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A charge-density wave loop threaded by the Aharonov-Bohm flux

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Abstract

The charge density wave (CDW) of the quasi- one-dimensional mesoscopic loop threaded by the Aharonov-Bohm magnetic flux is studied. It is found that the energetically favorable CDW-state is the state where two kinds of CDWs with different wave lengthes coexist in the loop. Two wave lengthes are complementarily shifted by the flux to each other. In accordance with this, the Aharonov-Bohm flux escapes from the flux-quantization.

Text

The quasi-one-dimensional conductor undergoes, at the critical temperature $T_C(>0)$, the charge dendity wave (CDW) transition [1]-[3]. Below T_C, the conductor is in the superconducting phase resulting from the CDW electronic state [4][5]. In this paper we study the CDW state of the loop threaded by the Aharonov-Bohm magnetic flux (A-B flux), and also examine the possibility of the A-B flux-quantization. The present investigations are carried out under the condition that the one-dimensional lattice contains no serious impurity. Especially inelastic impurity scatterers are assumed to be absent. That is, our discussion will be restricted to the regime of the *mesoscopic* region where the loop circumference L is smaller than the phase coherence length of the electron l_ϕ, $L \lesssim l_\phi$ [6] [7]. Accordingly, the free electron model will be adopted as an appropriate basis of calculations.

Let us consider an infinitely long and closely wound solenoid running along z axis. If the winding of the solenoid can be viewed as a current sheet, the magnetic field developed by an external current source is $\mathbf{B} = B\mathbf{e}_z$ in the solenoid and vanishes on the outside. Thus the A-B vector potential is $\mathbf{A}(r,\theta,t) = \Phi(t)/2\pi r \cdot \mathbf{e}_\theta$ for $\xi \leq r < \infty$. Here $\mathbf{e}_\theta$ is an unit vector in the direction of the azimuthal angle θ and ξ is a radius of the solenoid. The magnetic flux Φ is given by $\Phi = \oint \mathbf{A}\, d\mathbf{l}$ where $\oint \cdots d\mathbf{l}$ is a line integral bounded by the loop. The Hamiltonian of a free electron orbiting around the A-B flux is

$$H_{f.e} = \frac{1}{2m}[-i\hbar\nabla - e\mathbf{A}(\mathbf{r},t)]^2. \tag{1}$$

The wave function $\Psi(\mathbf{r},t)$ satisfying the Schrödinger equation $i\hbar\partial\Psi/\partial t = H_{f.e}\Psi$ is factorized as (here the time-dynamical vector potential is adopted for convenience)

$$\Psi(\mathbf{r},t) = \exp[ie\int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}(\mathbf{r}',t)\,d\mathbf{r}'/\hbar]\psi(\mathbf{r},t) \tag{2}$$

for $\xi \leq r < \infty$. In obtaining (2), $\nabla\times\mathbf{A} = 0$ for $\xi \leq r < \infty$ has been used. The factorized phase factor is called the Dirac phase, and the pseudo-wave function $\psi(\mathbf{r},t)$ satisfies the pseudo- Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = [-\frac{\hbar^2}{2m}\nabla^2 - e\int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{E}(\mathbf{r}',t)\,d\mathbf{r}']\psi(\mathbf{r},t), \tag{3}$$

where $\mathbf{E}$ is the electric field, $\mathbf{E} = -\partial\mathbf{A}/\partial t$. On combining (3) with Faraday's law $\oint \mathbf{E}\,d\mathbf{r} = -\partial\Phi(t)/\partial t$, we find the multi-valued circular condition:

$$\psi(r,\theta+2\pi,t) = \exp[-2\pi i\alpha(t)]\psi(r,\theta,t), \tag{4}$$

where $\alpha(t)$ is a scaled magnetic flux, $\alpha(t) = e\Phi(t)/h$ [8]. As seen from (4), $\alpha(t)$ can be restricted to $-1/2 \leq \alpha(t) \leq 1/2$ without losing generality. Furthermore $\alpha(t) > 0$ can be imposed on $\alpha(t)$, because the sign of $\alpha(t)$ simply identifies a positive direction of the magnetic flux Φ. Thus $0 \leq \alpha(t) \leq 1/2$ will be assumed in what follows. Our quasi-one-dimensional loop winds round the solenoid. Thereby a radius of the loop is ξ. Applying (3) and (4) to a free electron confined in this loop gives, for a time-static α, an energy spectrum $\epsilon_{n,\alpha} = \hbar^2 k_{n,\alpha}^2/2m$ with $k_{n,\alpha} = (n-\alpha)/\xi$. Here n is an integer, $n = 0, \pm1, \pm2, \pm3, \ldots$..

The Peierls structual transition in a quasi-one-dimensional conductor [9] is linked to the singular behavior in the time-static 1-D susceptibility [10][11]

$$\chi_1^0(q) = \sum_k \frac{f(E_k) - f(E_{k+q})}{E_{k+q} - E_k}, \tag{5}$$

where $f(E_k)$ is the Fermi distribution function, $f(E) = [\exp\beta(E-\mu) + 1]^{-1}$. To calculate $\chi_1^0(q)$, we will neglect, for the sake of simplicity, the effects of the time-static lattice potential, and so employ the energy spectrum $\epsilon_{n,\alpha}$ as E_k. On replacing the summation $\sum_k$ by an integral $(L/2\pi)\int_{-k_F}^{k_F} dk$ $(k \equiv n/\xi)$, we have, at $T = 0$,

$$\chi_1^0(q) = \frac{Lm}{2\pi\hbar^2}\frac{1}{q}\,[\,ln\left|\frac{2(k_F - \frac{\alpha}{\xi}) + q}{2(k_F - \frac{\alpha}{\xi}) - q}\right| + ln\left|\frac{2(k_F + \frac{\alpha}{\xi}) + q}{2(k_F + \frac{\alpha}{\xi}) - q}\right|\,]. \tag{6}$$

In the above expression, $L \equiv 2\pi\xi$ is a circumference of the loop, and $k_F = n_F/\xi$ (n_F is an integer) is the Fermi wave vector defined by the Fermi energy $\epsilon_F = \hbar^2k_F^2/2m$. Our $\chi_1^0(q)$, which is symmetric with respect to a reflection $\alpha \leftrightarrow -\alpha$, has two singularities respectively lying at $q = Q_{+\alpha} = 2(n_F+\alpha)/\xi$ and at $q = Q_{-\alpha} = 2(n_F-\alpha)/\xi$. Thus the CDW phase in question is somewhat more complicated than the one for $\alpha \equiv 0$. The background of the doubled singularities is as follows. For a finite α, the Fermi energy $\epsilon_F = \hbar^2k_F^2/2m$ given for $\alpha \equiv 0$ splits into a pair of 'Fermi energies', that is, $\hbar^2(Q_{-\alpha}/2)^2/2m$ and $\hbar^2(-Q_{+\alpha}/2)^2/2m$ (see Fig.1). As a result, our system has the doubled CDW gaps, $|\Delta_{+\alpha}|$ and $|\Delta_{-\alpha}|$, which are made at the respective 'Fermi energies'. The wave lengthes of these CDW are

$$\lambda_{\pm\alpha} = \frac{2\pi}{Q_{\pm\alpha}} = \frac{L}{2(n_F \pm \alpha)}. \tag{7}$$

No matter which mode may take place, the corresponding ratio $L/\lambda_{+\alpha}$ or $L/\lambda_{-\alpha}$ must be an integer as far as it occupies the loop by itself. This reflects the common assumption that the wave function is single-valued. In the absence of an A-B flux, this condition is automatically satisfied as $L/\lambda_0 = 2n_F$. In contrast to this, the condition can provide the flux quantization when the A-B flux is present. From (7), the quantized values $\alpha = 0$ and $\alpha = 1/2$ are readily obtained. [1]

There is an alternative case where the CDW system satisfies the single-valued condition without any flux quantization. Let us consider the loop in which two modes of the CDW coexist. If one half of L is occupied by $\lambda_{+\alpha}$-CDW and the other half by $\lambda_{-\alpha}$-CDW, a number of the waves in L is

$$\frac{\frac{L}{2}}{\lambda_{+\alpha}} + \frac{\frac{L}{2}}{\lambda_{-\alpha}} = (n_F + \alpha) + (n_F - \alpha) = 2n_F, \tag{8}$$

which, for a finite α, remains as it was for $\alpha \equiv 0$. Obviously, such a coexistence state escapes from the flux quantization. Which materializes in the loop ? The answer is, as will be observed, that the coexistence state (8) is promising. As to the flux-quantized state in either case $\alpha = 0$ or $\alpha = 1/2$, it necessarily accompanies the flux-screening flux $\Phi^{sc} = \{-\alpha \text{ or } (1/2 - \alpha)\} \times (h/e)$ which is produced by the induced persistent current J_{ind} on the loop. The flux-screening energy $E_{f,sc}$, which is an expence paid for the flux-quantization, is a function of a self-inductance of the loop $\mathcal{L}_\phi \approx 4\pi\mu_0\xi \ln(\xi/b)$ (μ_0 is a free-space permeability and b is a radius of the wire). It must be notable that the loop considered was assumed to be a mesoscopic one preserving the phase coherence (4). Hence ξ in $\mathcal{L}_\phi$ is very small, and so gives a large $E_{f,sc}$ whose expression is $E_{f,sc} = \{\alpha^2 \text{ or } (1/2 - \alpha)^2\} \times (h/e)^2 / 2\mathcal{L}_\phi$. Such a large $E_{f,sc}$ might act as an insuperable barrier to the flux-quantization. On the other hand, the formation energy of the coexistence state δE_{co} is much smaller than $E_{f,sc}$. In conclusion, our loop seems to prefer the coexistence state (8) to the flux-quantized states. The detailed discussions will be given at the end of the text.

Henceforth an α is not necessarily restricted to the quantized values. The much simplified theory for the CDW is the mean-field treatment described by the Hamiltonian [4][5]

$$\begin{aligned} H^{\pm\alpha}_{CDW} &= \sum_{|k'| \le Q_{\pm\alpha}} \epsilon_{k'} c^\dagger_{k'} c_{k'} + \sum_{0 \le k' \le Q_{\pm\alpha}} \Delta^*_{\pm\alpha} c^\dagger_{k'-Q_{\pm\alpha}} c_{k'} \\ &+ \sum_{-Q_{\pm\alpha} \le k' \le 0} \Delta_{\pm\alpha} c^\dagger_{k'+Q_{\pm\alpha}} c_{k'}, \end{aligned} \tag{9}$$

where $c^\dagger_{k'}$ and $c_{k'}$ are respectively creation and annihilation operators of electrons, and $k_{n,\alpha}$ are abbreviated by k'. The CDW gaps $\Delta_{\pm\alpha}$ will be determined by the so-called

[1] The 1-D susceptibility (6) is calculated in terms of the oversimplified electronic states. Not every (pair of) singularity(ies) in (6), as is well known, ensures the actual CDW transition. Here appearance of the CDW states is assumed.

gap equation(see (16)). When an α is finite, the numbers of the occupied states of $H^{\pm\alpha}_{CDW}$, which respectively lie in $[-n_F, n_F+2\alpha]$ and in $[-(n_F-2\alpha), n_F]$, differ from the actual one lying in $[-n_F, n_F]$ (see Fig.1). To be more precise, the state $n = n_F + 2\alpha$ belonging to the empty domain $n > n_F$ is treated as a fractionally occupied state in the $H^{+\alpha}_{CDW}$ case, while the fractional part of (two) electrons at $n = -n_F$ have been illegally removed in the $H^{-\alpha}_{CDW}$ case. The concept 'fractional occupation' is introduced as a convenient mathematical aid for calculating the diagonized fields. Things are readily understood from the symmetry property, $\epsilon_{n+2\alpha,\alpha} = \epsilon_{-n,\alpha}$ or equivalently $\epsilon_{-(n-2\alpha),\alpha} = \epsilon_{n,\alpha}$. For this reason, the special notice will be taken when the energy of $H^{+\alpha}_{CDW}$ or $H^{-\alpha}_{CDW}$ is calculated (see (12) and (14)).

With the aids of $\tilde{k} \equiv k' - Q_{\pm\alpha}/2$ and $\tilde{k} \equiv k' + Q_{\pm\alpha}/2$ respectively introduced for $0 \le \tilde{k} \le Q_{\pm\alpha}$ and for $-Q_{\pm\alpha} \le \tilde{k} \le 0$, $H^{\pm\alpha}_{CDW}$ can be converted into

$$H^{\pm\alpha}_{CDW} = \sum_{|\tilde{k}|\le Q_{\pm\alpha}/2} (c^{\dagger}_{\tilde{k}+Q_{\pm\alpha}/2}, c^{\dagger}_{\tilde{k}-Q_{\pm\alpha}/2}) \times \begin{pmatrix} \epsilon_{\tilde{k}+Q_{\pm\alpha}/2} & \Delta_{\pm\alpha} \\ \Delta^{*}_{\pm\alpha} & \epsilon_{\tilde{k}-Q_{\pm\alpha}/2} \end{pmatrix} \begin{pmatrix} c_{\tilde{k}+Q_{\pm\alpha}/2} \\ c_{\tilde{k}-Q_{\pm\alpha}/2} \end{pmatrix}. \tag{10}$$

Diagonalizing the above 2×2 matrix, we have the eigenvalues[5]

$$E^{\pm\alpha}_{\pm}(\tilde{k}) = \frac{\hbar^2}{2m}\{\tilde{k}^2 + (\frac{Q_{\pm\alpha}}{2})^2\} \pm \{(\frac{\hbar^2}{2m}\tilde{k}Q_{\pm\alpha})^2 + |\Delta_{\pm\alpha}|^2\}^{\frac{1}{2}}, \tag{11}$$

which satisfy an inequality $E^{-\alpha}_{\pm}(\tilde{k}) < E^{+\alpha}_{\pm}(\tilde{k})$. The energy for $H^{+\alpha}_{CDW}$ is, at $T = 0$, given by

$$E^{+\alpha}_{CDW} = 2\ [\ \sum_{|\tilde{k}|\le Q_{+\alpha}/2} E^{+\alpha}_{-}(\tilde{k}) - I_\alpha\, E^{+\alpha}_{-}(0)\ ], \tag{12}$$

where the weight function I_α ($0 \le I_\alpha \le 1$), which will be determined later, represents the fractional occupation. The summation spans over the whole states $|\tilde{k}| \le Q_{+\alpha}/2$, because after the transition all states considered in $H^{+\alpha}_{CDW}$ condense under the opened gap $2|\Delta_{+\alpha}|$. $E^{+\alpha}_{-}(0)$ is the energy of the quasi-particle with $n = n_F + 2\alpha$. The reason why $I_\alpha E^{+\alpha}_{-}$ is subtracted is, as was mentioned below (9), that the empty state $n = n_F + 2\alpha$ is superfluously counted as the fractionally occupied state. Replacing $\sum_{|\tilde{k}|\le Q_{+\alpha}/2}$ by $(L/2\pi)\int_{-Q_{+\alpha}/2}^{Q_{+\alpha}/2} d\tilde{k}$, we obtain, to lowest order in the small parameters $|\Delta_{+\alpha}|/\epsilon_F$ and α/n_F,

$$\begin{aligned} E^{+\alpha}_{CDW} &= 2n_F\ [\ \frac{2}{3}\epsilon_F - \frac{|\Delta_{+\alpha}|^2}{4\epsilon_F} - \frac{|\Delta_{+\alpha}|^2}{2\epsilon_F}\ln(\frac{4\epsilon_F}{|\Delta_{+\alpha}|})] \\ &+ \ 2(2\alpha - I_\alpha)\epsilon_F + 2I_\alpha\ [\ |\Delta_{+\alpha}| - \frac{2\alpha}{n_F}\epsilon_F]. \end{aligned} \tag{13}$$

Analogous consideration leading to (12) now gives the eneygy for $H^{-\alpha}_{CDW}$:

$$E^{-\alpha}_{CDW} = 2\ [\ \sum_{|\tilde{k}|\le Q_{-\alpha}/2} E^{-\alpha}_{-}(\tilde{k}) + I_\alpha\, E^{-\alpha}_{+}(-\frac{2\alpha}{\xi})\ ]. \tag{14}$$

The result calculated is

$$\begin{aligned} E^{-\alpha}_{CDW} &= 2n_F\ [\ \frac{2}{3}\epsilon_F - \frac{|\Delta_{-\alpha}|^2}{4\epsilon_F} - \frac{|\Delta_{-\alpha}|^2}{2\epsilon_F}\ln(\frac{4\epsilon_F}{|\Delta_{-\alpha}|})] \\ &- \ 2(2\alpha - I_\alpha)\epsilon_F + 2I_\alpha[\{(\frac{4\alpha}{n_F}\epsilon_F)^2 + |\Delta_{-\alpha}|^2\}^{\frac{1}{2}} - \frac{2\alpha}{n_F}\epsilon_F]. \end{aligned} \tag{15}$$

Here the reasonable choice of I_α is reached. It is easily understood that the term $2(2\alpha - I_\alpha)\epsilon_F$ in (13) and (15) should vanish. Consequently we obtain $I_\alpha = 2\alpha$.

The pairing energies $\Delta_{\pm\alpha}$ are determined by the well-known gap equation [4][5] which is given by

$$1 = 2\lambda \frac{\epsilon_F}{N_L} \sum_{|\tilde{k}| \leq Q_{\pm\alpha}/2} \frac{1}{E_+^{\pm\alpha}(\tilde{k}) - E_-^{\pm\alpha}(\tilde{k})} \tag{16}$$

at $T = 0$, where N_L is a number of the lattice sites in the loop and λ is the non-dimensional coupling constant between electrons and phonons. Under the approximated calculations which give (13) and (15), $|\Delta_{\pm\alpha}| = 4\epsilon_F \exp[-(1 \pm \alpha / n_F) / \lambda\nu]$ is obtained. Here $\nu \equiv 4n_F/N_L$, and $\alpha/n_F \ll \lambda (\ll 1)$ has been used. From (13) and (15) we have

$$\begin{aligned} E^\alpha_{CDW} - E^0_{CDW} &= 2I_\alpha(|\Delta_0| - \frac{2\alpha}{n_F}\epsilon_F) \\ &+ 2\frac{\alpha}{\lambda\nu}|\Delta_0|[\frac{|\Delta_0|}{\epsilon_F}\ln(\frac{4\epsilon_F}{|\Delta_0|}) - \frac{I_\alpha}{n_F}] \end{aligned} \tag{17}$$

in leading order. In a similar way, $E^{-\alpha}_{CDW} - E^0_{CDW}$ is readily obtained.

Let us define the formation energy of the coexistence state by $\delta E_{co} = [E^\alpha_{CDW} + E^{-\alpha}_{CDW}]_{I_\alpha=0}/2 - E^0_{CDW}$ where $[\cdots\cdots]_{I_\alpha=0}$ means that $I_\alpha = 0$ should be imposed on $E^{\pm\alpha}_{CDW}$. The reason of setting $I_\alpha = 0$ is that $2 \times 2\alpha$ electrons have *actually* transfered from the $\lambda_{-\alpha}$ -CDW region to the $\lambda_{+\alpha}$-CDW region in the coexistence state. In other words, two Hamiltonians $H^{+\alpha}_{CDW}$ and $H^{-\alpha}_{CDW}$ jointly but segregately govern the physics of the loop. In such a case, the compensations $-I_\alpha E_-^{+\alpha}(0)$ and $+I_\alpha E_+^{-\alpha}(-2\alpha/\xi)$ should be respectively removed from (12) and (14). Using (13) and (15) with $I_\alpha = 0$, we obtain

$$\delta E_{co} = -\frac{2}{n_F}(\frac{\alpha}{\lambda\nu})^2 \frac{|\Delta_0|^2}{\epsilon_F}[\ln(\frac{4\epsilon_F}{|\Delta_0|}) - \frac{1}{2}]. \tag{18}$$

When obtaining (18), we had no need to re-examine the terms that had already been discarded from (13) and (15) as higher ordered corrections. With use of $\lambda = 1.0\times10^{-1}$ and $\nu = 1$, we have $|\Delta_0|/\epsilon_F = 1.8\times10^{-4}$, and furthermore obtain $|\Delta_0| = 2.0\times10^0\,K$ for mesoscopic values $\xi = 1.0\times10^{-5}$ meter and $n_F = 5\times10^4$. An estimated value of the flux-screening energy $E_{f,sc}$ is $E_{f,sc} = 8.5\,\alpha^2 \times 10^2\,K$ for $\xi / b = 1.0\times10^2$, giving $E_{f,sc} \gg \delta E_{co}$ *and* $|E^{+\alpha}_{CDW} - E^0_{CDW}|$. As a consequence we are led to the conclusion that the coexistence state (8) is energetically much more promising than the flux-quantized state with either $\alpha = 0$ or $\alpha = 1/2$.

In our loop, inelastic scattering of the electrons is not allowed, and furthermore the mesoscopic condition $L \lesssim l_\phi$ is initially assumed. Accordingly, application of an accelerating field E will yield a change in $k_{n,\alpha}$, $dk_{n,\alpha}/dt = -eE/\hbar$, and produce the CDW-current [12]. If the field E is turned off (the flux α remains fixed), the produced CDW-current will be expected to flow persistently. All properties of the CDW-current seems to be periodic in the flux α with period $\alpha/2$. This period $\alpha/2$ is a direct result from two symmetry properties; one is discussed below (4) and the other is the symmetry property of $\epsilon_{n,\alpha}$ mentioned below (9) which survives after a reflection $\alpha \to -\alpha$. Following the epoch-making paper [6], the persistent currents in the mesoscopic loops have been widely studied theoretically [7][13]-[17]. The evidence for the persistent current also has been observed experimentally, which is periodic in α with period $\alpha/2$ [18]. It seems to be a further question whether or not the CDW-current proposed above is a possible explanation of the observed current.

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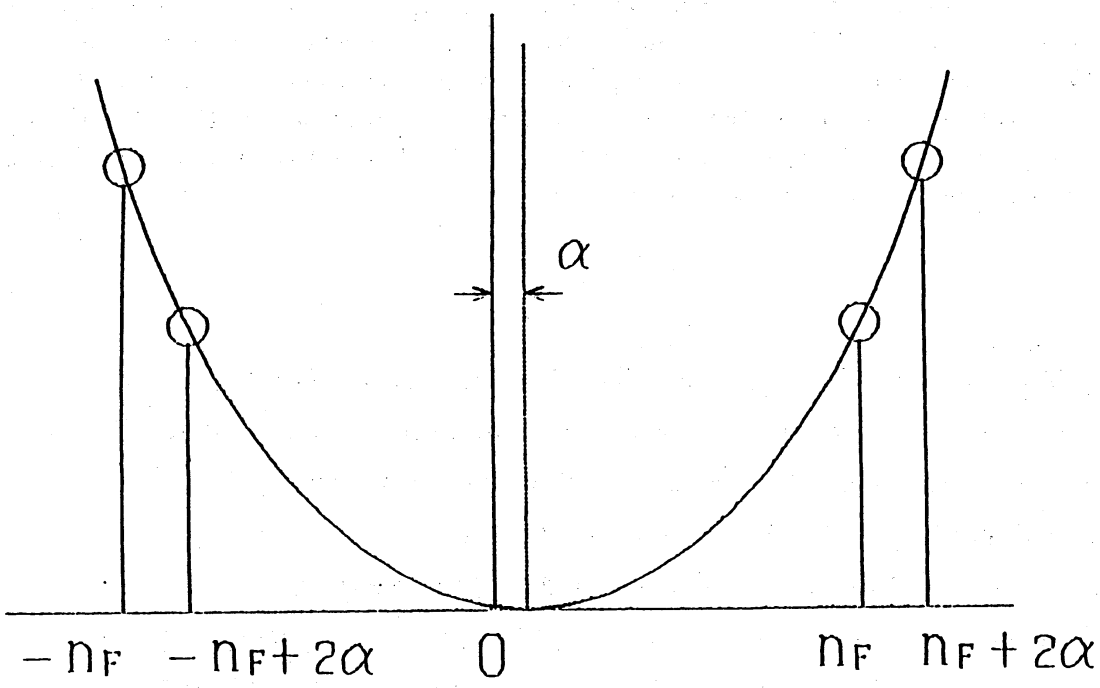

Fig. 1

Fig.1 The A-B flux gives rise to a splitting of the Fermi energy. The newly obtained 'Fermi energies' $\epsilon_F^{\pm\alpha} = \hbar^2 (\mp Q_{\pm\alpha}/2)^2/2m$ are respectively given at $n = \mp n_F$. Either of the $|\Delta_{\pm\alpha}|$, the CDW gaps, is opened at the corresponding 'Fermi energy'.