Implications of infrared instability in a two-dimensional electron gas

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We consider the tight-binding energy band in *sq* lattices and determine that in the half-filled case there exists an infrared instability in addition to the $2k_F$ (nesting)-type instability. In view of the pseudo-two-dimensional band structure of $La_{2-x}Ba_xCuO_4$ recently proposed by Jorgensen *et al.* and by Mattheiss, our conclusions should be relevant to this material which demonstrates the remarkable phenomenon of high-T_c superconductivity. To further analyze it, we devise a two-dimensional bosonization scheme. Three-dimensional bosonization is also briefly discussed.

In recent Letters, Jorgensen *et al.*[1] and Mattheiss[1] presented detailed descriptions of the structural and electronic properties of the family of materials $La_{2-x}Ba_x$-CuO_4, of which the composition $x=0.15$ demonstrates "high-temperature superconductivity" with $T_c \approx 35$ K. The discovery of this property by Bednorz and Müller[2] and its subsequent confirmation[3] has set off a flurry of experimental and theoretical activity, and has stimulated the discovery of a number of other high-T_c materials.[4]

Now the Letters in Ref. 1 propose a simple pseudo-two-dimensional band structure for the undoped (barium free, $x=0$) material, with the Fermi level at[5] $|k_x|+|k_y|=\pi$. This band structure allows nesting in the [110] and [$\bar{1}$10] directions and suggests that a distortion with $\mathbf{Q}=(\pi,\pi,0)$ or $(-\pi,\pi,0)$ will occur in this material. This is, in fact, observed and leads to an energy gap forming at the erstwhile Fermi surface, and hence to semiconducting behavior. However, doping with Ba shifts the initial Fermi surface eliminating nesting, thus presumably permitting BCS-type pairing to occur (although the precise mechanism causing superconductivity in these materials remains speculative or controversial).

The present Brief Report is a contribution to the theory of interacting electrons in tight-binding (TB) band structures which "nest" easily, such as the materials of Ref. 1. The archetype of this is the following well-known form: $\epsilon_{TB}(\mathbf{k}) = -t(\cos k_x + \cos k_y)$. For a half-filled band, the Fermi level lies along straight-line segments defined by $|k_x|+|k_y|=\pi$ as illustrated in Ref. 1. The states of $\epsilon<0$ are all occupied; those with $\epsilon>0$ are unoccupied in the ground state. Now it will be shown that the instability noted in Ref. 1 with respect to the above $\mathbf{Q}$'s is *not* the only instability caused by this band structure, and indeed that there exist important infrared ($\mathbf{q}\rightarrow\mathbf{0}$) instabilities. In the absence of a firm theory, it is supposed that these infrared modes may be somehow related to the high-temperature superconductivity, but this point cannot be addressed at present. This paper is in two parts. At first, the phenomenon will be demonstrated, and in the second part a model will be set up to deal with it semiquantitatively, by means of some familiar bosonization techniques extended into new territory.

Suppose we apply a perturbation $V(\mathbf{q})$ with $\mathbf{q}\equiv(q_x,q_y)$ and calculate the response to second order, $\delta E = -\frac{1}{2}\chi(\mathbf{q})|V(\mathbf{q})|^2$. We find the following for the long-wavelength ("infrared") response function or susceptibility $\chi(\mathbf{q})$ at low temperatures T:

$$\chi(\mathbf{q}) = \sum \frac{f[\beta\epsilon_{TB}(\mathbf{k}-\mathbf{q}/2)] - f[\beta\epsilon_{TB}(\mathbf{k}+\mathbf{q}/2)]}{\epsilon_{TB}(\mathbf{k}+\mathbf{q}/2) - \epsilon_{TB}(\mathbf{k}-\mathbf{q}/2)} ,$$

which, upon Taylor expansion of the Fermi functions, becomes

$$\chi(\mathbf{q}) = -\sum \partial f[\beta\epsilon_{TB}(\mathbf{k})]/\partial\epsilon_{TB}(\mathbf{k}) = (A/|t|)\ln(|t|)/(kT+Bt|q|) \quad (1)$$

(A,B being appropriate numerical constants). This long-wavelength divergence at $T=0$ reflects the well-known logarithmic singularity of the density of states at the center of the two-dimensional (2D) tight-binding band structure.

Once χ is singular, one can imagine higher-order terms being even more singular, and perturbation theory itself becomes suspect. The question is how to proceed? The many-body problem cannot be solved in general.

My approach is to simplify the form of ϵ so as to achieve an *exactly soluble model,* and with it some insights into the effects of electron-electron interactions, the electron-phonon interaction, pairing, etc. Our model will be based on the observation that ϵ_{TB} is separable—i.e., is written as $\epsilon(k_x)+\epsilon(k_y)$. Let us take the behavior of ϵ_{TB} near the Fermi surface as a guide, linearize so that energy transfer becomes proportional to momentum transfer everywhere, and define the following four-component field theory:

$$H_0 \equiv v_F \sum [(-\pi+k_x+k_y)(a^*_{\mathbf{k},+}a_{\mathbf{k},+}) - (\pi+k_x+k_y)(a^*_{\mathbf{k},-}a_{\mathbf{k},-}) + (-\pi+k_x-k_y)(b^*_{\mathbf{k},+}b_{\mathbf{k},+}) - (\pi+k_x-k_y)(b^*_{\mathbf{k},-}b_{\mathbf{k},-})] , \quad (2)$$

with $\mathbf{k}=(k_x,k_y)$ a two-dimensional vector and $\pm$ refers to right and left going. It is now necessary to fill the negative energy states of four Fermi seas; i.e., to *occupy* all states of type $a(\mathbf{k},+)$ with $k_x+k_y<\pi$, all states of type $a(\mathbf{k},-)$ with $k_x+k_y>-\pi$, all states of type $b(\mathbf{k},+)$ with $k_x-k_y<\pi$, and $b(\mathbf{k},-)$ with $k_x,k_y>-\pi$. The typical two-body interaction is

$$H'=(2\pi\lambda/L)\sum U(\mathbf{q})\rho^*(\mathbf{q})\rho(\mathbf{q}) \ , \tag{3}$$

the ρ's being the charge-density fluctuation operators:

$$\rho(\mathbf{q})\equiv\sum(a^*_{\mathbf{k}+\mathbf{q},+}a_{\mathbf{k},+}+a^*_{\mathbf{k}+\mathbf{q},-}a_{\mathbf{k},-} +b^*_{\mathbf{k}+\mathbf{q},+}b_{\mathbf{k},+}+b^*_{\mathbf{k}+\mathbf{q},-}b_{\mathbf{k},-}) \ . \tag{4}$$

For notational simplicity, the electrons' spin coordinates have been omitted, although this lack is easily remedied by doubling the number of fields. Now, following the well-known procedures of Tomonaga[6] and others[7,8] we replace the operators in (2)–(4), which are quadratic in fermions, by expressions in *boson* creation and annihilation operators $\alpha^*(\mathbf{q}),\alpha(\mathbf{q})$, and $\beta^*(\mathbf{q}),\beta(\mathbf{q})$, as follows:

$$H_0\rightarrow v_F\sum[|q_x+q_y|\alpha^*(\mathbf{q})\alpha(\mathbf{q})+|q_x-q_y|\beta^*(\mathbf{q})\beta(\mathbf{q})] \ , \tag{5}$$

the sums being over all $\mathbf{q}$, while

$$\rho(\mathbf{q})\rightarrow(L/2\pi)^{1/2}\sum{}'(q_x+q_y)^{1/2}[\alpha^*(\mathbf{q})+\alpha(-\mathbf{q})] +(L/2\pi)^{1/2}\sum{}''(q_x-q_y)^{1/2}[\beta^*(\mathbf{q})+\beta(-\mathbf{q})] \ , \tag{6}$$

where $'$ indicates that the first sum is over the half-plane $(q_x+q_y)>0$ and $''$ indicates that the second sum is over the half-plane $(q_x-q_y)>0$.

Equation (5) for H_0, and (3) for H' [using the ρ's given in (6) with the coupling constant set at $\lambda=1$] may be considered either as an approximate reformulation of the original tight-binding model in the presence of interactions (in the spirit of Tomonaga[6] or of random-phase approximation) or as an interesting, linearized, model in its own right, one which is exactly soluble, in the spirit of Luttinger.[7] In any event, it allows us to make use of the simplifying features of the 1D electron gas in 2D, reducing the calculations to the diagonalization of a quadratic form. The two dimensionality has not disappeared—it is reflected in the mixing of α and β operators at every $\mathbf{q}$.

We now evaluate a secular determinant to establish the eigenvalues which diagonalize this quadratic form. Omitting algebraic details, we obtain

$$H=v_F\sum[\omega_+(\mathbf{q})\alpha^*(\mathbf{q})\alpha(\mathbf{q})+\omega_-(\mathbf{q})\beta^*(\mathbf{q})\beta(\mathbf{q})]-W_0 \ , \tag{7}$$

in which the sum is again over all $\mathbf{q}$, W_0 is the change in zero-point energy as λ is increased from 0 to 1, and the $\omega_\pm$ are

$$\omega_\pm(\mathbf{q})=|q|\{(1+2u)\pm[(1+2u)^2-e^2(1+4u)]^{1/2}\}^{1/2} \ . \tag{8}$$

Here $u=u(\mathbf{q})\equiv\lambda U(\mathbf{q})/v_F$ and

$$e\equiv|q_x^2-q_y^2|/q^2=|\cos(2\theta)| \ .$$

Within the context of the given model, Eqs. (7) and (8) are exact to all orders.

The $\omega_+(\mathbf{q})$ normal modes along the $(\pm1,\pm1)$ directions ($e^2=0$) are never unstable. The $\omega_-(\mathbf{q})=0$ modes in these directions, which persist at all values of the interaction parameters u indicate a (harmless) *degeneracy* built into the model. In all other directions, the $\omega_-(\mathbf{q})$ modes can become complex when $u<-\frac{1}{4}$, in which case the linearized theory is without a ground state and must be replaced by a more realistic Hamiltonian.

Since superconductivity is understood to be an instability of the Fermi sea against electron pairing,[9] requiring arbitrarily weak, but attractive forces, it should already be exhibited in the range $-\frac{1}{4}<u\leq0$, i.e., for attractive forces within the range of validity of our model. In extensions of the present work, I intend to examine the electrons' spins, their interactions with short-wavelength ($q\approx\pi$) phonons, and the electron operators for evidence of electron-pairing or other superconducting phenomena.[9]

On the other hand, the present model does not exhibit the standard instabilities [spin-density waves (SDW's) and charge-density wave (CDW's)] against repulsive forces and even appears to be qualitatively (if not quantitatively) *indifferent* to them. This may not be a real problem at all. The *ad hoc* modifications (the model used in Ref. 10) required to incorporate such terms into the boson Hamiltonian are well known,[11,12] and it is not even necessary to take the space to discuss them here. We should also note the recent and most persuasive computational[13] and theoretical[14] evidence that the repulsive 2D electron gas is *indeed* featureless in many respects, exhibiting neither ferromagnetic nor antiferromagnetic short-range or long-range order (SRO, LRO).[13] What is more, Mermin and Wagner's most basic theorem[15] rigorously precludes CDW's, SDW's, *and any other form* of LRO in the 2D electron gas at any finite temperature, except insofar as such distortions are mediated by 3D phonons (or by fully three-dimensional, interplanar, electron-electron interactions).

The generalization of the above to the 3D tight-binding

$$\epsilon=-t(\cos k_x+\cos k_y+\cos k_z)$$

is feasible. The flat areas of the Fermi surface are connected by $\mathbf{Q}=(\pi,\pi,\pi)$. It is necessary to double the number of distinct fields [one for each of the orientations: $(\pm k_x,\pm k_y,\pm k_z)$]. To include the electrons' spin degrees of freedom requires additional doubling of the number of the fields. Although such embellishments pose no difficulty in principle, they do complicate the notation and, in a minor way, the algebra, so I regretfully leave them for future examination.

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