〔RESEARCH〕

Superconductivity of the 2D Hubbard Model with a Small U

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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 $V_{\mathbf{kk'}}=U+U^2\chi(\mathbf{k}+\mathbf{k}')$. The susceptibility $\chi(\mathbf{k})$ has been evaluated accurately and the gap equation, which reduces to a seqular 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 seqular equation with dimension of 10 to 25. 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 $n_e \to 0$. These results can be explained in terms of the following criterion: In order to have a superconducting energy gain for a repulsive interaction, the gap functions at $\mathbf{k}$ and $\mathbf{k}'$ should have different signs, when the interaction for pair scattering from $\mathbf{k}$ to $\mathbf{k}'$ is larger than its average and they should have the same sign when the pair scattering is smaller than its average.

§1 Introduction

Recent theoretical studies on the two-dimensional Hubbard model indicate that the ground state of the model seems to be superconducting for some range of parameters[1-10]. 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

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

where $V_{\mathbf{kk'}}$ 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 $V_{\mathbf{kk'}}$ is negative, one may take $u_{\mathbf{k}}v_{\mathbf{k}}$ positive. When it is positive, one must devide the 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 $V_{\mathbf{kk'}}$ 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. So our strategy is such that $u_{\mathbf{k}}v_{\mathbf{k}}$ and $u_{\mathbf{k'}}v_{\mathbf{k'}}$ should have different signs when $V_{\mathbf{kk'}}$ is larger than its average and the same sign when $V_{\mathbf{kk'}}$ is smaller than the average. Taking the BCS wave function for the Hubbard Hamiltonian, in which the interaction is k-independent, one cannot make the interaction energy negative even for the d-wave pairing. To have a $\mathbf{k}$, $\mathbf{k}'$-dependence of the interaction for the Hubbard Hamiltonian one may derive an effective interaction as in the spin fluctuation theory[11-12]. This theory tells us that the effective interaction is expressed as

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

up to the second order of U, where $\chi(\mathbf{k})$ is the wave number dependent susceptibility of the unperturbed band, and it also tells us that, when $\chi(\mathbf{k})$ has a peak at (π, π), a d-wave superconductivity is possible. Another way to have a $\mathbf{k}$, $\mathbf{k}'$-dependence of the interaction is to take account of the electron correlation. Yamaji et al.[5-7]

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took a BCS wave function with a Gutzwiller projection to take account of the electron correlation but with a bare Hubbard U and showed that the ground state is a d-wave superconductor for some parameter regions. In their theory the effective interaction, if the theory can be reformulated in terms of it, should have a $\mathbf{k}$, $\mathbf{k}'$-dependence favorable for the d-wave superconductivity.

In this paper we first derive Eq. (1) by taking account of the electron correlation correct up to the first order of U. Then we calculate $\chi(\mathbf{k})$ accurately and solve the self-consistency equation for the superconducting gap function $\Delta_{\mathbf{k}}$ as precisely as possible by taking the interaction as given in Eq. (1). We 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. This switch of the symmetry can clearly be explained in terms of the 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 $V_{\mathbf{kk}'}$ is larger than its average, and the same sign, when it is smaller than its average.*

§2 Formulation

We take the two-dimensional Hubbard model

$$H=H_0+H' , \tag{2}$$

$$H_0=\sum_{\sigma k}\varepsilon_k c_{\sigma k}^{\dagger} c_{\sigma k}, \tag{3}$$

$$\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-\mu, \tag{4}$$

$$H'=U\sum_n c_{n\uparrow}^{\dagger} c_{n\uparrow} c_{n\downarrow}^{\dagger} c_{n\downarrow}, \tag{5}$$

where t denotes the nearest-neighbour hopping integral and U is the on-site Coulomb repulsion. The total site number and the total electron number will be denoted by N and N_e, respectively. The electron states where all the N_e electrons are paired will be denoted by ϕ_n, ϕ_m etc. and those where only one pair is broken by ψ_i, ψ_j, etc. We look for the solution of the Schrödinger equation

$$H\Psi=E\Psi, \tag{6}$$

in which Ψ is expressed as

$$\Psi=\sum_n a_n\phi_n+\sum_i b_i\psi_i. \tag{7}$$

When U is small, we eliminate the second term with the use of a perturbation theory and obtain the equation for a_n as

$$(E-E_n)a_n=\sum_{m\neq n}\langle n\tilde{H}'m\rangle a_m , \tag{8}$$

where

$$\left\langle n\tilde{H}'\, m\right\rangle = \langle nH'\, m\rangle + \sum_i \frac{\langle nH'\, i\rangle\langle iH'\, m\rangle}{E-E_i}. \tag{9}$$

E_i denotes the energy of the excited state ψ_i: $E_i=\langle iHi\rangle$. When ϕ_n and ϕ_m differ only by a single pair, $(\mathbf{k}\uparrow,-\mathbf{k}\downarrow)$ for ϕ_m and $(\mathbf{k}'\uparrow,-\mathbf{k}'\downarrow)$ for ϕ_n, then the effective matrix element for the transition from ϕ_m to ϕ_n is obtained by calculating contributions from the two diagrams shown in **Fig.1**. The result is

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

where

$$\chi(\mathbf{k}) = \frac{2}{N}\sum_{\mathbf{q}}\frac{f_{\mathbf{q}}(1-f_{\mathbf{q}+\mathbf{k}})}{\varepsilon_{\mathbf{q}+\mathbf{k}}-\varepsilon_{\mathbf{q}}} = \frac{2}{N}\sum_{\mathbf{q}}\frac{f_{\mathbf{q}}}{\varepsilon_{\mathbf{q}+\mathbf{k}}-\varepsilon_{\mathbf{q}}}. \tag{10}$$

In deriving this result, we replaced E_i–E by the excitation energy necessary for going from ϕ_m to ψ_i, E_i–E_m, and furthermore neglected $\varepsilon_{\mathbf{k}}$–$\varepsilon_{\mathbf{k}'}$, because we consider $\mathbf{k}$ and $\mathbf{k}'$ both very close to the fermi surface.

Following the BCS theory we take the independent pair approximation :

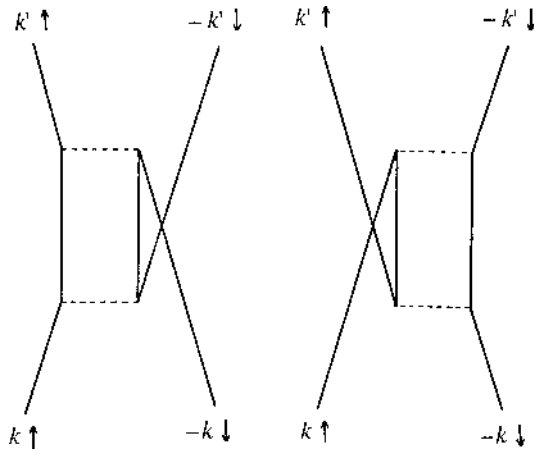

Fig.1 Diagrams contributing to the first order correction of the scattering amplitude.

$$\Psi_0 = \sum{}_n a_n \phi_n = P_{Ne}\Pi(u_{\mathbf{k}} + v_{\mathbf{k}} a_{\mathbf{k}\uparrow}{}^{\dagger} a_{-\mathbf{k}\downarrow}{}^{\dagger})|0\rangle. \quad (11)$$

Then the ground state energy is obtained as

$$\begin{aligned} E_s &= \langle \Psi H \Psi \rangle = \left\langle \Psi_0 \tilde{H} \Psi_0 \right\rangle \\ &= \sum{}_{\mathbf{k}} 2\varepsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum{}_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}. \end{aligned} \quad (12)$$

Minimizing this expression with respect to $v_{\mathbf{k}}$, we have

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{1}{2}\frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad (13)$$

with $E_{\mathbf{k}} = \sqrt{\varepsilon_k^2 + \Delta_k^2}$ and the self-consistency equation

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum{}_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}}. \quad (14)$$

As we solve this equation in the weak-coupling limit, namely the limit of small $\Delta_{\mathbf{k}}$, we note that the sum over **k**' in Eq.(14) is simplified in this limit. Consider the sum $\sum_{\mathbf{k}} \frac{A_{\mathbf{k}}}{E_{\mathbf{k}}}$, where $A_{\mathbf{k}}$ is a function of $\mathbf{k}=(k_x,k_y)$. We set $\Delta_{\mathbf{k}}$ as $\Delta_{\mathbf{k}}=\Delta\cdot z_{\mathbf{k}}$, where Δ denotes the magnitude of $\Delta_{\mathbf{k}}$ and $z_{\mathbf{k}}$ represents its k-dependence. For $\Delta\to 0$ the sum diverges as $\log\Delta$. We want to find the correct coefficent of $\log\Delta$ but are not concerned with non-divergent terms. This amounts to finding the correct exponent of the superconducting gap but its prefactor may be incorrect. For this purpose we use "polar" coordinates ε, θ instead of k_x,k_y, where $\varepsilon=\varepsilon_{\mathbf{k}}$ and θ is the angle between **k** and the k_x axis (see **Fig.2**). Replacing the sum over k by an integral over ε and θ by using the density of states $\rho(\varepsilon,\theta)$, we have

$$\sum{}_{\mathbf{k}} \frac{A_{\mathbf{k}}}{E_{\mathbf{k}}} = N\iint \frac{A(\varepsilon,\theta)}{\sqrt{\varepsilon^2 + \Delta^2 z(\varepsilon,\theta)^2}} \rho(\varepsilon,\theta) d\varepsilon d\theta. \quad (15)$$

For very small Δ the main contribution to the integral over ε comes from ε close to zero, so Eq.(15) gives us a term involving $\log[\Delta\cdot z(0,\theta)]$. This implies that, to find the coefficient of $\log\Delta$, we can set $z(\varepsilon,\theta)$ to a constant, say, unity. Thus we have

$$\int \frac{g(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} d\varepsilon = -2g(0)\log\Delta + \text{non-divergent terms}. \quad (16)$$

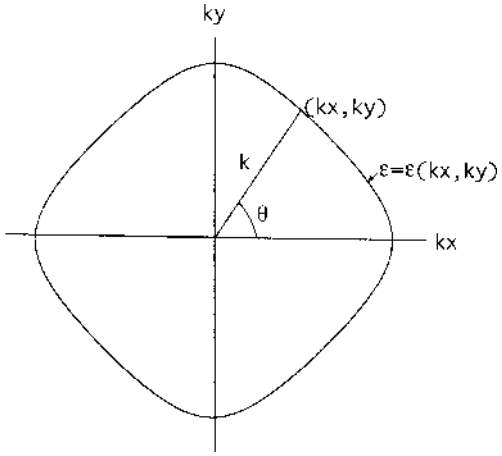

Fig.2 Definition of the "polar" coordinates, ε and θ.

This result tells us that for the limit of small Δ we can set as

$$\sum{}_{\mathbf{k}} \frac{A_{\mathbf{k}}}{E_{\mathbf{k}}} = -2\log\Delta \sum{}_{\mathbf{k}} A_{\mathbf{k}} \delta(\varepsilon_{\mathbf{k}}) \quad (17)$$

in the accuracy of retaining only the $\log\Delta$ term. Consequently, in the same accuracy Eq.(14) is written as

$$z_{\mathbf{k}} = \log\Delta \cdot \sum{}_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \delta(\varepsilon_{\mathbf{k}'}) z_{\mathbf{k}'}. \quad (18)$$

§3 Methods of solving the self-consistency equation

3.1 Fourier transform

We decompose all the quantities that depend on the wave number **k** into components depending on integers *n* and *m*. Thus

$$z_{\mathbf{k}} = \sum{}_{nm} z_{nm} e^{i(k_x n + k_y m)}, \quad (19)$$

$$\begin{aligned} V_{\mathbf{k}\mathbf{k}'} &= V(\mathbf{k} + \mathbf{k}') = V\left(k_x + k_x', k_y + k_y'\right) \\ &= \sum{}_{nm} v_{nm} e^{i\left(k_x n + k_y m\right)} e^{i\left(k_x' n + k_y' m\right)}. \end{aligned} \quad (20)$$

Eq.(18) now reads in terms of the Fourier components

$$z_{nm} = \log\Delta \cdot v_{nm} \sum{}_{n'm'} \left(\sum{}_{\mathbf{k}} \delta(\varepsilon_{\mathbf{k}}) e^{i\left[k_x (n+n') + k_y (m+m')\right]}\right) z_{n'm'}. \quad (21)$$

This is a homogeneous linear equation and can be solved

by a standard method, 1/logΔ being the eigenvalue. We have solved this equation by taking more than 1000 z_{nm}'s into account. (Independent z_{nm}'s are about 120.) Convergence of the results is satisfactory for $n_e \equiv N_e/N$ larger than 0.4. To obtain a reliable result for $n_e < 0.4$ we resort to the second method. The results of the eigenvalues and the gap functions for $n_e > 0.4$ are almost the same for both methods. Since the second method takes less computation time and is more transparent to obtain a physical insight, we will concentrate on it after this.

3.2 Use of the "polar" coordinates

We decompose $z_{\mathbf{k}}$ as

$$z_{\mathbf{k}}=z(\varepsilon,\theta)=\sum_l z_l(\varepsilon)e^{il\theta} \tag{22}$$

and express $V_{\mathbf{kk}'}$ in terms of the "polar" coordinates:

$$\begin{aligned} V_{\mathbf{kk}'}&=V(\mathbf{k}+\mathbf{k}')=V(k_x+k_x',\ k_y+k_y') \\ &=V(k(\varepsilon,\theta)\cos\theta+k(\varepsilon',\theta')\cos\theta',\ k(\varepsilon,\theta)\sin\theta \\ &\quad +k(\varepsilon',\theta')\sin\theta') \\ &\equiv\tilde{V}(\varepsilon,\theta,\varepsilon',\theta'), \end{aligned} \tag{23}$$

where $k(\varepsilon,\theta)$ is the magnitude of $\mathbf{k}$ expressed in terms of ε and θ. With the use of the "polar" coordinates Eq. (18) reads

$$z(\varepsilon,\theta)=\log\Delta\cdot N\iint\rho(\varepsilon',\theta')\tilde{V}(\varepsilon,\theta,\varepsilon',\theta')\delta(\varepsilon')z(\varepsilon',\theta')d\varepsilon'd\theta'. \tag{24}$$

One may be interested only in the gap function on the fermi surface $z(0,\theta)$. Defining z_l by $z_l=z_l(0)$ and expressing Eq.(24) in terms of it, we obtain

$$z_l=\log\Delta\cdot\sum_{l'}H_{ll'}z_{l'}, \tag{25}$$

where

$$H_{ll'}=\frac{N}{2\pi}\iint\tilde{V}_F(\theta,\theta')\rho_F(\theta')e^{il'\theta'-il\theta}d\theta d\theta', \tag{26}$$

$$\tilde{V}_F(\theta,\theta')\equiv\tilde{V}(0,\theta,0,\theta'), \tag{27}$$

and

$$\rho_F(\theta)\equiv\rho(0,\theta). \tag{28}$$

Solving this equation gives us Δ and z_l except their absolute magnitude. However, 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. A proof that it is real will be given in the following. Define $\rho_{l-l'}$ by $\rho_{l-l'}\equiv\int\rho_F(\theta)e^{i(l-l')\theta}d\theta$. Multiplying both sides of Eq.(25) by $\tilde{z}_{l'}\rho_{l-l'}$ and summing over l and l', one obtains

$$\sum_{ll'}\tilde{z}_{l'}\rho_{l-l'}z_l=\log\Delta\cdot\sum_{ll'l''}\tilde{z}_{l'}\rho_{l-l'}H_{ll''}z_{l''}. \tag{29}$$

Using the formula $\sum_l e^{il(\theta-\theta')}=2\pi\delta(\theta-\theta')$, one can show that

$$\sum_l\rho_{l-l'}H_{ll''}=N\iint\rho_F(\theta)\rho_F(\theta')\tilde{V}_F(\theta,\theta')e^{il''\theta'-il'\theta}d\theta d\theta', \tag{30}$$

which is now hermitian when l' and l'' are regarded as suffixes. Thus one sees that both sums in Eq.(29) are real and so is logΔ.

§4 Irreducible representations of even parity

We now concentrate on superconductivity of even parity in the square lattice. The eigenfunction of the gap equation (25) 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:

$$z(0,\theta)=\sum_{L=1}z_{4L}\cos 4L\theta \qquad a_{1g} \tag{31}$$

$$z(0,\theta)=\sum_{L=1}z_{4L}\sin 4L\theta \qquad a_{2g} \tag{32}$$

$$z(0,\theta)=\sum_{L=1}z_{4L-2}\cos(4L-2)\theta \qquad b_{1g} \tag{33}$$

$$z(0,\theta)=\sum_{L=1}z_{4L-2}\sin(4L-2)\theta \qquad b_{2g} \tag{34}$$

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

Following these limitations on the values of l, the seqular equations are also modified. We present the case of the b_{1g} representaion as an example:

$$z_{4L-2}=\log\Delta\sum_{L'=1}G_{LL'}z_{4L'-2}, \qquad L=1,2,\cdots \tag{35}$$

where

$$G_{LL'} = \frac{N}{\pi}\iint \rho_F(\theta')\tilde{V}_F(\theta,\theta')\cos(4L-2)\theta \cdot \cos(4L'-2)\theta'\, d\theta d\theta' . \quad (36)$$

We now express $\tilde{V}_F(\theta,\theta')$ in terms of $\chi(\mathbf{k}+\mathbf{k}')$ using Eq.(1). We first note that the constant term in Eq.(1), U/N, does not contribute to the integral in Eq.(36), because the integrand involves $\cos 2\theta$ or higher cosine terms. 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:

$$\chi_F(\theta,\theta') = \chi(k_F(\theta)\cos\theta + k_F(\theta')\cos\theta',\ k_F(\theta)\sin\theta + k_F(\theta')\sin\theta') , \quad (37)$$

where

$$k_F(\theta) = k(0,\theta). \quad (38)$$

Since the U term vanishes, we expect an attractive interaction occurs at U^2. So we set

$$\log\Delta = -\frac{2t^2}{xU^2}, \quad (39)$$

where x is to be determined. With these definitions we have a seqular equation for b_{1g} symmetry:

$$x\cdot z_{4L-2} = \sum_{L'=1} F_{LL'} z_{4L'-2}, \qquad L=1,2\cdots \quad (40)$$

where

$$F_{LL'} = -\frac{2}{\pi}\iint \rho_F(\theta')\chi_F(\theta,\theta')\cos(4L-2)\theta \cdot \cos(4L'-2)\theta'\, d\theta d\theta' . \quad (41)$$

Eq.(40) is a homogeneous linear equation with the eigenvalue being x. If we have a positive eigenvalue, we can conclude that the superconducting state with b_{1g} symmetry is stable. The most stable superconducting state is what has the largest eigenvalue x.

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 $0\le\theta\le\pi$ and $-\pi/2\le\theta'\le\pi/2$. 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. (41), in which the integration ranges are $0\le\theta\le 2\pi$ and $0\le\theta'\le 2\pi$. This is allowed by symmetry properties of $\chi_F(\theta,\theta')$. In the usual case we took L up to 15 and in some cases to 25. We note that, when we take 160×160 points instead of 200×200, the final results of x and z_l differ only less than 1 %.

§5 Results

The fermi surface (or the fermi line) in the k_x–k_y plane is shown in **Fig.3** for the upper right part of the plane. The electron number per site n_e was varied from 0.9 to 0.1.

Fig.4 shows the logarithm of the largest eigenvalue x as a function of n_e for the four representations. 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

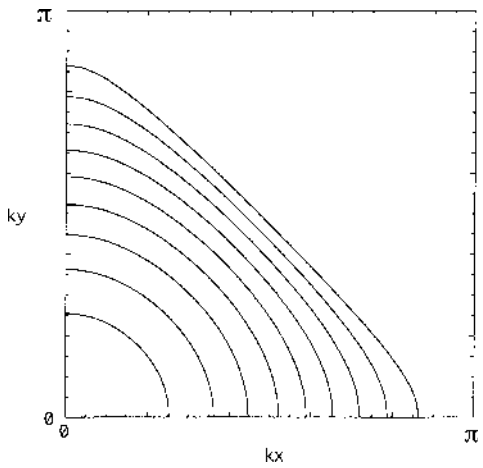

Fig.3 The fermi surfaces for n_e=0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9.

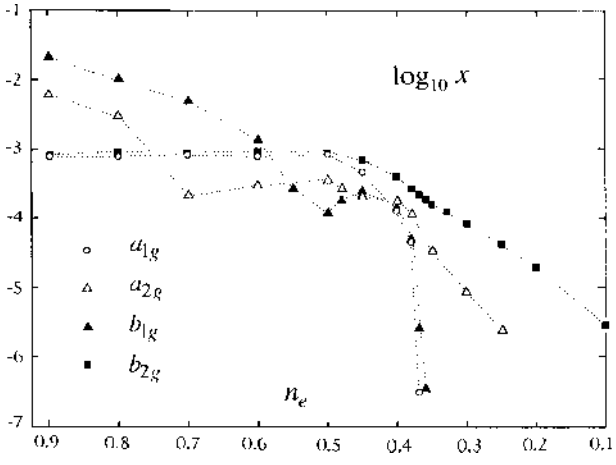

Fig.4 Logarithm of x vs n_e for four symmetries of the gap function.

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.

Figs.5-8 show the susceptibility $\chi(k_x,k_y)$ as a function of k_x and k_y for n_e=0.9 to 0.3, in which one may notice several ridges. The projection of the ridges onto the k-plane is shown in **Figs.9-10** for n_e=0.9 and 0.4. Point A in Fig.9 corresponds to the fermi surface shifted as indicated in **Fig.11** and point B to that also as indicated in Fig.11. Thus the ridge is a locus of the center of the shifted fermi surface, that is always in touch with one of the original fermi surfaces. At point B the shifted fermi surface is in contact with two of them and the susceptibility has a peak there. If the fermi surface were a perfect square, the positions of the peaks are expressed by $(\pi(1\pm\xi), \pi(1\pm\xi))$, where $\xi = 2-2\sqrt{n_e}$. We note ξ is close to the hole number δ=1-n_e, when δ is small.

For a small electron number (e. g. n_e=0.4) the fermi surface is nearly a circle and the projection of the ridges

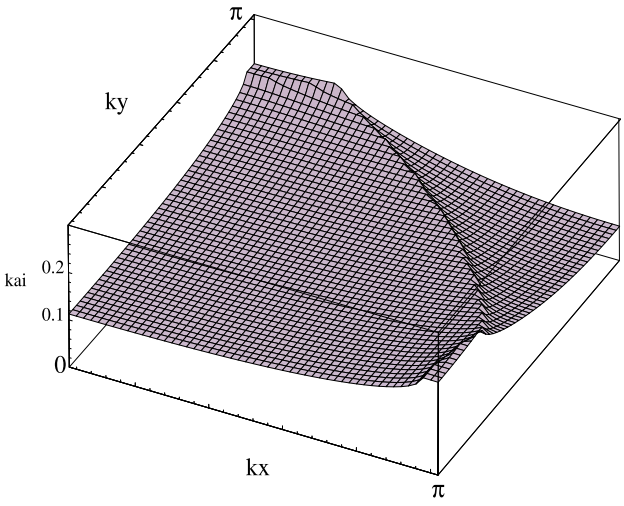

Fig.7 $\chi(k_x,k_y)$ for n_e = 0.4

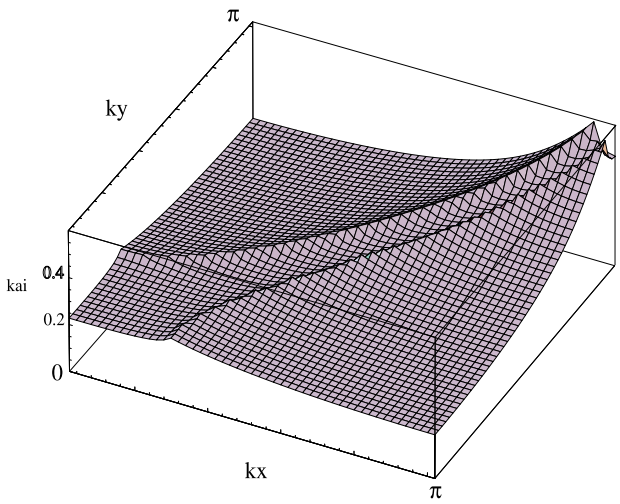

Fig.5 $\chi(k_x,k_y)$ for n_e = 0.9

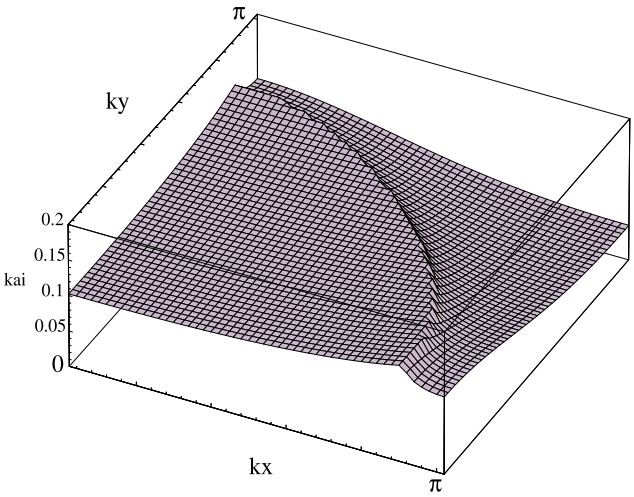

Fig.8 $\chi(k_x,k_y)$ for n_e = 0.3

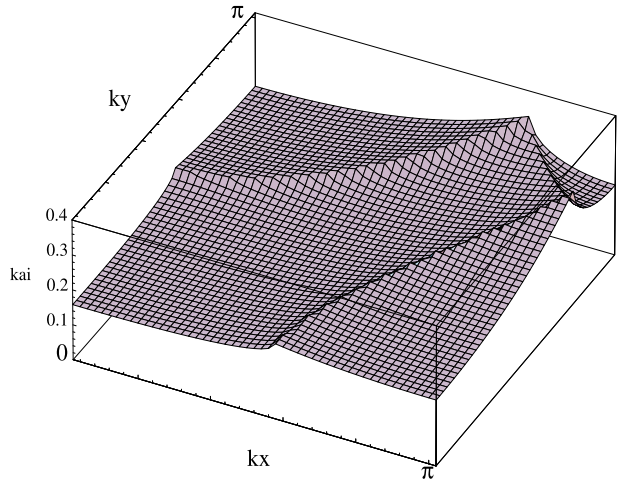

Fig.6 $\chi(k_x,k_y)$ for n_e = 0.7

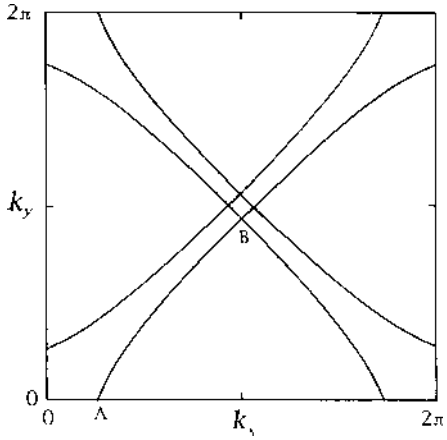

Fig.9 Projection of the ridges of $\chi(k_x,k_y)$ for n_e=0.9. "A" and "B" correspond to the shifted fermi surface indicated as "A" and "B" in Fig.11, respectively.

is essentially a circle of the radius $2k_F$, which overlaps with other ones centered on other reciprocal lattice points (see Fig.10). Crossing of the $2k_F$ circles occurs at points close to $(\pm\pi,0)$ or $(0,\pm\pi)$, where the susceptibility is the largest (see Fig.7). This is in sharp contrast to the case n_e=0.9, where the crossing (point B) occurs close to $(\pm\pi, \pm\pi)$ and the susceptibility has a peak there. We will see later that this is the reason for switching the most stable symmetry from b_{1g} to b_{2g} as the electron number decreases. Further reduction of the electron number results in non-crossing of the $2k_F$ circles as is seen in Fig.8 for the case of $n_e = 0.3$. Even in this case the susceptibility retains the symmetry of the square lattice. It is larger on the k_x or k_y axis than on the line 45 degrees from these axes. (This is not clearly seen in Fig.8.) This fact becomes important when one considers the origin of superconductivity for very small n_e and is due to the effect of one of the near-by $2k_F$ lines, which does not cross but approaches the central $2k_F$ line along the principal axes.

Fig.12 (a) 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 $(\pi/4, \pi/4)$. Point $(0, \pi/2)$ in the θ–θ' plane, for example, represents transition from **k** on the k_x axis to **k**' on the k_y axis. Then **k**+**k**' is very close to point B in Fig.9 (see **Fig.13**), where the susceptibility is the largest. For point (θ,θ')on the line from $(\pi/2,0)$ to $(0,\pi/2)$, the

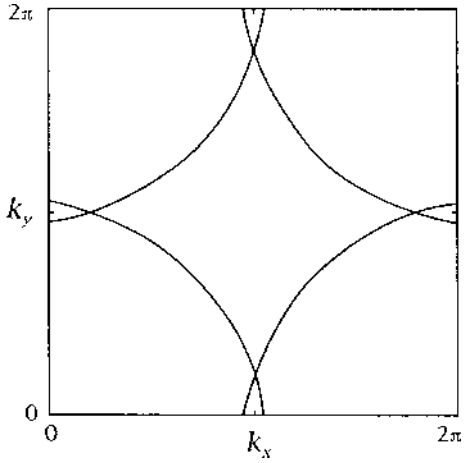

Fig.10 Projection of the ridges of $\chi(k_x,k_y)$ for n_e=0.4.

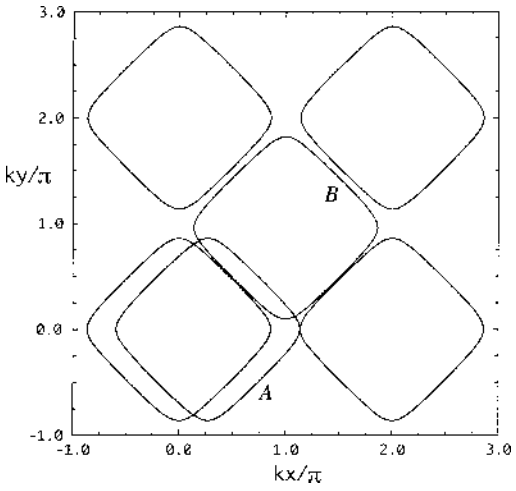

Fig.11 The fermi surfaces in the extended zone. The fermi surface denoted by "A" is shifted from the central zone so as to touch with a neighbouring fermi surface. "B" is in touch with two of the neighbouring fermi surfaces.

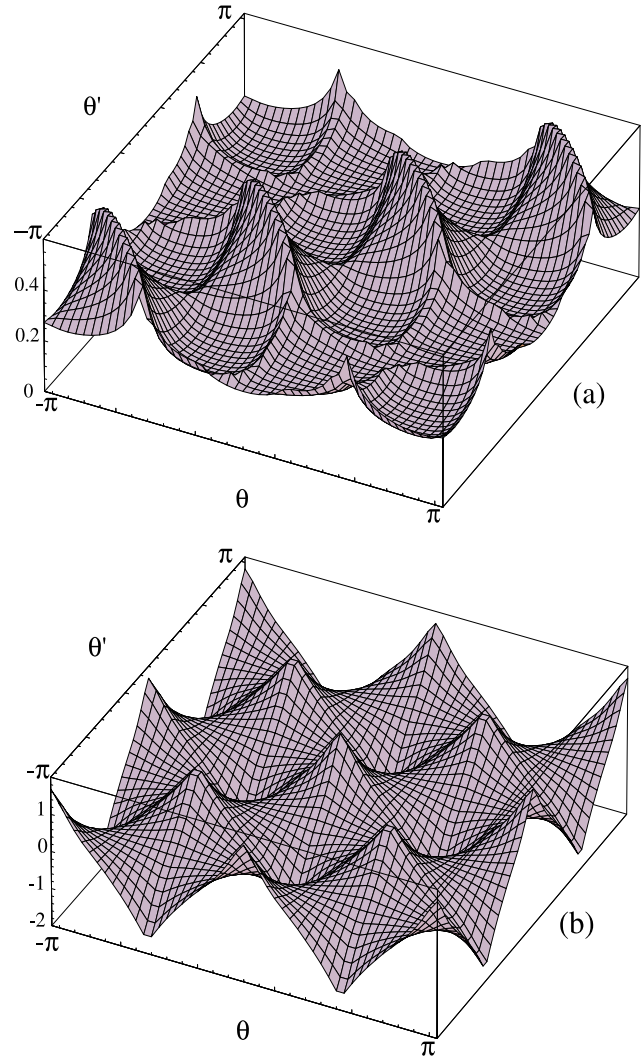

Fig.12 (a) $\chi_F(\theta,\theta')$ for n_e=0.9.
(b) $z(0,\theta)\times z(0,\theta')$ for n_e=0.9, where $z(0,\theta)$ is the gap function of b_{1g} symmetry. Note that the peaks and the valleys along the diagonal ($\theta = \theta'$) are 180 degrees out of phase from those of (a).

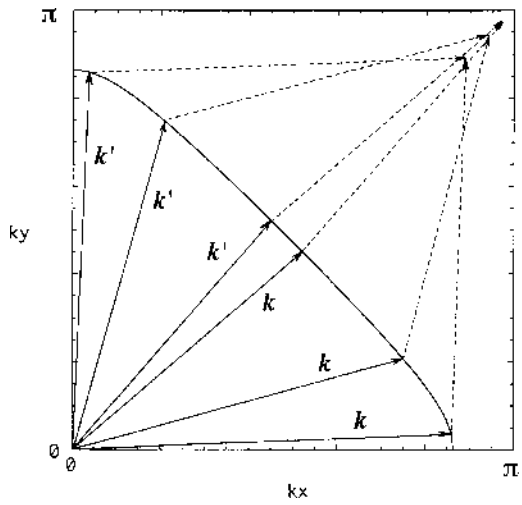

Fig.13 Scatterings from **k** to **k**' where $\theta+\theta'=\pi/2$. In this case **k**+**k**' always points to (π,π).

corresponding **k**+**k**' is also close to the peak points (see Fig.13). On the other hand, along the line from (π,0) to (0,−π) or equivalent lines **k**+**k**' is zero (backward scattering), so the susceptibility is the smallest there. One may notice deep valleys running along these lines in Fig.12(a).

Fig.14(a) and **Fig.15**(a) show $\chi_F(\theta,\theta')$ for n_e=0.7 and n_e=0.5, respectively. The ridges now split and go down and the regions around (0,0) and (±π/2, ±π/2) swell up. In **Fig.16**(a), which shows $\chi_F(\theta,\theta')$ for n_e=0.4, one sees mesas centered at (0,0) and (±nπ/2, ±nπ/2). The origin of the mesas is seen from Fig.7. Point (0,0), for example, implies that both **k** and **k**' are on the k_x axis. Since $k_F(\theta=0)$ is about 0.51π for n_e= 0.4, **k**+**k**' is close

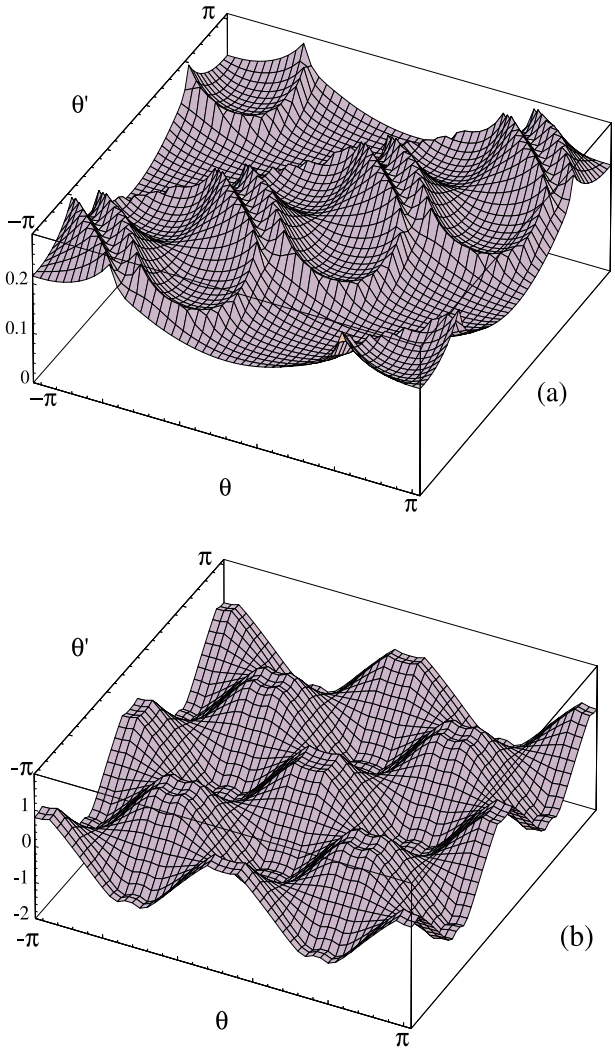

Fig.14 (a) $\chi_F(\theta,\theta')$ for n_e=0.7.
(b) $z(0,\theta)\times z(0,\theta')$ for n_e=0.7, where $z(0,\theta)$ is the gap function of b_{1g} symmetry.

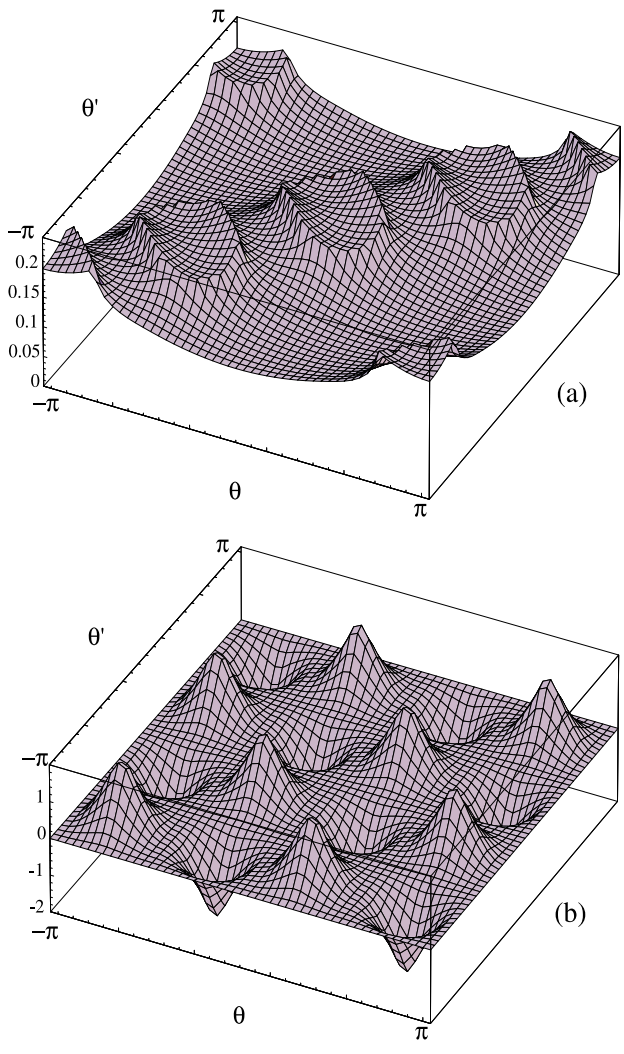

Fig.15 (a) $\chi_F(\theta,\theta')$ for n_e=0.5.
(b) $z(0,\theta)\times z(0,\theta')$ for n_e=0.5, where $z(0,\theta)$ is the gap function of b_{2g} symmetry.

to (1.02π, 0), where the susceptibility is the largest. On the other hand, point (π/4, π/4) implies **k**+**k**' is at 45 degrees from the k_x axis, where the susceptibility is smaller than that on the principal axes as mentioned previously. As one goes to n_e=0.3, one still finds ruined mesas along the diagonal. (See **Fig.17**(a). Note the extended scale of the ordinate.) This weak undulation (maxima at (0,0) and (±π/2,±π/2) and mimima at (±π/4, ±π/4) also comes from the fact that the susceptibility is larger on the principal axes than on the line at 45 degrees from them. We have found such undulation even for n_e=0.1.

We now present the results of diagonalization of Eq.(40) for b_{1g} symmetry and similar equations for other symmetries. We first discuss the case of n_e=0.9, for which the gap function with the b_{1g} symmtry gives us the most stable superconducting state. In **Fig.18**(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 was 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.12(a) and Fig.18(a), we find that the gap function $\cos 2\theta$ really satisfies this criterion. In fact we find F_{11}=0.0187, which is positive and implies a superconducting energy gain. By taking terms up to L=10 we find the largest eigenvalue of Eq.(40) is x=0.0204. The gap function, Eq.(33), with L summed

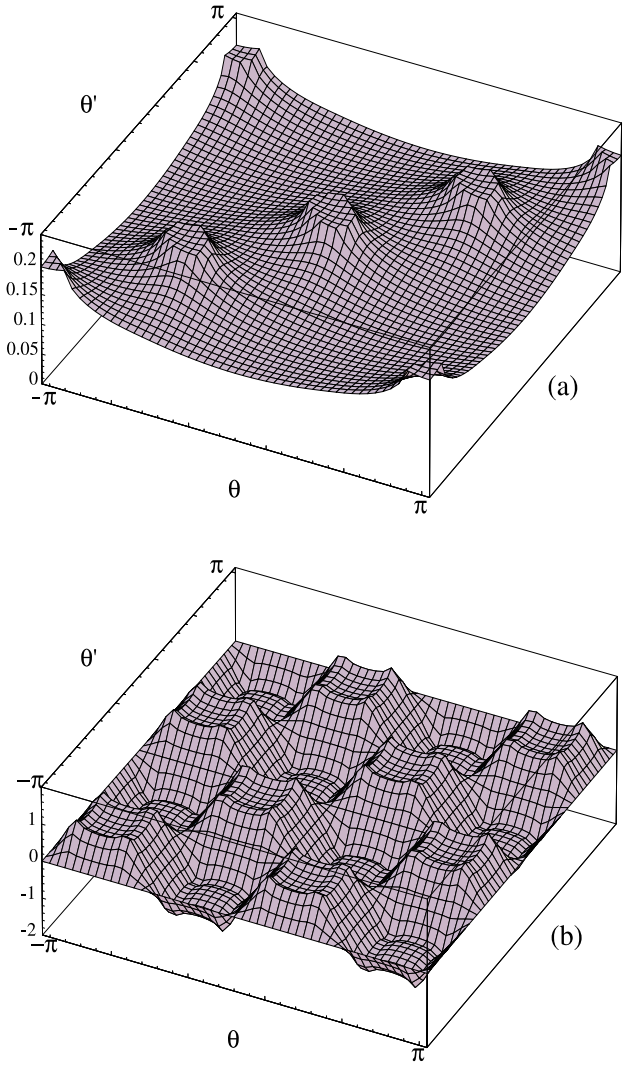

Fig.16 (a) $\chi_F(\theta,\theta')$ for n_e = 0.4.
(b) $z(0,\theta)\times z(0,\theta')$ for n_e=0.4, where $z(0,\theta)$ is the gap function of b_{2g} symmetry. Note that the mesas of (a) are placed in the middle of those of (b).

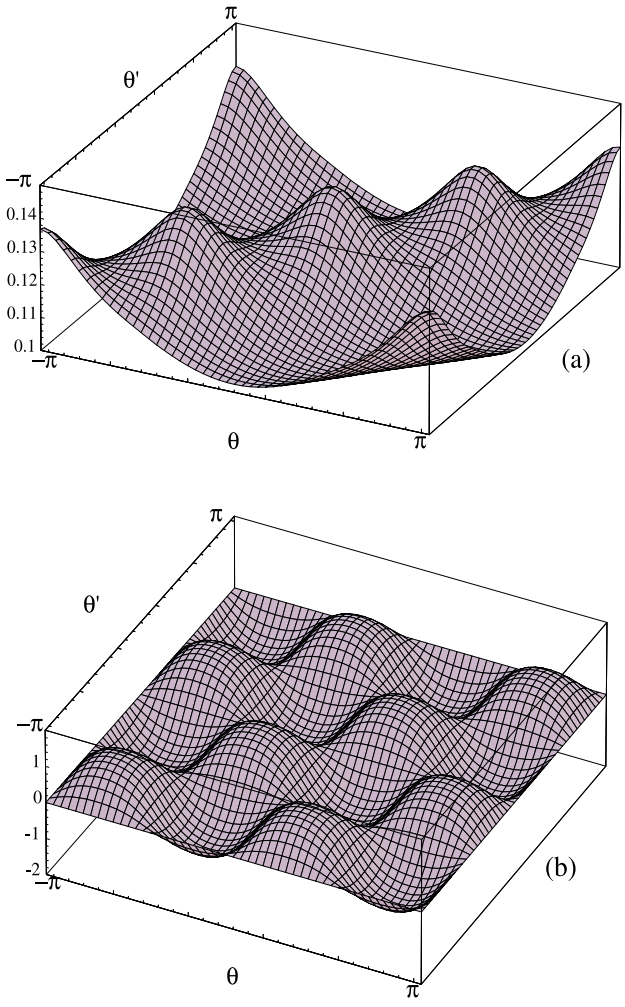

Fig.17 (a) $\chi_F(\theta,\theta')$ for n_e=0.3. Note the extended scale of the ordinate.
(b) $z(0,\theta)\times z(0,\theta')$ for n_e=0.3, where $z(0,\theta)$ is the gap function of b_{2g} symmetry. Note that the undulations along the diagonal (θ= θ') of (a) and (b) are mutually out of phase.

up to 10 is shown in **Fig.19**, which is basically of cos2θ type. Fig.12(b) shows $z(0,\theta)\times z(0,\theta')$ with this gap function, which is consistent with Fig.18(a).

Let us next consider the case of n_e=0.4. In contrast to the case of n_e=0.9 the susceptibility $\chi_F(\theta,\theta')$ is now small at ($\pm\pi/4$, $\pm\pi/4$)and equivalent points on diagonals (Fig.16(a)). This fits to the gap function sin2θ. In fact, the undulation of sin2$\theta\times$sin2θ' 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.18(b) and Fig.16(a).) This is favourable for a superconducting energy gain. By diagonalizing the seqular equation for the b_{2g} symmetry with L up to 10 we find the largest eigenvalue x=0.00039 and the gap function as shown in **Fig.20**. $z(0,\theta)\times z(0,\theta')$ for this case is shown in Fig.16(b).

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 mimima at ($\pm\pi/4$, $\pm\pi/4$) etc. (see Fig.17(a)) and the gap function is better represented by a single sin2θ term. An example is shown in **Fig.21** for n_e=0.2. 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 sin2$\theta\times$ sin2θ' along the diagonal, the gap function sin2θ picks up such a small undulation and gives rise to a superconducting energy gain.

As one sees in Fig.4 the eigenvalues of the a_{1g} symmetry and the b_{1g} symmetry are almost degenerate at n_e=0.38. The corresponding gap functions and the

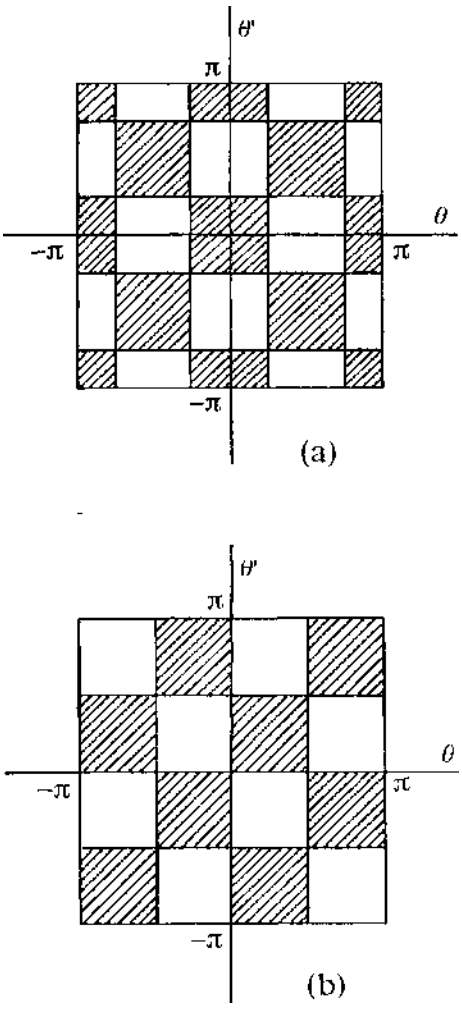

Fig.18 The signs of cos2$\theta\times$cos2θ' (a) and sin2$\theta\times$sin2θ' (b). In the shaded regions the sign is plus and in the open regions it is minus.

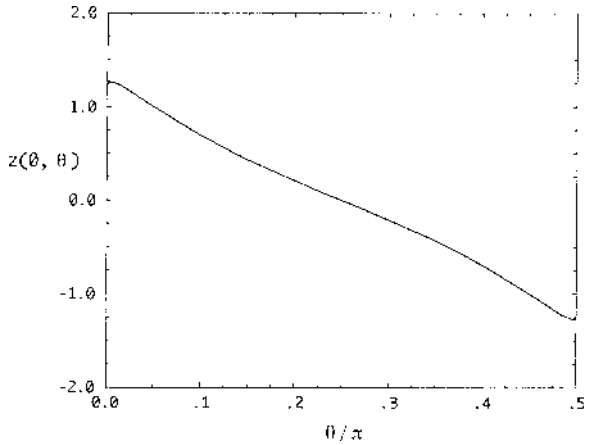

Fig.19 The gap function $z(0,\theta)$ of b_{1g} symmetry for n_e = 0.9. L is summed up to 10 in Eq.(33).

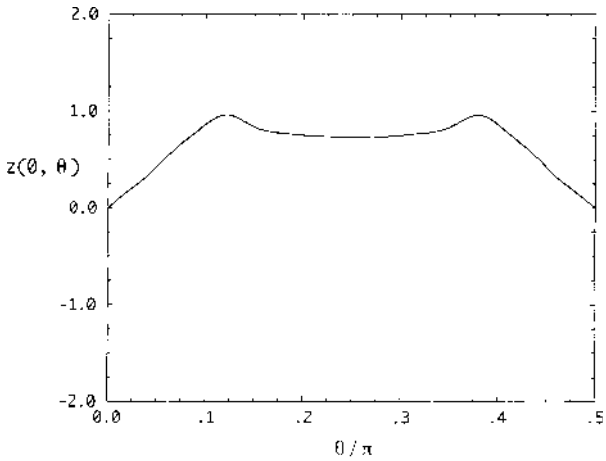

Fig.20 The gap function $z(0,\theta)$ of b_{2g} symmetry for n_e=0.4. L is summed up to 10 in Eq.(34).

products of them are shown in **Figs**.**22-25**. $\chi_F(\theta,\theta')$ for $n_e = 0.38$ is also shown in **Fig.26**, where one sees mesas at (0,0) and ($\pm n\pi/2$, $\pm n\pi/2$). From these figures one can imagine that each mesa determines the form of the gap function in its vicinity independently of other mesas. This is confirmed by treating a simple model, where we take $\chi_F(\theta,\theta')=V+V_0$ for $\theta^2+\theta'^2\le\beta^2$ and $\chi_F(\theta,\theta')=V_0$ otherwise with $V>0$. Our task is to obtain a superconducting energy gain with such a repulsive interaction. We take a gap function which is normalized and whose average is zero:

$$z(\theta)=\frac{2}{\sqrt{3}}\sqrt[4]{\frac{2\alpha}{\pi}}(1-2\alpha\theta^2)e^{-\alpha\theta^2}. \qquad (42)$$

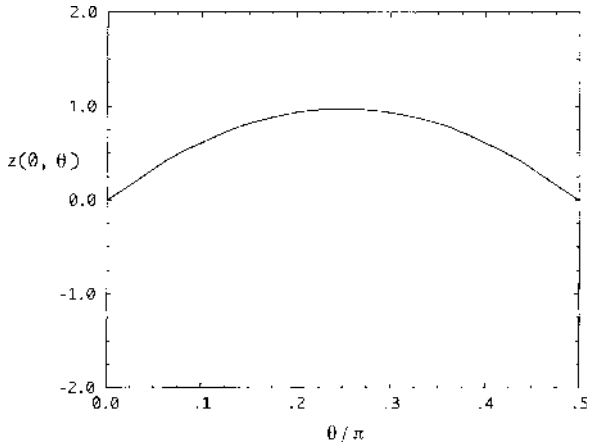

Fig.21 The gap function $z(0,\theta)$ of b_{2g} symmetry for n_e=0.2. L is summed up to 10 in Eq.(34). The main contribution comes from L=1.

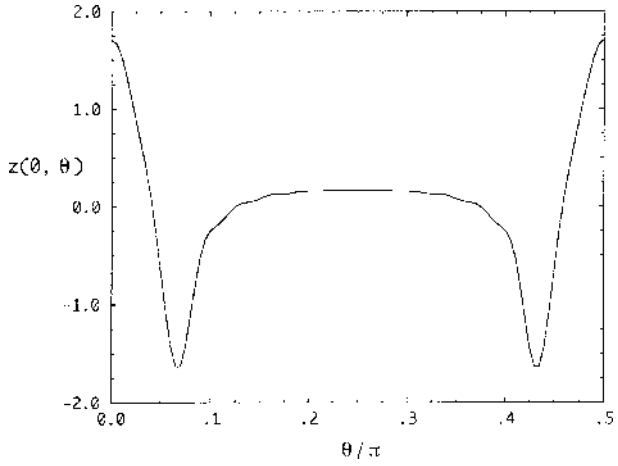

Fig.22 The gap function $z(0,\theta)$ of a_{1g} symmetry for n_e=0.38. L is summed up to 15 in Eq.(31).

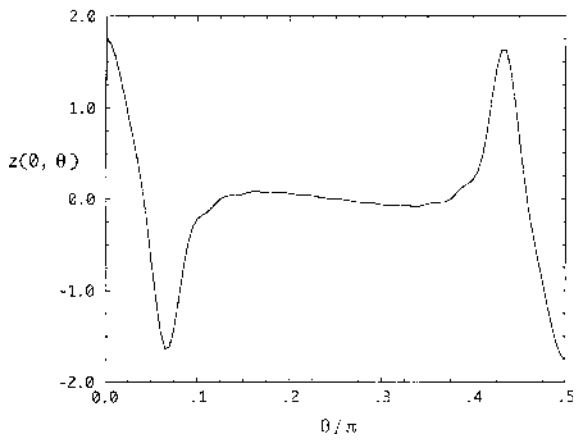

Fig.23 The gap function $z(0,\theta)$ of b_{1g} symmetry for n_e=0.38. L is summed up to 15 in Eq.(33). Note that this is regarded as the antisymmetric combination of the local gap function around θ= 0 and that around θ= π/2.

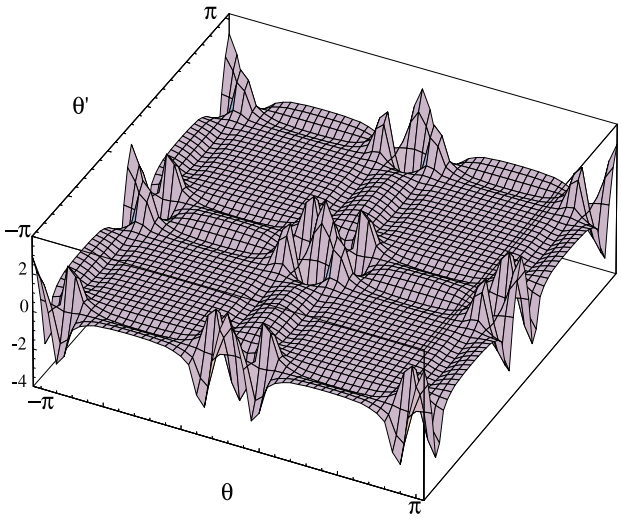

Fig.24 $z(0,\theta)\times z(0,\theta')$for n_e=0.38, where $z(0,\theta)$ is the gap function of a_{1g} symmetry.

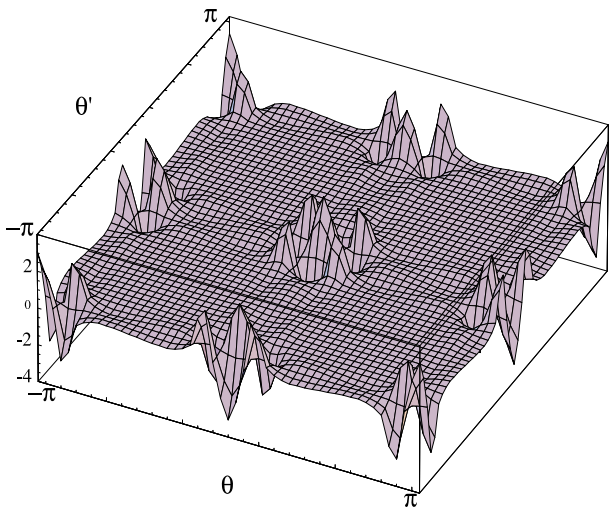

Fig.25 $z(0,\theta)\times z(0,\theta')$ for n_e= 0.38, where $z(0,\theta)$ is the gap function of b_{1g} symmetry.

The hint is the form of $z(0,\theta)$ near $\theta = 0$ or $\theta = \pi/2$ in Fig.22 and Fig.23. Our concern is whether the integral

$$\iint \chi_F(\theta,\theta')z(\theta)z(\theta')d\theta d\theta' = \iint_{\theta^2+\theta'^2 \le \beta^2} V \cdot z(\theta)z(\theta')d\theta d\theta' \quad (43)$$

can be negative. Calculation shows that it is negative for $\alpha\beta^2>2$ and is a minimum at $\alpha\beta^2=3.18$. This result is well understood by watching **Fig.27**, where the signs of $z(\theta)\times z(\theta')$ are shown together with the integration region. If the integration extends over the entire plane ($\beta\to\infty$), the integral vanishes. For small β it is positive. But when β is as indicated in Fig.27, one can imagine it may be negative. This is one of the cases, where the negative contributions arising from pair transitions between states with different signs of the gap function overcome positive ones arising from transitions between states with the same sign of the gap function.

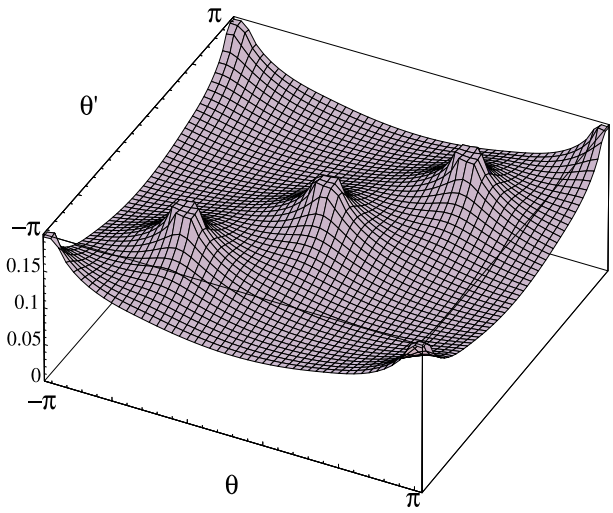

Fig.26 $\chi_F(\theta,\theta')$ for n_e=0.38

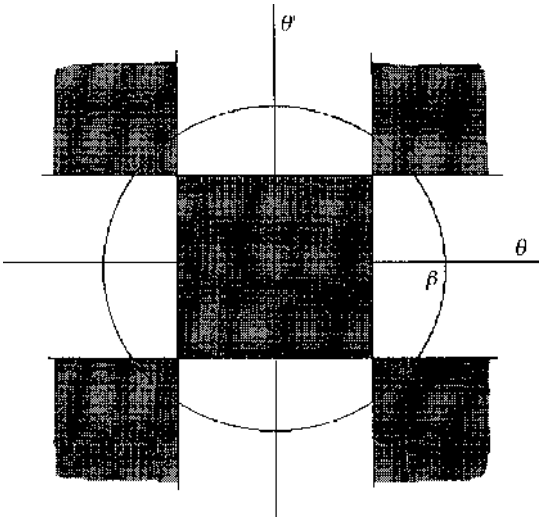

Fig.27 The signs of $z(\theta)\times z(\theta')$, where $z(\theta)$ is defined in Eq.(42). In the shaded regions the sign is plus and in the open regions it is minus. Inside the circle of the radius β the integration in Eq.(43) is carried out.

§6 Discussion

In this paper we have concerned with the way to obtain a superconducting energy gain for a repulsive interaction. The idea of deviding the 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[13,14]. 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 a superconductor with some symmetry of the gap function 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 accounnt 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. 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 in the wave number dependent susceptibiliy. In this respect it is interesting to note that inelastic neutron scattering experiments[15] on Sr_2RuO_4 revealed a significant spin fluctuation at an incommensurate k-point, whereas it is a triplet superconductor.

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Superconductivity of the two-dimensional Hubbard model with t'=0 has been examined in the small U limit. We found that the ground state is superconducting at least for the electron density between 0.9 and 0.1.