

Superconductivity of the Two-Dimensional Hubbard Model with a Small U

Jun KONDO*

Electrotechnical Laboratory, Tsukuba, Ibaraki 305-8568

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Superconductivity of the two-dimensional Hubbard model with $t' = 0$ has been examined in the small U limit, where the matrix element of pair scattering is expressed as $V_{\mathbf{k}\mathbf{k}'} = U + U^2\chi(\mathbf{k} + \mathbf{k}')$. The susceptibility $\chi(\mathbf{k})$ of the unperturbed band has been evaluated accurately and the gap equation, which reduces to a secular equation, has been solved precisely. The gap is found to be of the form $\propto \exp(-2t^2/xU^2)$, where x is the eigenvalue of the secular equation. We have found the largest eigenvalue x is always positive (superconductive). The symmetry of the gap function is b_{1g} for the electron density $n_e > 0.6$ and b_{2g} for $n_e < 0.6$, depending on the peak position of $\chi(\mathbf{k})$. It is roughly (π, π) for the former case and $(\pi, 0)$ for the latter. The superconductivity seems to prevail even for $n_e \rightarrow 0$. These results can be explained with a simple criterion.

KEYWORDS: superconductivity, Hubbard model, two dimension, theory

§1. Introduction

There has been a controversy on whether the two-dimensional Hubbard model leads to a superconducting state or not. Recent theoretical studies^{1–16)} on this model (and the d-p model) seem to indicate that the answer is yes for some range of parameters. However, a definitive conclusion must be reserved, because all of these studies involve some kind of approximation as RPA,^{1,2)} FLEX,^{3–5)} variation method,^{6–8)} finite systems,^{9–11)} perturbation theory with large U ,^{12–14)} and $1/N$ expansion.^{15,16)} In this paper we rely on a perturbation theory and limit ourselves to the small U limit of the model and will give a definitive answer to this question in this limit.

Our concern is how superconductivity is possible when the interaction is repulsive. We set the problem in the following way. Let us write the interaction energy of the BCS theory as

$$\langle H' \rangle = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}},$$

where $V_{\mathbf{k}\mathbf{k}'}$ is the matrix element for the pair transition from \mathbf{k} to \mathbf{k}' and $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are variational parameters of the theory. If one can make the above energy negative, then we regard the ground state of the model is superconducting. When $V_{\mathbf{k}\mathbf{k}'}$ is negative, one may just take $u_{\mathbf{k}} v_{\mathbf{k}}$ positive. When it is positive, one must divide the \mathbf{k} -space into two regions, where $u_{\mathbf{k}} v_{\mathbf{k}}$ is either positive or negative. Then the sum has contributions of both signs. How can the negative contributions overcome the positive ones? First we note that, when $V_{\mathbf{k}\mathbf{k}'}$ is independent of \mathbf{k} and \mathbf{k}' , the sum is expressed as $V(\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}})^2$, which is positive or at best zero. Consequently, in order to have a superconducting energy gain for the Hubbard model, where the bare interaction U is independent of \mathbf{k} and \mathbf{k}' , we must take account of the electron correla-

tion and derive a \mathbf{k} and \mathbf{k}' dependent interaction. There have been three ways to do this. Anderson proposed the t - J model which takes account of a strong correlation effect.¹⁷⁾ On the other hand, the spin fluctuation theory takes account of the correlation perturbatively.^{18–20)} A variation method was used by Yamaji *et al.*, who took a BCS wave function with a Gutzwiller projection.^{6–8)}

Once we have a \mathbf{k} and \mathbf{k}' dependent interaction $V_{\mathbf{k}\mathbf{k}'}$, our next task is to find $u_{\mathbf{k}} v_{\mathbf{k}}$ such that $u_{\mathbf{k}} v_{\mathbf{k}}$ and $u_{\mathbf{k}'} v_{\mathbf{k}'}$ should have different signs when $V_{\mathbf{k}\mathbf{k}'}$ is larger than its average and the same sign when $V_{\mathbf{k}\mathbf{k}'}$ is smaller than the average. This task is not always successful. As we will show in the following, however, the two dimensional Hubbard model with a small U is well suited for this purpose. By taking the correlation effect correct up to the first order of U , we find that $V_{\mathbf{k}\mathbf{k}'}$ is expressed by the wave number dependent susceptibility of the unperturbed band, as the spin fluctuation theory indicated:^{18–20)}

$$V_{\mathbf{k}\mathbf{k}'} = \frac{U}{N} + \frac{U^2}{N} \chi(\mathbf{k} + \mathbf{k}'), \quad (1)$$

$$\chi(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{q}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{q}}}{\varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}. \quad (2)$$

We neglect the next-nearest-neighbour transfer t' so that $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$. Evaluating the susceptibility accurately for arbitrary \mathbf{k} and solving the gap equation precisely, we shall find that the ground state is superconducting at least for the electron number per site between 0.9 and 0.1. The symmetry of the gap function changes from b_{1g} to b_{2g} at the electron number ≈ 0.6 . The superconductivity seems to prevail even for very small electron number. This switch of the symmetry and robustness of the superconductivity can clearly be explained with the following criterion: *In order to have a superconducting energy gain for a repulsive interaction, the gap functions $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{k}'}$ should have different signs, when the interaction $V_{\mathbf{k}\mathbf{k}'}$ is larger than its average, and*

*Correspondence should be sent to 2-2-29 Kamitakaido, Suginamiku, Tokyo 168-0074.

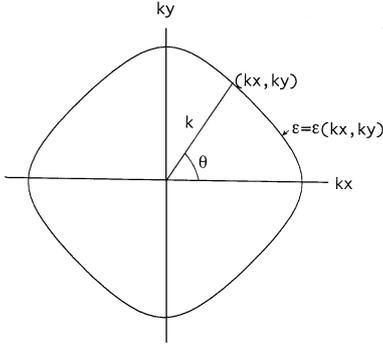


Fig. 1. Definition of the *polar* coordinates, ε and θ .

the same sign, when it is smaller than its average.

§2. Formulation

We take the BCS state $\Psi = P_{N_e} \Pi(u_{\mathbf{k}} + v_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger) |0\rangle$ and find the average of the energy as

$$E_S = \sum_{\mathbf{k}} 2\varepsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}. \quad (3)$$

Minimizing this energy with respect to $v_{\mathbf{k}}$ we obtain the gap equation

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \quad (4)$$

with $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. We consider the case of weak coupling (small U) and set $\Delta_{\mathbf{k}} = \Delta \cdot z_{\mathbf{k}}$, where Δ denotes the magnitude of $\Delta_{\mathbf{k}}$ and $z_{\mathbf{k}}$ represents its \mathbf{k} -dependence. In the weak coupling limit the sum in eq. (4) involves a $\log \Delta$ term and terms that remain a constant as $\Delta \rightarrow 0$. In the approximation of retaining only the $\log \Delta$ term, we can rewrite eq. (4) as

$$z_{\mathbf{k}} = \log \Delta \cdot \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \delta(\varepsilon_{\mathbf{k}'}) z_{\mathbf{k}'}. \quad (5)$$

This is a linear homogeneous equation for the gap function $z_{\mathbf{k}}$, the eigenvalue being $1/\log \Delta$.

In order to solve this equation we use *polar* coordinates ε , θ instead of k_x , k_y , where $\varepsilon = \varepsilon_{\mathbf{k}}$ and θ is the angle between \mathbf{k} and the k_x axis (see Fig. 1), and express $z_{\mathbf{k}}$ as $z_{\mathbf{k}} = z(\varepsilon, \theta)$. We also express $V_{\mathbf{k}\mathbf{k}'}$ with the *polar* coordinates as $V_{\mathbf{k}\mathbf{k}'} = \tilde{V}(\varepsilon, \theta, \varepsilon', \theta')$. Then eq. (5) reads

$$z(\varepsilon, \theta) = \log \Delta \cdot N \iint \rho(\varepsilon', \theta') \tilde{V}(\varepsilon, \theta, \varepsilon', \theta') \times \delta(\varepsilon') z(\varepsilon', \theta') d\varepsilon' d\theta', \quad (6)$$

where the sum over \mathbf{k} has been replaced by the integral over ε and θ with the use of the density of states $\rho(\varepsilon, \theta)$. One may be interested only in the gap function on the Fermi surface $z(0, \theta)$, which we decompose as

$$z(0, \theta) = \sum_l z_l e^{il\theta}, \quad (7)$$

and express eq. (6) for $\varepsilon = 0$ as

$$z_l = \log \Delta \cdot \sum_{l'} H_{ll'} z_{l'}, \quad (8)$$

where

$$H_{ll'} = \frac{N}{2\pi} \iint \tilde{V}_F(\theta, \theta') \rho_F(\theta') e^{il'\theta' - il\theta} d\theta d\theta', \quad (9)$$

with $\tilde{V}_F(\theta, \theta') \equiv \tilde{V}(0, \theta, 0, \theta')$ and $\rho_F(\theta) \equiv \rho(0, \theta)$. Although the absolute magnitude of z_l is not fixed by eq. (8), z_l fixes the angular dependence of the gap function. Note that $\tilde{V}_F(\theta, \theta')$ is the interaction strength for the transition of the pair from θ -direction to θ' -direction and is the most important quantity in the following argument. Since the matrix $H_{ll'}$ is not hermitian, one may wonder if its eigenvalue is real or not. However, one can easily show that it is real.

§3. Irreducible Representations of Even Parity

We now concentrate on superconductivity of even parity in the square lattice. The eigenfunction of the gap equation (8) is specified by one of the irreducible representations, a_{1g} , a_{2g} , b_{1g} and b_{2g} , of the square lattice. Symmetry requirements of each representation pose constraints on the form of the gap function:

$$z(0, \theta) = \sum_{L=1} z_{4L} \cos 4L\theta \quad a_{1g}, \quad (10)$$

$$z(0, \theta) = \sum_{L=1} z_{4L} \sin 4L\theta \quad a_{2g}, \quad (11)$$

$$z(0, \theta) = \sum_{L=1} z_{4L-2} \cos(4L-2)\theta \quad b_{1g}, \quad (12)$$

$$z(0, \theta) = \sum_{L=1} z_{4L-2} \sin(4L-2)\theta \quad b_{2g}, \quad (13)$$

The $L=0$ term of the a_{1g} representation was omitted to suppress a strong s-type repulsive term U/N in eq. (1).

We now express $\tilde{V}_F(\theta, \theta')$ in terms of $\chi(\mathbf{k} + \mathbf{k}')$ using eq. (1). We define $\chi_F(\theta, \theta')$ by the value of $\chi(\mathbf{k} + \mathbf{k}')$, where \mathbf{k} and \mathbf{k}' are on the Fermi surface and θ and θ' are their polar angles:

$$\chi_F(\theta, \theta') = \chi(k_F(\theta) \cos \theta + k_F(\theta') \cos \theta', \quad (14)$$

$$k_F(\theta) \sin \theta + k_F(\theta') \sin \theta'),$$

where $k_F(\theta)$ is the magnitude of \mathbf{k} on the Fermi surface with the *polar* angle θ . Since the U term vanishes, we expect an attractive interaction occurs at U^2 and set

$$\log \Delta = -2t^2/xU^2, \quad (15)$$

where x is to be determined. With these definitions the secular equation reads

$$xz_l = \sum_{l'} G_{ll'} z_{l'}, \quad (16)$$

$$G_{ll'} = -\frac{1}{\pi} \iint \chi_F(\theta, \theta') \rho_F(\theta') e^{il'\theta' - il\theta} d\theta d\theta'. \quad (17)$$

The solution of eq. (16) is specified by one of the four types of the symmetry. When the eigenvalue x for one of them is positive, the superconductivity of that symmetry is stable and what has the largest eigenvalue x is the most stable one.

We have first made a computer program to calculate $\chi(k_x, k_y)$ for arbitrary k_x and k_y . Using this program we calculated $\chi_F(\theta, \theta')$ for 200×200 points in the intervals of $0 \leq \theta \leq \pi$ and $-\pi/2 \leq \theta' \leq \pi/2$. With these data the double integral was evaluated using an interpolation method. Finally the result is multiplied by 4 to obtain the integral in eq. (17), in which the integration ranges are $0 \leq \theta \leq 2\pi$ and $0 \leq \theta' \leq 2\pi$. This is allowed by symmetry properties of $\chi_F(\theta, \theta')$. We note that, when

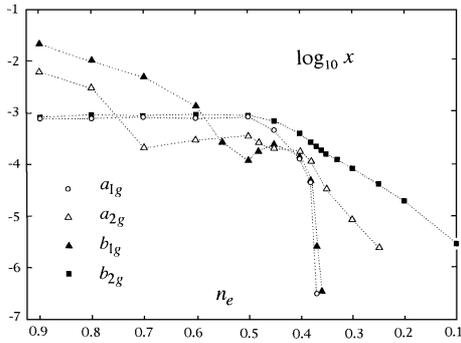


Fig. 2. Logarithm of x vs n_e for the four symmetry types.

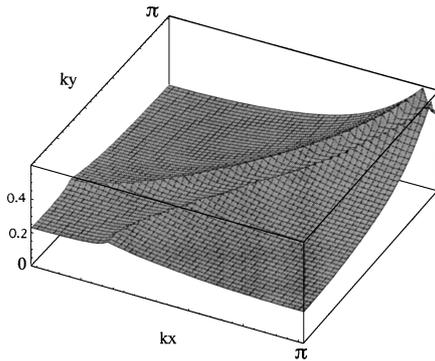


Fig. 3. $\chi(k_x, k_y)$ for $n_e = 0.9$.

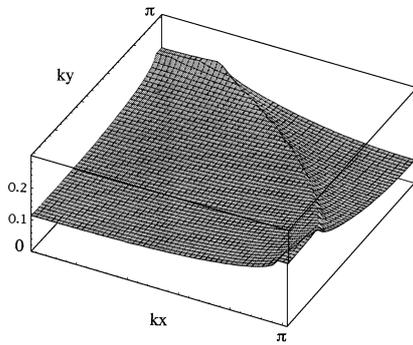


Fig. 4. $\chi(k_x, k_y)$ for $n_e = 0.4$.

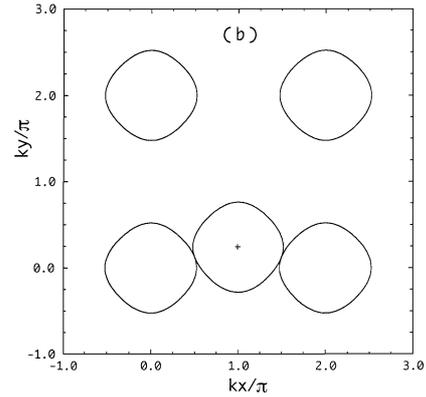
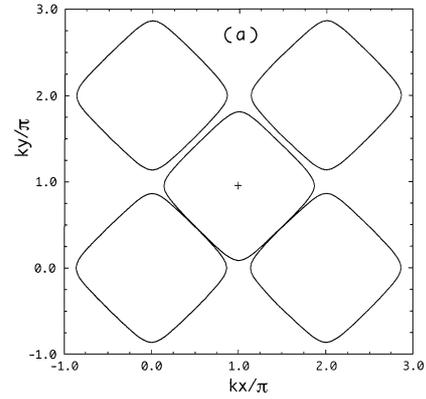


Fig. 5. The peak of χ is at the center of the nesting fermi surface (a) $n_e = 0.9$ (b) $n_e = 0.4$.

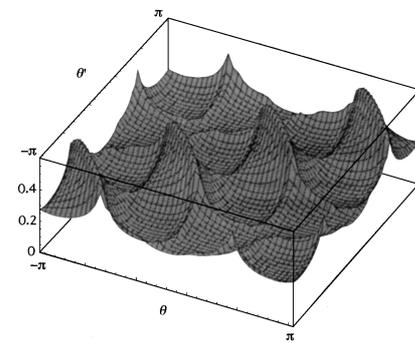


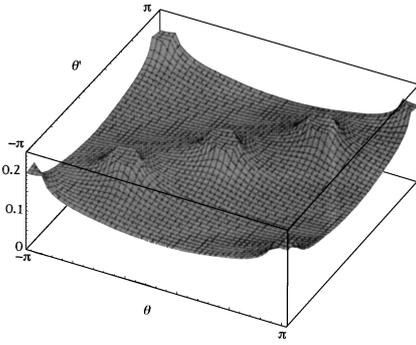
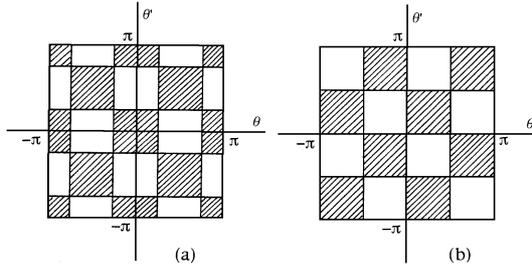
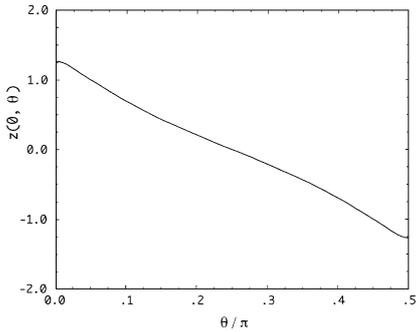
Fig. 6. $\chi_F(\theta, \theta')$ for $n_e = 0.9$.

we take 160×160 points instead of 200×200 , the final results of x and z_l differ only less than 1%.

§4. Results

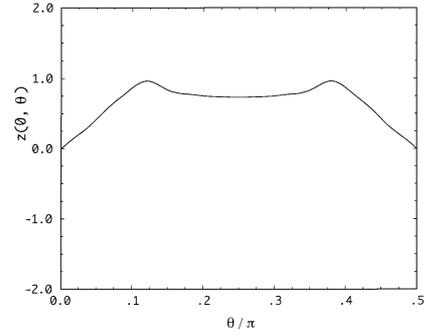
As we solve eq. (16), we first take account of constraints on the value of l ($l = 4L$ or $4L - 2$ with $L = 1, 2, \dots$). In the usual case we took L up to 10 and in some cases to 25. Figure 2 shows the logarithm of the largest eigenvalue x vs the electron density n_e for the four symmetries of the gap function. One sees that the b_{1g} state is the most stable for $n_e = 0.9$ to 0.6 but the b_{2g} state takes place for n_e less than 0.6. It is remarkable that the ground state of the Hubbard model is superconducting down to $n_e = 0.1$, where the fermi surface is almost a circle as in the jellium model.

Figures 3 and 4 show the susceptibility $\chi(k_x, k_y)$ as a function of k_x and k_y for $n_e = 0.9$ and 0.4, respectively. The peaks near (π, π) in the case of $n_e = 0.9$ and the flat ones near $(\pi, 0)$ or $(0, \pi)$ for $n_e = 0.4$ are the result of the nesting of the fermi surface (see Fig. 5). Figure 6 shows $\chi_F(\theta, \theta')$ for $n_e = 0.9$. One sees that a very sharp ridge runs along the line from $(\pi/2, 0)$ to $(0, \pi/2)$ or along equivalent lines, the highest point being at $(\pi/4, \pi/4)$ and equivalent points. Point $(0, \pi/2)$ in the θ - θ' plane, for example, represents transition from \mathbf{k} on the k_x axis to \mathbf{k}' on the k_y axis. Then $\mathbf{k} + \mathbf{k}'$ is very close to the peak in Fig. 3, where the susceptibility is the largest. For point (θ, θ') on the line from $(\pi/2, 0)$ to $(0, \pi/2)$, one has $\theta + \theta' = \pi/2$ and the corresponding $\mathbf{k} + \mathbf{k}'$ is also close to the peak. On the other hand, along the line from $(\pi, 0)$ to $(0, -\pi)$ or along equivalent lines $\mathbf{k} + \mathbf{k}'$ is zero (backward

Fig. 7. $\chi_F(\theta, \theta')$ for $n_e = 0.4$.Fig. 8. The signs of (a) $\cos 2\theta \times \cos 2\theta'$ and (b) $\sin 2\theta \times \sin 2\theta'$. The sign is plus (shaded) or minus (open).Fig. 9. The gap function $z(0, \theta)$ of b_{1g} symmetry for $n_e = 0.9$.

scattering), so the susceptibility is the smallest there. One may notice deep valleys running along these lines in Fig. 6. In Fig. 7, which shows $\chi_F(\theta, \theta')$ for $n_e = 0.4$, one sees mesas centered at $(0, 0)$ and $(\pm\pi/2, \pm\pi/2)$. The origin of the mesas is seen from Fig. 4. Point $(0, 0)$, for example, implies that both \mathbf{k} and \mathbf{k}' are on the k_x axis. Since $k_F(\theta = 0)$ is about 0.51π for $n_e = 0.4$, $\mathbf{k} + \mathbf{k}'$ is close to $(1.02\pi, 0)$, where the susceptibility is the largest. On the other hand, point $(\pi/4, \pi/4)$ implies $\mathbf{k} + \mathbf{k}'$ is at 45 degrees from the k_x axis, where the susceptibility is smaller than that on the principal axes. As one goes to $n_e = 0.3$, one still finds ruined mesas along the diagonal (not shown). Weak undulation (maxima at $(0, 0)$ and $(\pm\pi/2, \pm\pi/2)$, etc. and minima at $(\pm\pi/4, \pm\pi/4)$, etc.) also comes from the fact that the susceptibility is larger on the principal axes than on the lines at 45 degrees from them. We have found such undulation even for $n_e = 0.1$.

We now present the results of diagonalization of

Fig. 10. The gap function $z(0, \theta)$ of b_{2g} symmetry for $n_e = 0.4$.

eq. (16). We first discuss the case of $n_e = 0.9$, for which the gap function with the b_{1g} symmetry gives us the most stable superconducting state. In Fig. 8(a) we show the signs of $\cos 2\theta \times \cos 2\theta'$ on the θ - θ' plane. Our criterion to obtain an energy gain for the superconducting state is that the product of the gap functions, $z(0, \theta) \times z(0, \theta')$, should be negative where the susceptibility $\chi_F(\theta, \theta')$ is large and vice versa. Watching Fig. 6 and Fig. 8(a), we find that the gap function $\cos 2\theta$ really satisfies this criterion. In fact we find $G_{22} = 0.0187$, which is positive and implies a superconducting energy gain. By taking terms up to $L = 10$ ($l = 38$) we find the largest eigenvalue of eq. (16) is $x = 0.0204$. The gap function, eq. (12), with L summed up to 10 is shown in Fig. 9, which is basically of $\cos 2\theta$ type.

In contrast to the case of $n_e = 0.9$ the susceptibility $\chi_F(\theta, \theta')$ for $n_e = 0.4$ is now small at $(\pm\pi/4, \pm\pi/4)$ and equivalent points on diagonals (Fig. 7). This fits to the gap function $\sin 2\theta$. In fact, the undulation of $\sin 2\theta \times \sin 2\theta'$ along the diagonal axis ($\theta = \theta'$) is 180 degrees out of phase from that of $\chi_F(\theta, \theta')$ along the same axis (see Fig. 7 and Fig. 8(b)). This is favorable for a superconducting energy gain. By diagonalizing the secular equation for the b_{2g} symmetry with L up to 10 ($l = 38$) we find the largest eigenvalue $x = 0.00039$ and the gap function as shown in Fig. 10.

As n_e becomes smaller further, $\chi_F(\theta, \theta')$ shows undulation of a smaller amplitude along the diagonal with maxima at $(0, 0)$, $(\pm\pi/2, \pm\pi/2)$ etc. and minima at $(\pm\pi/4, \pm\pi/4)$ etc. and the gap function is better represented by a single $\sin 2\theta$ term. Such a small undulation of $\chi_F(\theta, \theta')$ is the result of $\chi(\mathbf{k})$ having the symmetry of the square lattice even for very small n_e , being larger on the principal axes than on the lines 45 degrees from them. Since this undulation is out of phase from that of $\sin 2\theta \times \sin 2\theta'$ along the diagonal, the gap function $\sin 2\theta$ picks up such a small undulation and gives rise to a superconducting energy gain.

§5. Discussion

Superconductivity arising from a short-ranged repulsive interaction was first pointed out by Kohn and Luttinger for the three dimensional electron gas.²¹⁾ Their result is correct within the second order perturbation theory for low electron density and they stated that the superconductivity originates from the sharpness of

the fermi surface. Chubukov²²⁾ applied their theory to the two dimensional fermi liquid and predicted that a (triplet) pairing instability should occur only at the third (or higher) order perturbation calculation. In this paper we have shown that a singlet pairing should occur at the second order of the interaction U for the electrons in a lattice. It originates from the square lattice symmetry of the wave number dependent susceptibility of the unperturbed band.

In this paper we have tried to visualize how the superconducting energy gain arises from a repulsive interaction. The idea of deviding the \mathbf{k} -space into two regions where the gap function is either positive or negative is similar to that of the two-band superconductivity, where the sign of the gap function is different for different bands.²³⁾ In order to have a net energy gain the interaction must have an appropriate wave number dependence. In this respect we have found that the two-dimensional Hubbard model is ideal. At least for a small U one can say that the ground state is superconducting with some symmetry without worrying about SDW. We have also seen that the wave number dependence of the interaction in the Hubbard model arises from the electron correlation, which may be taken into account either by a perturbation theory or by a Gutzwiller projection. For a large U limit it may also be taken by another perturbation theory, which gives us the t - J model. We have limited our study to the second order of U . The spin fluctuation theory is a way to take account of higher-order terms in U . It is not certain, however, that the effect of the electron correlation is fully taken into account by the wave number dependent susceptibility. Hotta¹²⁾ and Jujo, Koikegami and Yamada¹³⁾ showed that the vertex correction has an important effect to reduce the T_c .

In this paper we have been concerned only with the even parity superconductivity. To treat the case of the triplet superconductivity in the small U limit one just replaces $\chi(\mathbf{k} + \mathbf{k}')$ by $-\chi(\mathbf{k} - \mathbf{k}')$.^{19,20)} Then it is easily seen that the triplet superconducting state is not stable in this limit for any electron density. That a triplet pairing in two dimension occurs at the third order of the interaction has been shown by Chubukov²²⁾ for the low

density fermi liquid and by Nomura and Yamada¹⁴⁾ for the Hubbard model away from the half-filling.

A detailed account of this study has been published in Bulletin of the Electrotechnical Laboratory (special issue) vol. 64 (2000) 67.

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