposed to describe it. The Hubbard model simply describes electrons hopping on a square lattice subject to strong, local, coulombic repulsion. Since it is known that the condensed charge carriers have charge $2e$, and thus some kind of Cooper pairing is involved, the main open problem is to identify the precise pairing mechanism. Several mechanisms were proposed early on, in particular mechanisms based on spin fluctuations\cite{1-3}, charge fluctuations\cite{5-7}, and other more exotic ideas such as resonating valence bonds\cite{8}. A more recent work studies the possibility of superconductivity at small coupling, where here the mechanism goes back to ideas of Kohn-Luttinger\cite{9,10}.

Since the Mott-insulating anti-ferromagnetic phase at half-filling is well understood, much of the theoretical literature attempts to understand how doping “melts” the anti-ferromagnetic (AF) order, and how the resulting state can become superconducting. This has proven to be difficult to study, perhaps in part due to the fact that AF order is spatial, whereas superconducting order is in momentum space. (For a review and other references, see \cite{11}.) Furthermore, superconductivity exists at reasonably low densities far from the AF order at half-filling, which suggests that one can perhaps treat the model as a gas, with superconductivity arising as a condensation of Cooper pairs as in the BCS theory, and we will adopt this point of view in the present work.

Since there is as yet no consensus on the precise pairing mechanism in the cuprates, it is worthwhile continuing the search for new ones. In this paper we take a very conservative approach within the Hubbard model, wherein we do not postulate any
particular quasi-particle excitations that would play the role of the phonons, and we ignore the AF order at very low doping. In a field-theoretic approach to the BCS theory, the pairing instability arises from the sum of the ladder diagrams for phonon exchange, as shown in Figure 1. The sum of these diagrams has a pole at energy equal to the gap, and this pole is sufficient to cause the instability, and signifies gapped charge 2 excitations. This will be reviewed in section III. (See e.g. [12, 13]).

FIG. 1: Feynman diagrams that lead to the BCS pairing instability, where dashed lines are phonons.

Suppose that the electron-phonon interaction were treated as an effective, short-ranged electron-electron interaction, so that exchange of a single phonon were replaced by an effective 4-electron vertex. Then the diagrams in Figure 1 become the diagrams in Figure 2. In this work we explore the possibility of pairing instabilities arising from certain similar classes of Feynman diagrams in the Hubbard model. Whereas the diagrams in Figure 2 lead to the BCS pairing instability for bare attractive interactions (see below), for repulsive interactions they merely screen the strength of the Coulomb interaction. However, as we will show, the sum of another class of diagrams shown in Figure 3 do indeed exhibit poles possibly signifying pairing instabilities very near the Fermi surface. An obvious criticism of the present work is that for the cuprates, the coupling is large, and one should not trust perturbation theory. In answer to this, the diagrams we will focus upon can be summed up, and have a well-defined limit as the coupling goes to infinity. Furthermore, since we are focussing on sums of diagrams that lead to poles in the effective pairing potential, it
is possible that these singular diagrams dominate the perturbative expansion. Certainly our calculation can be improved upon; we wish here to present a possible pairing mechanism in its simplest form. For instance, we ignore the effect of interactions on the quasi-particle energies, and take $\xi_k$ to be that of the free theory, ignoring self-energy corrections.

The remainder of this paper is organized as follows. In the next section we define the Cooper ‘pairing’ Green functions of interest. In section III we first review how the Cooper pairing instability manifests itself as poles in such Green’s functions in the BCS theory. The remainder of this section specializes to the Hubbard model, where analogous poles are found for a different class of diagrams. The gap is related to the location of these poles, and solutions are found numerically. We find non-zero gap solutions in the anti-nodal directions in the range of hole doping $0 < h < 0.24$ with a dome-like shape. The maximum of the gap is approximately $\Delta/t = 0.01$ and occurs around $h = 0.18$.

FIG. 2: Feynman diagrams contributing to $V_{\text{eff}}^{(sc)}$.

FIG. 3: Feynman diagrams contributing to $V_{\text{eff}}^{(ex)}$. 
II. GREEN FUNCTIONS AND THE EFFECTIVE COOPER PAIR POTENTIAL

We study the two-dimensional Hubbard model, with an additional next-to-nearest neighbor hopping $t'$, with hamiltonian:

$$H = -t \sum_{<i,j>,\alpha=\uparrow,\downarrow} c_{i,\alpha}^\dagger c_{j,\alpha} - t' \sum_{<i,j>'\alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$  \hspace{1cm} (1)

where $i, j$ label sites of a two-dimensional square lattice, $<i,j>$ and $<i,j>'$ denote nearest and next-nearest neighbors respectively, and $n_{i,\alpha} = c_{i,\alpha}^\dagger c_{i,\alpha}$. Our convention for neighboring interactions is e.g. $\sum_{<i,j>} c_i^\dagger c_j = c_1^\dagger c_2 + c_2^\dagger c_1 + ...$ such that $H$ is hermitian.

The lattice operators $c_{r_i,\alpha}$ where $r_i$ is a lattice site, will correspond to the continuum fields

$$\psi_\alpha(x,t) = \int \frac{d^2k}{2\pi} c_{k,\alpha}(t) e^{ik\cdot x}$$  \hspace{1cm} (2)

The free hopping terms are diagonal in momentum space:

$$H_{\text{free}} = \int d^2k \omega_k \sum_{\alpha=\uparrow,\downarrow} c_{k,\alpha}^\dagger c_{k,\alpha}$$  \hspace{1cm} (3)

with the 1-particle energies

$$\omega_k = -2t(\cos(k_x a) + \cos(k_y a)) - 4t' \cos(k_x a) \cos(k_y a),$$  \hspace{1cm} (4)

where $a$ is the lattice spacing. We henceforth scale out the dependence on $t$ and $a$ such that all energies, temperatures and chemical potentials are in units of $t$. The interactions then depend on the dimensionless coupling $g \equiv U/t$, which is positive for repulsive interactions. Henceforth $\xi_k \equiv \omega_k - \mu$ is the 1-particle energy measured relative to the Fermi surface, where $\mu$ is the chemical potential. For the most part, our analysis will be for $t' = 0$, unless otherwise stated.
In order to probe possible Cooper pairing instabilities, we consider the Green function \( \langle \psi_{\uparrow}^\dagger(x_1)\psi_{\downarrow}^\dagger(x_2)\psi_\downarrow(x_3)\psi_\uparrow(x_4) \rangle \) where \( x = (x,t) \). The Fourier transform in both space and time of these functions are correlation functions of the operators \( c_{k,\alpha}^\dagger(\xi) = \int \frac{dt}{\sqrt{2\pi}} e^{-i\xi t} c_{k,\alpha}(t) \), and their hermitian conjugates. We study Green functions specialized to Cooper pairs: \( \langle c_{-k'\uparrow}(\xi')c_{k\downarrow}(\xi) c_{-k\downarrow}(\xi')c_{k'\uparrow}(\xi) \rangle \). It should be emphasized that since the above Green functions are just Fourier transforms of the spatial/temporal Green functions, although the \( \xi \) are energy variables, they are not necessarily ‘on-shell’, i.e. \( \xi \) is not necessarily \( \xi_k \) (borrowing the relativistic terminology). The only constraint is energy conservation: \( \xi + \xi' = \xi_k + \xi_{k'} \).

There are two important types of quantum corrections to the vertex, which we denote as \( V^{(sc)}_{\text{eff}} \) and \( V^{(ex)}_{\text{eff}} \), where, for reasons explained below, \( sc \) refers to screened and \( ex \) to exchange. \( V^{(sc)}_{\text{eff}} \) is defined as

\[
V^{(sc)}_{\text{eff}} = \langle c_{-k'\uparrow}(\xi')c_{k\downarrow}(\xi) c_{-k\downarrow}(\xi')c_{k'\uparrow}(\xi) \rangle \text{trunc}^{(sc)}
\]

where \( \text{trunc} \) refers to the truncated Green function, i.e. stripped of external propagators and energy-momentum conserving delta functions, and \( sc \) refers to the diagrams in Figure 2. Incoming (outgoing) arrows correspond to annihilation (creation) operator fields. The other class of diagrams are shown in Figure 3 and define \( V^{(ex)}_{\text{eff}} \) as in eqn. (5).

When ‘on-shell’, i.e. \( \xi = \xi_k = \xi_{k'} \) and \( \xi' = \xi_{k'} = \xi_k' \), then these truncated Green functions contribute to the matrix element, i.e. form-factor, of the integrated interaction hamiltonian density:

\[
V(k,k') = \int d^2x \langle -k' \uparrow, k' \downarrow | H_{\text{int}}(x) | k \uparrow, -k \downarrow \rangle
\]

Since there is no integration over time in the above equation, \( \xi_k \) and \( \xi_{k'} \) are not necessarily equal. To lowest order, \( V = g \). The form factor \( V^{(sc)}(k,k') \) corresponding to the diagrams of \( V^{(sc)}_{\text{eff}} \) is equal to \( V^{(sc)}_{\text{eff}} \) (as computed below) with \( \xi \rightarrow (\xi_k + \mathcal{O}(\xi_k^2)) \).
\( \xi_{k'}/2 \), whereas \( V^{(\text{ex})} \) is simply \( V^{(\text{ex})}_{\text{eff}} \) placed on shell. For both, one has the necessary symmetry: \( V(k, k') = V(k', k) \).

The evaluation of \( V^{(\text{ac,ex})}_{\text{eff}} \) at finite density and temperature is standard, however for completeness we provide some details. Consider first \( V^{(\text{ac})}_{\text{eff}} \). These diagrams factorize into 1-loop integrals and form a geometric series. There is no fermionic minus sign coming from each loop since the arrows do not form a closed loop. Momentum conservation at each vertex gives a loop integral that is independent of \( k, k' \):

\[
V^{(\text{ac})}_{\text{eff}}(\xi) = \frac{g_1 - gL^{(\text{ac})}(\xi)}{1 - gL^{(\text{ac})}(\xi)}
\]

(7)

where \( L^{(\text{ac})} \) is the one-loop integral:

\[
L^{(\text{ac})}(\xi) = -T \sum_n \int \frac{d^2\mathbf{p}}{(2\pi)^2} \left( \frac{1}{i\nu_n - \xi} \right) \left( \frac{1}{2\xi - i\nu_n - \xi_{-\mathbf{p}}} \right)
\]

(8)

where \( T \) is temperature, \( \nu_n \) is a fermionic Matsubara frequency, \( \nu_n = 2\pi(n + \frac{1}{2})T \) with \( n \) an integer, and \( \xi_{\mathbf{p}} = \omega_{\mathbf{p}} - \mu \) where \( \mu \) is the chemical potential. One needs the following identity:

\[
T \sum_n \left( \frac{1}{i\nu_n - \xi_{\mathbf{p}}} \right) \left( \frac{1}{2\xi - i\nu_n - \xi_{-\mathbf{p}}} \right) = \frac{f(\xi_{\mathbf{p}}) - 1/2}{\xi - \xi_{\mathbf{p}}}
\]

(9)

where \( f(\xi) = 1/(e^{\xi/T} + 1) \) is the fermionic occupation number, and we have used \( \xi_{\mathbf{p}} = \xi_{-\mathbf{p}} \). The above identity is valid before analytic continuation from imaginary to real time, i.e. when \( 2\xi \) is twice a fermionic Matsubara frequency. The final result is then:

\[
L^{(\text{ac})}(\xi) = \frac{1}{2} \int \frac{d^2\mathbf{p}}{(2\pi)^2} \left( \frac{1}{\xi - \xi_{\mathbf{p}} + i\eta} \right) \tanh(\xi_{\mathbf{p}}/2T)
\]

(10)

where \( \eta \) is infinitesimally small and positive. Integration is over the first Brillouin zone, \( -\pi \leq p_{x,y} \leq \pi \).

The diagrams for \( V^{(\text{ex})}_{\text{eff}} \), though simply an 'exchanged' version of those for \( V^{(\text{ac})}_{\text{eff}} \), have a rather different and more complicated structure. Here there is a fermionic
minus associated with each loop since the arrows form a closed loop. Momentum and energy conservation at each vertex now leads to a loop integral that depends on $q \equiv k' - k$ and $\Delta \xi \equiv \xi' - \xi$:

$$V_{\text{eff}}^{(\text{ex})}(q, \Delta \xi) = \frac{g}{1 - gL^{(\text{ex})}}$$

(11)

where

$$L^{(\text{ex})}(q, \Delta \xi) = T \sum_n \int \frac{d^2 p}{(2\pi)^2} \left( \frac{1}{i\nu_n - \xi_p} \right) \left( \frac{1}{\Delta \xi + i\nu_n - \xi_{p+q}} \right)$$

(12)

Now one needs the identity

$$T \sum_n \left( \frac{1}{i\nu_n - \xi_p} \right) \left( \frac{1}{i\nu_n + i\omega_m - \xi_{p+q}} \right) = \frac{f(\xi_p) - f(\xi_{p+q})}{i\omega_m + \xi_p - \xi_{p+q}}$$

(13)

which is valid for $\omega_m$ twice a bosonic Matsubara frequency. After analytic continuation $i\omega_m \rightarrow \Delta \xi + i\eta$, one has

$$L^{(\text{ex})}(q, \Delta \xi) = \int \frac{d^2 p}{(2\pi)^2} \left( \frac{f(\xi_p) - f(\xi_{p+q})}{\Delta \xi + \xi_p - \xi_{p+q} + i\eta} \right)$$

(14)

In the above formulas it is implicit that $V^{(\text{sc,ex})}$ is defined by the real part of $L^{(\text{sc,ex})}$ in the limit $\eta \rightarrow 0$. In the limit of zero density, i.e. $f = 0$, note that $V_{\text{eff}}^{(\text{ex})} = 0$, whereas $V_{\text{eff}}^{(\text{sc})}$ is non-zero.

III. COOPER PAIRING INSTABILITIES AS POLES IN THE EFFECTIVE POTENTIAL

It is well-known that the Cooper pairing instability of the BCS theory can be understood as a pole in $V_{\text{eff}}^{(\text{sc})}$ [12, 13]. This can be seen by inserting a complete set of states between the pair creation and annihilation operators in eqn. (5), and noting that poles in the energy $\xi$ signify bound states of electric charge 2, which...
are interpreted as the Cooper pairs. To see that this gives the correct result for the gap, let us leave behind the Hubbard model and specialize the coupling \( g \) to that of the BCS theory, where it arises from the interaction with phonons. For simplicity, \( g = -|g| \) is taken to be negative, signifying attractive interactions, in a narrow region near the Fermi surface \( |\xi| < \omega_D \), where \( \omega_D \) is the Debye frequency, otherwise zero. We approximate the integral over \( p \) near the Fermi surface as \( \int \rho(\xi_p) d\xi_p \approx \rho(0) \int d\xi_p \), where \( \rho(\xi) \) is the density of states. Letting \( \xi = \Delta/2 \), in the limit of zero temperature, \( L^{(sc)} \approx \rho(0) \frac{1}{2} \left( \int_{0<\xi_p<\omega_D} d\xi_p \frac{1}{\Delta/2 - \xi_p} - \int_{-\omega_D<\xi_p<0} d\xi_p \frac{1}{\Delta/2 - \xi_p} \right) \approx \rho(0) \log \left( \frac{\Delta}{2\omega_D} \right) \) (15)

(The first integral should be interpreted as the principal value.) There is a pole in \( V^{(sc)}_{\text{eff}} \) because both \( L^{(sc)} \) and \( g \) are negative. The location of the pole is given by \( 1 + |g| \rho(0) \log(\Delta/2\omega_D) = 0 \), which leads to the standard result for the gap: \( \Delta = 2\omega_D \exp(-1/(|g|\rho(0))) \). Note that there is a gap \( \Delta \) for arbitrarily small negative coupling \( g \).

Returning to the positive \( g \) Hubbard model, i.e. with repulsive interactions, there are no poles in \( V^{(sc)}_{\text{eff}} \) since \( L^{(sc)} \) turns out to be negative at finite temperature and density. These quantum corrections merely screen the Coulomb potential. It is meaningful to define a screened coupling near the Fermi surface as \( g_R = V^{(sc)}_{\text{eff}}(\xi = 0) \). The extent of the screening is quite large, on the order of a factor of 10. For instance for \( g = 13 \), appropriate to the cuprates, \( g_R = 0.95 \) at half-filling. For the numerical analysis in this section, we fixed \( g_R = 1 \). We wish to point out that at zero density, i.e. \( f = 0 \), and \( T = 0 \), \( L^{(sc)} \) can become positive, which means that \( V^{(sc)}_{\text{eff}} \) can be attractive. This was explored in [14], and with the help of a hypothesized gap equation, one finds anisotropic solutions with properties suggestive of the pseudo-gap.

We now turn to the investigation of the possibility of analogous pairing instabilities
in $V_{\text{eff}}^{(ex)}$. Namely we look for poles in $V_{\text{eff}}^{(ex)}$ for positive $g$, which only exist if $L^{(ex)}$ can be positive. For $\Delta_\xi = 0$, the integrand in $L^{(ex)}$ is always negative, thus $L^{(ex)}$ is negative and there are no poles for positive $g$. However we are precisely interested in the case $\Delta_\xi \neq 0$ since $\Delta_\xi$ represents a difference of incoming and outgoing energies, and it is thus poles at non-zero values of $\Delta_\xi$ that could signify Cooper paired bound states. As we will see, there are indeed regions of the parameter space near the Fermi surface where $L^{(ex)}$ is positive.

The integral defining $L^{(ex)}$ is rather delicate in comparison with $L^{(sc)}$. For $q$ and $\Delta_\xi$ unrelated, the integral is easily evaluated numerically, and has a smooth, well-defined limit as $\eta \to 0$. However physically we are interested in this function on-shell, i.e. the corresponding form factor $V^{(ex)}$ with $\Delta_\xi = \xi_{k'} - \xi_k$ when $q = k' - k$. In this case there is a pole in the integrand when $p = k$. Thus the $p$ integral should be understood as the Cauchy principal value (PV). Namely, inside an integral over a variable $x$, one has the identity:

$$\lim_{\eta \to 0^+} \frac{1}{x + i\eta} = \text{PV} \left( \frac{1}{x} \right) - i\pi \delta(x)$$

(16)

Recall the PV is defined by excising a small region around the pole: $\int dp_x \to \lim_{\delta \to 0} \left( \int_{-\pi}^{k_x - \delta} dp_x + \int_{k_x + \delta}^{\pi} dp_x \right)$ and similarly for $\int dp_y$.

In order to better understand other features of the function $L^{(ex)}$ on-shell, it is instructive to study the one-dimensional version of $L^{(ex)}$, appropriate to a chain of lattice sites, since here the integral can be performed analytically. This is described in the Appendix. (It should be emphasized that this exercise is not meant to capture the physics of the one-dimensional Hubbard model, which is exactly solvable [15], but rather simply to gain intuition on the function $L^{(ex)}$ in two dimensions.) As shown analytically in the appendix, the on-shell $L^{(ex)}$ actually diverges as the temperature goes to zero in one dimension. The reason is that in the limit of zero $T$, the occupation number $f$ is a step function, and the $\int_{k_F + \delta}^{\pi} dp$ piece of the PV is absent, leading it to
be ill-defined. The temperature $T$ should thus be viewed as an infra-red regulator in one dimension. In two dimensions we will also not take $T \to 0$ for analogous reasons. For arbitrarily small $T$, we verified that $L^{(ex)}$ is well defined numerically as $\delta \to 0$. As shown in the appendix, one can demonstrate analytically that there is a narrow region around the Fermi surface where $L^{(ex)}$ is positive and thus $V^{(ex)}_{\text{eff}}$ has poles. As we now show, the same is true in two dimensions.

We are interested in potential instabilities when $k, k'$ are near the Fermi surface. To be more specific, let $k = k_F(\mu)$ be right on the Fermi surface, i.e. $\xi_k = 0$, and $k'$ be slightly off the surface, with some small $\xi_{k'}$, so that $\Delta_\xi = \xi_{k'}$. See Figure 4. $L^{(ex)}$ is now a function only of the angular directions $\theta, \theta'$ of $k, k', \Delta_\xi, \mu$ and $T$. As usual, the $\theta = \pi/4$ direction will be referred to as nodal, whereas the $\theta = 0$ as anti-nodal.

The chemical potential will be related to the hole doping $h$ by the formula:

$$1 - h = 2 \int \frac{d^2k}{(2\pi)^2} \frac{1}{e^{\xi(k)/T} + 1}$$

(17)

This is clearly an approximation since there are self-energy corrections that modify $\xi_k$ which we ignore; however, since the experimentally measured Fermi surfaces can be fit to a $\xi_k$ of a tight-binding form, we do not expect these corrections to drastically affect the main features of our results. Henceforth, we express various properties in terms of $h$ defined by the above equation in the limit $T \to 0$.

Let us first illustrate our findings at the fixed doping $h = 0.21$. In Figure 5 we plot $L^{(ex)}$ for both $k, k'$ in the anti-nodal direction as a function of $\Delta_\xi$ at the low temperature $T = 0.001$ (compared to the bandwidth). One sees that for small enough $\Delta_\xi$, i.e. close enough to the Fermi surface, $L^{(ex)}$ becomes positive. As in the case of the BCS instability reviewed above, let us identify the gap $\Delta_{\text{gap}} = \Delta_\xi$ with the location of the pole in $V^{(ex)}_{\text{eff}}$ in the anti-nodal direction, i.e. the solution to the equation:

$$\frac{1}{g_{sc}} = L^{(ex)}(\Delta_{\text{gap}}, \mu, T)$$

(18)
FIG. 4: Geometry near the Fermi surface in the first quadrant of the Brillouin zone.

where it is implicit that $\theta = \theta' = 0$. For $g_{sc} = 1$, appropriate to an unscreened (bare) $g$ on the order of 10, one sees from Figure 5 that $\Delta_{gap} \approx 0.003$.

Two other features are apparent from Figure 5:

(i) There is a solution to eqn. (18) for arbitrarily large $g_{sc}$ since $L^{(ex)}$ passes through zero. Furthermore, as $g_{sc} \to \infty$, $\Delta_{gap}$ saturates to where $L^{(ex)}$ crosses the real axis, in this case $\Delta_{gap} \approx 0.003$.

(ii) Since $L^{(ex)}$ has a maximum, there are only solutions to eqn. (18) for $g_{sc}$ larger than a minimum value, in this case $g_{sc}$ greater than approximately $1/7$. Since no such threshold was found in [1], one should conclude that the pairing mechanism presented here is essentially different.

The solutions $\Delta_{gap}$ to eqn. (18) depend on the temperature. However since we view $T$ as an infra-red cut-off, one should think of this in terms of the renormalization group. Namely, $g$ can be made to depend on $T$ in such a manner as to keep the solution $\Delta_{gap}$ fixed. One finds that $g$ increases with decreasing $T$. For instance, at $\hbar = 0.15$, if $g_{sc} = 1$ at $T_0 = 10^{-3}$, then $g_{sc} \approx 2.3$ for $T_0 = 10^{-4}$. Henceforth we fix
the reference temperature $T_0 = 0.001$, keeping $g_{sc} = 1$.

![Graph](attachment:graph.png)

FIG. 5: The loop integral $L^{(ex)}$ in the anti-nodal direction as a function of $\Delta \xi$ for hole doping $h = 0.21$ and temperature $T = 0.001$.

In order to understand how $\Delta_{\text{gap}}$ depends on doping, in Figure 6 we plot $L^{(ex)}$ for $h = 0.05, 0.15$ and 0.24. One sees that as $h$ is decreased, $L^{(ex)}$ crosses zero at smaller values of $\Delta \xi$, signifying a smaller $\Delta_{\text{gap}}$. Finally, when $h$ is large enough, $L^{(ex)}$ is nowhere positive, signifying no solution to eqn. (18). In Figure 7 is shown the anti-nodal solution $\Delta_{\text{gap}}$ as a function of doping $h$. It is important to note that reasonable values for $\Delta_{\text{gap}}$ were obtained without introducing any explicit cut-off.

Numerically, we found no solutions to the eqn. (18) in the nodal direction. In fact, solutions only exist in a narrow direction around the anti-nodal region. Since the anti-nodal direction is along a 1-dimensional chain of lattice sites, this suggests that the effect we are describing is closely tied to the properties of the 1-dimensional chains studied in the appendix. Although this may help to explain the d-wave nature of the gap in the cuprates, it by no means establishes it. In order to study this further, one needs a BCS-like gap equation built upon the effective interaction $\nu^{(ex)}_{\text{eff}}$, or equations
FIG. 6: The loop integral $L^{(ex)}$ in the anti-nodal direction as a function of $\Delta_\xi$ for hole doping $h = 0.05, 0.15$ and $0.24$. Analagous to those in [9], which is beyond the scope of this paper.

A non-zero $t'$ has a strong influence on the above results. In order to obtain a comparable value of the gap, one needs a significantly higher $g_{sc}$. For instance, to obtain a gap $\Delta_{\text{gap}} = 0.01$ at doping $h = 0.15$, one needs $g_{sc} \approx 10$.

We wish to point out that the function $L^{(ex)}$ off-shell, i.e. with $\Delta_\xi$ equal to an arbitrary frequency $\omega$ unrelated to $q$ appears in the RPA expression for the dielectric response function $\varepsilon_{\text{RPA}}(\omega, q) = 1 - g L^{(ex)}(\Delta_\xi = \omega, q)$ [13]. Here, $\omega$ is the frequency of an external probe, such as an electric field. Plasmons, i.e. quantized electric charge fluctuations, are manifested as delta-function peaks in $-\text{Im}(1/\varepsilon_{\text{RPA}})$ as a function of $\omega$. The pairing mechanism studied here thus appears closest to the idea of plasmon mediated superconductivity [5, 16]. However our analysis differs in important ways: no low energy plasmons were postulated, and the properties of the on-shell $L^{(ex)}$ are very different from those of $\varepsilon_{\text{RPA}}$. 

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IV. CONCLUSIONS

In summary, we identified the possibility of Cooper pairing instabilities which arise as poles in certain Green functions in the two dimensional Hubbard model, in a manner analogous to the BCS theory. Reasonable magnitudes for the gap in the anti-nodal direction were found, $\Delta_{\text{gap}}/t \approx 0.01$, without introducing an explicit cut-off.

In the BCS theory, the analogous poles are ‘resolved’ by the BCS gap equation. The latter has not been developed in the present case, thus this should be investigated as a next step in exploring the consequences of the pairing mechanism identified in this work. Since it is not clear that the usual BCS gap equation with the effective pair potential studied in this paper is valid, this has not been pursued here. Certainly the very existence of these poles imply that the effective pairing potential can change sign thereby becoming attractive, thus non-zero solutions to the proper gap equation should exist.
V. ACKNOWLEDGMENTS

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VI. APPENDIX: CHAINS: THE LOOP INTEGRALS IN ONE DIMENSION.

In this appendix we study the one-dimensional version of the integrals for \( L^{(ex)} \), i.e. eq. (14) with \( \int d^2p/(2\pi)^2 \to \int dp/2\pi \) where \( p \) is now a one-dimensional vector, and \( \omega_k = -2 \cos k \). In the limit of zero temperature, the occupation number \( f \) becomes a step function, and the integral can be performed analytically. Namely,

\[
L^{(ex)} = L_+ - L_-
\]

where

\[
L_+ = \frac{1}{2\pi} \int_{|p| \leq k_F(\mu)} \left( \frac{dp}{\Delta_\xi + \xi_p - \xi_{p+q}} \right), \quad L_- = \frac{1}{2\pi} \int_{|p+q| \leq k_F(\mu)} \left( \frac{dp}{\Delta_\xi + \xi_p - \xi_{p+q}} \right)
\]

where \( k_F(\mu) = \arccos(\mu/2) \) is the Fermi momentum. In the region of small \( q \) that we are interested in, the appropriate branch of the above integrals are given in terms of the functions

\[
I(p) = \frac{1}{\pi \sqrt{\Delta_\xi^2 - 8(1 - \cos q)}} \arctan \left( \frac{(\Delta_\xi + 2 - 2 \cos q) \tan(p/2) - 2 \sin q}{\sqrt{\Delta_\xi^2 - 8(1 - \cos q)}} \right),
\]

as follows:

\[
L_+ = I(k_F(\mu)) - I(-k_F(\mu)), \quad L_- = I(k_F(\mu) - q) - I(-k_F(\mu) - q)
\]
In the limit of zero temperature, $L^{(ex)}$ is then only a function of $q, \Delta_\xi$ and the chemical potential $\mu$, by using the identities

$$\tan(k_F(\mu)/2) = \sqrt{\frac{2 + \mu}{2 - \mu}}, \quad \tan((k_F(\mu) - q)/2) = \frac{\sqrt{2 + \mu} - \sqrt{2 - \mu} \tan(q/2)}{\sqrt{2 - \mu} + \sqrt{2 + \mu} \tan(q/2)}$$  \hspace{1cm} (23)$$

Using the above expressions, one can show that $L^{(ex)}$ can indeed be positive, which is required for pole singularities in $V_{\text{eff}}^{(ex)}$. For instance, for small $q/\Delta_\xi$, $L^{(ex)}$ has the following asymptotic form:

$$L^{(ex)}(q, \Delta_\xi, \mu) \approx \frac{q^2 \sqrt{4 - \mu^2}}{\Delta_\xi \pi} \left(1 + \frac{q^2}{\Delta_\xi^2} \left(4 - \mu^2 - \Delta_\xi^2/12\right)\right)$$  \hspace{1cm} (24)$$

Whereas $q$ and $\Delta_\xi$ were treated as independent in the above formulas, physically we are interested in the situation where $q = k' - k$ and $\Delta_\xi = \xi_{k'} - \xi_k$, referred to as ‘on-shell’ above. In this case there is a divergence in $L^{(ex)}$ which arises from the pole in the integrand when $p = k$. Since we are interested in $k, k'$ near the Fermi surface, let us be more specific and let $k = k_F(\mu)$ be right on the Fermi surface, and $k'$ be slightly off of it, for a small $\xi_{k'}$. Here $\Delta_\xi = \xi_{k'}$ and the singularity occurs at $q_F \equiv \arccos(-(\xi_{k'} + \mu)/2) - k_F(\mu)$. For $\xi_{k'} = 0.01$ and $\mu = -0.618$, which corresponds to hole doping $h = 0.2$, the singularity is at $q_F = \pm 0.0053$, which is shown in Figure 8. Analytically, this divergence arises as arctan($i$) in the above formulas.

The $p$-integral for $L^{(ex)}$ should thus be understood as the Cauchy principal value (PV), i.e. $\int dp \rightarrow \lim_{\delta \to 0} \left(\int_{-\pi}^{k_F-\delta} dp + \int_{k_F+\delta}^{\pi} dp\right)$. For finite temperature $T$, one can check numerically that this PV integral is well-defined and finite. However it is important to note that $L^{(ex)}$ continues to be divergent as $T \to 0$, which the above analytic formulas demonstrate. The reason is that in the limit of zero $T$, $f$ is a step function and the $\int_{k_F+\delta}^{\pi} dp$ piece of the PV is absent, leading it to be ill-defined. This is interpreted as an infra-red divergence that needs to be regulated by a finite $T$, however small.
Let now turn to the 1-d analogs of the gap $\Delta_{\text{gap}}$ defined in section III. In this 1d case, because of the divergence as $T \to 0$, it makes sense to define $\Delta_{\text{gap}}$ as solutions to eqn. (18) with $T = \Delta_{\text{gap}}$, i.e. to determine $\Delta_{\text{gap}}$ at a temperature comparable to it. The result is shown in Figure 9 where $g_{\text{sc}}$ was taken to be the screened coupling for a bare $g = 1$. In Figure 10 we plot $\Delta_{\text{gap}}$ as a function of the bare coupling $g$; here, contrary to the 2d case, there is no minimal value of $g$ required for the existence of solutions. On the other hand the $\Delta_{\text{gap}}$ saturates with increasing $g$ as in the two-dimensional case.

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FIG. 9: The $\Delta_{\text{gap}}$ pole in $\mathcal{V}_{\text{eff}}^{(\text{ex})}$ as a function of hole doping $h$ for bare coupling $g = 1$.

FIG. 10: The $\Delta_{\text{gap}}$ pole in $\mathcal{V}_{\text{eff}}^{(\text{ex})}$ as a function of coupling $g$ for hole doping $h = 0.15$.

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