Electron acceleration, effective masses, and sum rule in the polar model

M. S. Svirskii and L. M. Svirskaya

Chelyabinsk State Teaching Institute

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Using the polar model, we obtain expressions for the effective mass which characterize the inertial properties of a system of electrons and show that this effective mass affects the high-frequency conductivity as well as the heat capacity and paramagnetic susceptibility of the electron system. We also derive a sum rule which allows us to determine the sign of the effective mass both in the ground state and in the highest excited state, and determine the way the effective mass varies in these states as we vary the transfer integral (L) and the Coulomb repulsion integral (A) between electrons with opposite spin projections on the same lattice site.

1. EFFECTIVE MASS OF AN ELECTRON SYSTEM IN THE POLAR MODEL

According to the polar model,[1] the Hamiltonian of a system of electrons in a one-dimensional lattice, including the transfer integral (L) and Coulomb repulsion integral (A) of electrons with oppositely-directed spin projections at the same lattice site, has the form

$$H_0=H_L+H_A, \tag{1}$$

where

$$H_L=-|L|\sum_g\sum_\sigma (c_{g\sigma}{}^+c_{g+1,\sigma}+c^+_{g+1,\sigma}c_{g\sigma}), \tag{2}$$

$$H_A=A\sum_g s_g, \tag{3}$$

and $c^+_{g\sigma}(c_{g\sigma})$ is a creation (annihilation) operator for an electron with spin projection σ at site g, $s_g=n_g$, $n_{g\downarrow}$, $n_{g\sigma}=c^+_{g\sigma}c_{g\sigma}$. The Hamiltonian (1) has also been discussed within the context of the Hubbard model,[2] in which the quantities $|L|$ and A are denoted t and U.

We assume that

$$c_{g\sigma}=\frac{1}{N^{1/2}}\sum_k e^{ikga}c_{k\sigma}, \tag{4}$$

where a is the lattice constant, k is the wave vector, and N is the number of lattice sites. Then we can transform Eq. (2) for H_L to the form

$$H_L=-2|L|\sum_k (\cos ka)\, n_k, \tag{5}$$

where

$$n_k=\sum_\sigma n_{k\sigma}.$$

According to (5),

$$H_L=\sum_k \varepsilon_0(k)\, n_k, \tag{6}$$

where

$$\varepsilon_0(k)=-2|L|\cos ka \tag{7}$$

is the energy of a band electron when $A=0$,

It follows from (7) that

$$\frac{\partial^2\varepsilon_0(k)}{\partial k^2}=2a^2|L|\cos \kappa a. \tag{8}$$

Taking (8) into account, we can rewrite Eq. (5) for H_L as follows:

$$H_L=-\frac{\hbar^2}{a^2}\sum_k \frac{1}{\hbar^2}\frac{\partial^2\varepsilon_0(k)}{\partial k^2}n_k. \tag{9}$$

It is well known that

$$\frac{1}{\hbar^2}\frac{\partial^2\varepsilon_0(k)}{\partial k^2}=\frac{1}{m^*(k)}, \tag{10}$$

where $m^*(k)$ is the effective mass of an electron as defined in band theory. Therefore, it follows from (9) that

$$H_L=-\frac{\hbar^2}{a^2}\sum_k \frac{1}{m^*(k)}n_k. \tag{11}$$

According to (11),

$$\langle\alpha|H_L|\alpha\rangle=-\frac{\hbar^2}{a^2}\sum_k\frac{1}{m^*(k)}\langle\alpha|n_k|\alpha\rangle, \tag{12}$$

where $|\alpha\rangle$ is an eigenfunction of the Hamiltonian (1).

The right side of Eq. (12) contains effective masses $m^*(k)$ of band electrons for all states $|k\rangle$. In band theory, there are a number of properties of electronic systems (see, e.g., Eq. 13.36 of Ref. 3) whose study leads to analogous sums over all states $|k\rangle$ weighted by the effective masses $m(k)$. however unlike those encountered in band theory, for the sums we will deal with here when electron correlations are absent ($A=0$) we have $|\alpha\rangle=|k\rangle$, implying that the matrix element $\langle\alpha|n_k|\alpha\rangle=\langle k|n_k|k\rangle$ coincides with some eigenvalue of the operator n_k. In the polar model with $A\neq 0$, the operator n_k does not commute with the Hamiltonian H_0 from (1), and thus the matrix element $\langle\alpha|n_k|\alpha\rangle$ does not coincide with an eigenvalue of the operator n_k.

The proper way to characterize the inertial properties of a system of electrons is to introduce an effective mass m_α determined by the expression

$$\frac{1}{m_\alpha}=\left[\sum_k\frac{1}{m^*(k)}\langle\alpha|n_k|\alpha\rangle\right]\Big/\sum_k\langle\alpha|n_k|\alpha\rangle. \tag{13}$$

According to (4),

$$\sum_k\langle\alpha|n_k|\alpha\rangle=\sum_g\langle\alpha|n_g|\alpha\rangle=N. \tag{14}$$

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It follows from (13) and (14) that

$$\frac{1}{m_\alpha}=\frac{1}{N}\sum_k \frac{1}{m^*(k)}\langle\alpha|n_k|\alpha\rangle. \tag{15}$$

It is clear from (15) that $1/m_\alpha$ has the physical meaning of an average value of the inverse effective mass of a band electron. In the average the quantity $1/m^*(k)$ enters in with probability

$$W_{k,\alpha}=\langle\alpha|n_k|\alpha\rangle/N.$$

It follows from (15) and (12)

$$m_\alpha=-\frac{N\hbar^2}{a^2\langle\alpha|H_L|\alpha\rangle}, \tag{16}$$

i.e., the effective mass m_α we have introduced is inversely proportional to the average value of the transfer Hamiltonian H_L.

2. COEFFICIENT OF HIGH-FREQUENCY ELECTRONIC CONDUCTIVITY IN THE POLAR MODEL

In the presence of an external spatially uniform electric field intensity with periodic time dependence $E=E_0\cos\omega t$, where ω is the frequency and t the time, the time dependence of the current I is determined by the expression [see, e.g., Eq. (4.23) in Ref. 4]

$$I(t)=-\frac{1}{\hbar}\operatorname{Re}\left\{\langle[I(0)H_E(0)]_-\rangle\frac{\exp[(i\omega+\varepsilon)t]}{\omega-i\varepsilon}+\int_{-\infty}^{\infty}\langle\!\langle I(t)\dot{H}_E(\tau)\rangle\!\rangle\frac{\exp[(i\omega+\varepsilon)\tau]}{i\omega+\varepsilon}d\tau\right\}, \tag{17}$$

where

$$H_E(t)=-eE_0\sum_{l=1}^{N}x_l(t), \tag{18}$$

$$I(t)=e\sum_{l=1}^{N}\dot{x}_l(t), \tag{19}$$

here x_l is the coordinate of the l th electron, and $\varepsilon>0$ goes to zero.

Assuming

$$x_c=\frac{1}{N}\sum_{l=1}^{N}x_l, \tag{20}$$

we obtain from (17)–(19):

$$I(t)=\frac{NeE_0}{\hbar}\operatorname{Re}\left\{\langle[I(0)x_c(0)]_-\rangle\frac{\exp[(i\omega+\varepsilon)t]}{\omega-i\varepsilon}+\int_{-\infty}^{\infty}\langle\!\langle I(t)I(\tau)\rangle\!\rangle\frac{\exp[(i\omega+\varepsilon)\tau]}{i\omega+\varepsilon}d\tau\right\}. \tag{21}$$

In the high-frequency region, the second term on the right side of (21) decreases faster than the first term (see, e.g., p. 86 of Ref. 4). Therefore

$$I(t)=\operatorname{Re}\{\sigma(\omega)E_0\exp[(i\omega+\varepsilon)t]\}, \tag{22}$$

where the electron conductivity equals

$$\sigma(\omega)=\frac{Ne}{\hbar\omega}\langle[I(0)x_c(0)]_-\rangle. \tag{23}$$

In a system with the Hamiltonian (1) the electron current operator I is determined by the expression (see, e.g., Refs. 5,6):

$$I=\frac{ie|L|a}{\hbar}\sum_g\sum_\sigma(c^+_{g+1,\sigma}c_{g\sigma}-c_{g\sigma}{}^+c_{g+1,\sigma}). \tag{24}$$

In the second-quantized representation, the operator x_c from (20) can be written in the form

$$x_c=\frac{1}{N}\sum_{g_1,g_2,\sigma}\langle g_1|x|g_2\rangle c^+_{g_1\sigma}c_{g_2\sigma}. \tag{25}$$

It follows from (25) that

$$x_c=\frac{1}{N}\sum_g\langle g|x|g\rangle n_g+\frac{1}{N}\sum_{g_1\neq g_2}\sum_\sigma\langle g_1|x|g_2\rangle c^+_{g_1\sigma}c_{g_2\sigma}. \tag{26}$$

Here $\langle g|x|g\rangle=ga$. Therefore, within the nearest-neighbor approximation implied by this Hamiltonain, we obtain from (26)

$$x_c=\frac{a}{N}\sum_g gn_g+\frac{1}{N}\sum_g\Big(\langle g+1|x|g\rangle\sum_\sigma c^+_{g+1,\sigma}c_{g\sigma}+\langle g|x|g+1\rangle\sum_\sigma c^+_{g\sigma}c_{g+1,\sigma}\Big). \tag{27}$$

The matrix elements $\tilde{M}=\langle g+1|x|g\rangle$ do not depend on g under the assumption that $|L|$ and A are also g-independent. Therefore it follows from (27) that

$$x_c=\frac{a}{N}\sum_g gn_g+\frac{1}{N}\Big(\tilde{M}\sum_{g,\sigma}c^+_{g+1,\sigma}c_{g\sigma}+\tilde{M}^*\sum_{g,\sigma}c_{g\sigma}{}^+c_{g+1,\sigma}\Big). \tag{28}$$

According to (28), (24) and (1)

$$[Ix_c]_-=\frac{iea^2}{N\hbar}H_L+\frac{ie|L|a}{N\hbar}(\tilde{M}+\tilde{M}^*)(n_{N_a}-n_1), \tag{29}$$

where N_a is the number of sites in the lattice. It follows from (29) that

$$\langle\alpha|[Ix_c]_-|\alpha\rangle=\frac{iea^2}{N\hbar}\langle\alpha|H_L|\alpha\rangle. \tag{30}$$

In obtaining Eq. (30) from (29), we have taken into account the fact that $\langle\alpha|n_{Na}|\alpha\rangle=\langle\alpha|n_1|\alpha\rangle$ by virtue of the equivalence of the lattice sites. It follows from (30) and (23) that

$$\sigma(\omega)=\frac{ie^2a^2}{\omega\hbar^2}\langle H_L\rangle. \tag{31}$$

Taking (17) into account, we obtain from (31)

$$\sigma(\omega)=\frac{Ne^2}{i\omega}\left\langle\frac{1}{m}\right\rangle. \tag{32}$$

Thus, it is the effective mass defined in Sec. 1 which enters into the expressions for the electronic conductivity and which characterizes the effect of inertia of the many-electron system on its response to an external high-frequency field. The electronic conductivity (32) corresponds to the equation

$$\frac{dI}{dt}=\Lambda E, \tag{33}$$

where

$$\Lambda=Ne^2\left\langle\frac{1}{m}\right\rangle. \tag{34}$$

3. SUM RULE IN THE POLAR MODEL

Let us discuss the operator

$$x_{c,0}=\frac{a}{N}\sum_g gn_g. \tag{35}$$

From (35), (1), and (24) there follows the commutation relation

$$[x_{c,0}H_0]_-=\frac{i\hbar}{Ne}I. \tag{36}$$

Taking into account that

$$\frac{dx_{c,0}}{dt}=\frac{1}{i\hbar}[x_{c,0}H_0]_-,$$

we obtain from (36) the following relation between I and $dx_{c,0}/dt$:

$$I=Ne\frac{dx_{c,0}}{dt}. \tag{37}$$

Taking a matrix element of (36) between eigenstates $|\alpha\rangle$ and $|\beta\rangle$ of the Hamiltonian H_0 which correspond to the energies E_α and E_β, we obtain the equation

$$\langle\alpha|x_{c,0}|\beta\rangle=\frac{i\hbar}{Ne}\frac{\langle\alpha|I|\beta\rangle}{E_\beta-E_\alpha}. \tag{38}$$

According to (24) and (35),

$$[Ix_{c,0}]_-=\frac{iea^2}{N\hbar}H_L. \tag{39}$$

From (39), taking into account (38), there follows the sum rule:

$$2\left(\frac{\hbar}{ea}\right)^2\sum_{\beta\neq\alpha}\frac{|\langle\beta|I|\alpha\rangle|^2}{E_\alpha-E_\beta}=\langle\alpha|H_L|\alpha\rangle. \tag{40}$$

According to (17), the sum rule (40) can be cast in the form

$$2\frac{m_\alpha}{e^2}\sum_{\beta\neq\alpha}\frac{|\langle\beta|I|\alpha\rangle|^2}{E_\beta-E_\alpha}=N. \tag{41}$$

This equation is an analog of the Thomas-Reich-Kuhn (TRK) sum rule. In contrast to the TRK sum rule, the right side of (41) is multiplied not by the mass of a free electron, but by the effective mass m_α, which depends on the state $|\alpha\rangle$ and is determined both by the transfer integral L and the Coulomb repulsion integral A for the two electrons with opposite spin projections on the same site of the crystal lattice.

It is clear from (41) that in the ground state, when $E_\alpha=E_{\rm gr}$ and the difference $E_\beta-E_\alpha$ is positive, the effective mass $m_{\rm gr}$ is positive. In the highest excited state, when $E_\alpha=E_{\rm h.ex.}$ and the difference $E_\beta-E_\alpha$ is negative, the effective mass $m_{\rm h.ex.}$ is negative.

4. VARIATION OF THE EFFECTIVE MASS AS A FUNCTION OF THE COULOMB REPULSION INTEGRAL BETWEEN TWO ELECTRONS WITH OPPOSITE SPIN PROJECTIONS ON THE SAME LATTICE SITE

Differentiating (16) with respect to A for fixed L, we obtain

$$\frac{\partial m_\alpha}{\partial A}=\frac{N\hbar^2}{a^2\langle\alpha|H_L|\alpha\rangle^2}\frac{\partial\langle\alpha|H_L|\alpha\rangle}{\partial A}. \tag{42}$$

The expression for the derivative $\partial\langle\alpha|H_L|\alpha\rangle/\partial A$ can be found by taking into account the equation

$$\langle\alpha|H_L|\alpha\rangle=E_\alpha-A\langle\alpha|s|\alpha\rangle, \tag{43}$$

which follows from (1)–(3), where

$$s=\sum_g s_g.$$

Differentiating (43) with respect to A, we obtain

$$\frac{\partial\langle\alpha|H_L|\alpha\rangle}{\partial A}=\frac{\partial E_\alpha}{\partial A}-\langle\alpha|s|\alpha\rangle-A\frac{\partial\langle\alpha|s|\alpha\rangle}{\partial A}. \tag{44}$$

According to the Gell-Mann–Feynman relation (see §11, Ref. 7), in the case of the Hamiltonian (1) the following relation is fulfilled:

$$\frac{\partial E_\alpha}{\partial A}=\left\langle\alpha\left|\frac{\partial H}{\partial A}\right|\alpha\right\rangle=\langle\alpha|s|\alpha\rangle. \tag{45}$$

It follows from (44) and (45) that

$$\frac{\partial\langle\alpha|H_L|\alpha\rangle}{\partial A}=-A\frac{\partial\langle\alpha|s|\alpha\rangle}{\partial A}. \tag{46}$$

Taking (46) into account, we find from (42) that

$$\frac{\partial m_\alpha}{\partial A}=-\frac{N\hbar^2A}{a^2\langle\alpha|H_L|\alpha\rangle^2}\frac{\partial\langle\alpha|s|\alpha\rangle}{\partial A}. \tag{47}$$

In order to determine the sign of the derivative $\partial\langle\alpha|s|\alpha\rangle/\partial A$, we use the results of Ref. 8. According to Ref. 8, for a Hamiltonian of the form

$$H=H_1-fG, \tag{48}$$

where H_1 does not depend on f, the derivative $\partial\langle\alpha|G|\alpha\rangle/\partial f$ is positive in the ground state, while it is negative in the highest excited state. A comparison of (1) and (48) shows that in the case under discussion we have $f=-A$ and $G=s$. Therefore, the derivative $\partial\langle\alpha|s|\alpha\rangle/\partial A$ is negative in the ground state, while it is positive in the higher excited state. Correspondingly, we obtain from (47)

$$\frac{\partial m_{\rm gr}}{\partial A}>0,\quad\frac{\partial m_{\rm h.ex.}}{\partial A}<0, \tag{49}$$

where $m_{\rm gr}$ and $m_{\rm h.ex.}$ are effective masses in the ground and highest excited states, respectively.

Thus, we are led to the conclusion that, within the framework of the polar model with the Hamiltonian (1), the effective mass in the ground state increases as A increases, while the effective mass in the highest excited state decreases as A increases.

5. RELATION BETWEEN EFFECTIVE MASSES IN THE GROUND AND HIGHEST EXCITED STATES

According to Ref. 9, the energy $E_{\text{h.ex}}$ of the highest excited state and the energy E_{gr} of the ground state are related by the equation

$$E_{\text{h.ex.}}(M)+E_{\text{gr}}(N_a-M)=(N-M)A, \tag{50}$$

where M is the number of electrons with negative spin projection. Differentiating (50) with respect to A, and taking (45) into account, we obtain

$$\bar{s}_{\text{h.ex.}}(M)+\bar{s}_{\text{gr}}(N_a-M]=N-M, \tag{51}$$

where $\bar{s}_{\text{h.ex.}}$ and $\bar{s}_{\text{gr}}$ are the average number of "pairs" in the highest excited state and in the ground state.

On the other hand, it follows from (1) and (50) that

$$\begin{aligned}&\langle F(M)|H_L|F(M)\rangle+\langle 0(N_a-M)|H_L|0(N_a-M)\rangle\\&\quad=A[N-M-\bar{s}_{\text{h.ex.}}(M)-\bar{s}_{\text{gr}}(N_a-M)],\end{aligned} \tag{52}$$

where F denotes the highest excited state and 0 the ground state. From (51) and (52) we obtain:

$$\langle F(M)|H_L|F(M)\rangle=-\langle 0(N_a-M)|H_L|0(N_a-M)\rangle. \tag{53}$$

Combining (53) and (16) leads to the relation

$$m_{\text{h.ex.}}(M)=-m_{\text{gr}}(N_a-M). \tag{54}$$

For the special case where $M=\frac{1}{2}N_a$, which implies that $N_a-M=M$, it follows from (54) that

$$m_{\text{h.ex.}}=-m_{\text{gr}}. \tag{55}$$

Therefore, in this case the effective masses in the ground state and in the highest excited state are equal in value and opposite in sign.

6. VARIATION OF THE EFFECTIVE MASS AS A FUNCTION OF TRANSFER INTEGRAL

Differentiating (16) with respect to $|L|$ at fixed A, we obtain

$$\frac{\partial m_\alpha}{\partial|L|}=\frac{N\hbar^2}{a^2\langle\alpha|H_L|\alpha\rangle^2}\frac{\partial\langle\alpha|H_L|\alpha\rangle}{\partial|L|}. \tag{56}$$

According to (2)

$$H_L=-|L|\Pi, \tag{57}$$

where the transfer operator equals

$$\Pi=\sum_g\sum_\sigma(c_{g\sigma}{}^+c_{g+1,\sigma}+c_{g+1,\sigma}^+c_{g\sigma}). \tag{58}$$

It follows from (57) that

$$\langle\alpha|H_L|\alpha\rangle=-|L|\langle\alpha|\Pi|\alpha\rangle. \tag{59}$$

Setting $f=|L|$ and $G=\Pi$ [see (48)], and taking into account the results of Ref. 8, we obtain

$$\frac{\partial\langle 0|\Pi|0\rangle}{\partial|L|}>0,\quad \frac{\partial\langle F|\Pi|F\rangle}{\partial|L|}<0. \tag{60}$$

It follows from (59) and (60) that

$$\frac{\partial\langle 0|H_L|0\rangle}{\partial|L|}<0. \tag{61}$$

Taking (61) into account, we obtain from (56)

$$\frac{\partial m_{\text{gr}}}{\partial|L|}<0. \tag{62}$$

Thus, we are led to the conclusion that in the polar model with Hamiltonian (1), as in band theory, the effective mass in the ground state decreases with increasing $|L|$.

A comparison of (62) and (49) shows that variation of the integral A produces a variation of m_{gr} which is opposite the corresponding variation produced by varying $|L|$. It follows from (53) that for the case $M=\frac{1}{2}N_a$ the following equation holds:

$$\frac{\partial\langle F|H_L|F\rangle}{\partial|L|}=-\frac{\partial\langle 0|H_L|0\rangle}{\partial|L|}. \tag{63}$$

It follows from (63), (61), and (56) that

$$\frac{\partial m_{\text{h.ex.}}}{\partial|L|}>0. \tag{64}$$

Thus, $m_{\text{h.ex.}}$ increases as $|L|$ increases in this case as well, just as in band theory.

A comparison of (64) and (49) shows that in the highest excited state a variation of the integral A produces a variation of $m_{\text{h.ex.}}$ which is opposite the corresponding variation produced by varying $|L|$, as in the case of the ground state.

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APPENDIX 1

EFFECTIVE MASS AND SUM RULE IN A SYSTEM MADE UP OF TWO SITES AND TWO ELECTRONS

In the case of the system where the number of sites is $N_a=2$ and the number of electrons with opposite spin projections is $N_e=2$ (such a system is discussed, e.g., in page 305 of Ref. 3 within the context of the Hubbard model), the energy spectrum and wave functions have the form

$$\begin{aligned}E_1&=\frac{1}{2}A-K,\quad \psi_1=\frac{1}{2}\left(1-\frac{A}{2K}\right)^{1/2}(|20\rangle+|02\rangle)\\&\quad+\frac{1}{2}\left(1+\frac{A}{2K}\right)^{1/2}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle),\\E_2&=0,\quad \psi_2=\frac{1}{2^{1/2}}(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle),\\E_3&=A,\quad \psi_3=\frac{1}{2^{1/2}}(|20\rangle-|02\rangle),\\E_4&=\frac{A}{2}+K,\quad \psi_4=\frac{1}{2}\left(1+\frac{A}{2K}\right)^{1/2}(|20\rangle+|02\rangle)\\&\quad-\frac{1}{2}\left(1-\frac{A}{2K}\right)^{1/2}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle),\end{aligned} \tag{65}$$

where

$$\begin{aligned}&K=\left[\left(\frac{A}{2}\right)^2+4L^2\right]^{1/2},\\&|20\rangle=c_{1\uparrow}{}^+c_{1\downarrow}{}^+|0\rangle,\quad |02\rangle=c_{2\uparrow}{}^+c_{2\downarrow}{}^+|0\rangle,\\&|\uparrow\downarrow\rangle=c_{1\uparrow}{}^+c_{2\downarrow}{}^+|0\rangle,\quad |\downarrow\uparrow\rangle=c_{1\downarrow}{}^+c_{2\uparrow}{}^+|0\rangle.\end{aligned} \tag{66}$$

It follows from (57), (58), and (65) that

$$\begin{aligned}&\langle\psi_1|H_L|\psi_1\rangle=-4L^2/K,\quad \langle\psi_2|H_L|\psi_2\rangle=0,\\&\langle\psi_3|H_L|\psi_3\rangle=0,\quad \langle\psi_4|H_L|\psi_4\rangle=4L^2/K;\end{aligned} \tag{67}$$

correspondingly, we obtain from (16)

$$m_1=\frac{\hbar^2}{2a^2L^2}\left[\left(\frac{A}{2}\right)^2+4L^2\right]^{1/2},$$
$$m_2=-\frac{\hbar^2}{2a^2L^2}\left[\left(\frac{A}{2}\right)^2+4L^2\right]^{1/2} \tag{68}$$

Thus, in agreement with the conclusions of Sec. (3), $m_{gr}=m_1$ is found to be a positive quantity, while $m_{h.ex.}=m_4$ is negative. In this case Eq. (55) is fulfilled. As A increases the effective mass $m_1=m_{gr}$ increases while the effective mass $m_4=m_{h.ex.}$ decreases (i.e., increases in absolute value). This agrees with (49).

In the states (65), the average value of the currents equal zero:

$$\langle 1|I|1\rangle=\langle 2|I|2\rangle=\langle 3|I|3\rangle=\langle 4|I|4\rangle=0. \tag{69}$$

The nondiagonal matrix elements are determined by the equations

$$\langle 2|I|1\rangle=0,\quad \langle 3|I|2\rangle=0,$$
$$\langle 3|I|1\rangle=-\left[2\left(1+\frac{A}{2K}\right)\right]^{1/2},\quad \langle 4|I|2\rangle=0,$$
$$\langle 4|I|1\rangle=0,\quad \langle 4|I|3\rangle=-\left[2\left(1-\frac{A}{2K}\right)\right]^{1/2}. \tag{70}$$

Correspondingly, including the energy levels from (65)

$$2\left(\frac{\hbar}{ea}\right)^2\sum_{\beta\neq 1}\frac{|\langle\beta|I|4\rangle|^2}{E_1-E_\beta}=-\frac{4L^2}{K},$$
$$2\left(\frac{\hbar}{ea}\right)^2\sum_{\beta\neq 2}\frac{|\langle\beta|I|2\rangle|^2}{E_2-E_\beta}=0,$$
$$2\left(\frac{\hbar}{ea}\right)^2\sum_{\beta\neq 3}\frac{|\langle\beta|I|3\rangle|^2}{E_3-E_\beta}=0, \tag{71}$$
$$2\left(\frac{\hbar}{ea}\right)^2\sum_{\beta\neq 4}\frac{|\langle\beta|I|4\rangle^2}{E_4-E_\beta}=\frac{4L^2}{K}.$$

It is clear from (71) and (67) that the sum rule (40) is fulfilled.

In Eq. (65) the average value of the number of "pairs" (i.e., sites with two electrons having opposite spin projections) is determined by the equations

$$\bar{s}_1=\frac{1}{2}\left(1-\frac{A}{2K}\right),$$
$$\bar{s}_2=0,$$
$$\bar{s}_3=0, \tag{72}$$
$$\bar{s}_4=\frac{1}{2}\left(1+\frac{A}{2K}\right).$$

It is clear from (72) that, in agreement with the conclusion of Sec. 4, the quantity $\bar{s}$, decreases with increasing A in the ground state, while in the highest excited state $\bar{s}_4$ increases with increasing A.

In the case under discussion here, we have $M=1$ and $N-M=1$. Therefore, according to (50), the following equation should hold:

$$E_4+E_1=A. \tag{73}$$

The energies E_4 and E_1 from (65) satisfy this equation. According to (51), we should have

$$\bar{s}_4+\bar{s}_1=1. \tag{74}$$

This equation is also satisfied for the values of $\bar{s}_1$ and $\bar{s}_4$ from (72).

It follows from (68) that

$$\frac{\partial m_1}{\partial|L|}<0,\quad \frac{\partial m_4}{\partial|L|}>0, \tag{75}$$

which is in agreement with (62) and (64).

In the $|k\rangle$ representation, the wave functions ψ_1 and ψ_4 from (65) have the form

$$\psi_1=\frac{1}{2}\left\{\left[\left(1+\frac{A}{2K}\right)^{1/2}+\left(1-\frac{A}{2K}\right)^{1/2}\right]c^+_{k_1\uparrow}c^+_{k_1\downarrow}\right.$$
$$\left.+\left[\left(1-\frac{A}{2K}\right)^{1/2}-\left(1+\frac{A}{2K}\right)^{1/2}\right]c^+_{k_2\uparrow}c^+_{k_2\downarrow}\right\}|0\rangle,$$
$$\psi_4=\frac{1}{2}\left\{\left[\left(1+\frac{A}{2K}\right)^{1/2}-\left(1-\frac{A}{2K}\right)^{1/2}\right]c^+_{k_1\uparrow}c^+_{k_1\downarrow}\right. \tag{76}$$
$$\left.+\left[\left(1+\frac{A}{2K}\right)^{1/2}+\left(1-\frac{A}{2K}\right)^{1/2}\right]c^+_{k_2\uparrow}c^+_{k_2\downarrow}\right\}|0\rangle,$$

with $k_1=0$, $k_2=\pi/a$. It follows from (76) and (65) that for $A=0$, in agreement with Sec. 1, the occupation numbers n_{k_1} and n_{k_2} are good quantum numbers. In the ground state

$$\psi_1|_{A=0}=\psi_1^{(0)}=c^+_{k_1\uparrow}c^+_{k_1\downarrow}|0\rangle \tag{77}$$

we have $n_{k_1}=2$ and $n_{k_2}=0$, which corresponds to occupation of two $|k_1\rangle$ states with opposite spin projections at the Fermi level. In the highest excited state, we have $n_{k_1}=0$ and $n_{k_2}=2$, which corresponds to the occupation of two $|k_2\rangle$ states with opposite spin projections. In this case

$$\psi_4|_{A=0}=\psi_4^{(0)}=c^+_{k_2\uparrow}c^+_{k_2\downarrow}|0\rangle. \tag{78}$$

In the states (77) and (78)

$$E_1|_{A=0}=E_1^{(0)}=-2|L|,$$
$$E_4|_{A=0}=E_4^{(0)}=2|L|. \tag{79}$$

When electron correlations are taken into account ($A\neq 0$), the number n_k is no longer a good quantum number. According to (76), ψ_1 is no longer purely the ground state $\psi_1^{(0)}$ for $A=0$ with $n_{k_1}=2$ and $n_{k_2}=0$, but also has an admixture of the highest excited state $\psi_4^{(0)}$ for $A=0$ with $n_{k_1}=0$ and $n_{k_2}=2$. Analogously, ψ_4 is no longer purely the highest excited state $\psi_4^{(0)}$ for $A=0$ with $n_{k_1}=0$ and $n_{k_2}=2$, but also has an admixture of the ground state $\psi_1^{(0)}$ for $A=0$ with $n_{k_1}=2$ and $n_{k_2}=0$.

In this state we have

$$\langle\psi_1|n_{k_1}|\psi_1\rangle=1+\frac{2|L|}{K},$$
$$\langle\psi_1|n_{k_2}|\psi_1\rangle=1-\frac{2|L|}{K}. \tag{80}$$

In this case $\langle\psi|n_{k_1}+n_{k_2}|\psi_1\rangle=2$, which agrees with (14).

In the case under discussion here, according to (15) and (80)

$$\frac{1}{m_1}=\frac{1}{m(k_1)}W_{k_1,1}+\frac{1}{m(k_2)}W_{k_2,1}, \tag{81}$$

where the probabilities are

$$W_{k_1,1}=\frac{1}{2}\left(1+\frac{2|L|}{K}\right),$$
$$W_{k_2,1}=\frac{1}{2}\left(1-\frac{2|L|}{K}\right). \tag{82}$$

It is clear from (80)–(82) that, although we have used the many-electron wave function (in this case a two-electron wave function) to calculate the probabilities $W_{k_1,1}$ and $W_{k_2,1}$, the quantity $1/m_1$ still has the physical meaning of an average value of inverse effective mass for a band electron, in agreement with Sec. 1. The many-electron character of the wave function used here allows us to take into account the contribution due to electron correlations.

Actually, the probability (82) can be cast in the form

$$W_{k_1,1}=W_{k_1,1}|_{A=0}+\Delta_{k_1,1}, \quad W_{k_2,1}=W_{k_2,1}|_{A=0}+\Delta_{k_2,1}, \tag{83}$$

where

$$W_{k_1,1}|_{A=0}=1, \quad W_{k_2,1}|_{A=0}=0,$$
$$\Delta_{k_1,1}=-\frac{1}{2}\left(1-\frac{2|L|}{K}\right), \quad \Delta_{k_2,1}=-\Delta_{k_1,1}. \tag{84}$$

It follows from (84), (83), and (81) that

$$\frac{1}{m_1}=\frac{1}{m_1}\Big|_{A=0}+\Delta\left(\frac{1}{m(k_1)}\right), \tag{85}$$

where

$$\frac{1}{m_1}\Big|_{A=0}=\frac{1}{m(k_1)},$$
$$\Delta\left(\frac{1}{m_1}\right)=\Delta_{k_1,1}\left(\frac{1}{m(k_1)}-\frac{1}{m(k_2)}\right). \tag{86}$$

According to (84) and (86), the corrections to the probability $\Delta_{k_1,2}$ and therefore to $\Delta(1/m_1)$ vanish in the absence of correlations. However, for $A\neq 0$, the corrections to this probability and therefore to $\Delta(1/m_1)$ do not equal zero. In this case $\Delta(1/m_1)$ describes the change in the average value of the inverse effective mass of a band electron due to electron correlations.

In the case under discussion here we have $m(k_2)=-m(k_1)$. Therefore, it follows from (86), (85), and (84) that

$$m_1=m(k_1)\frac{K}{2|L|}, \tag{87}$$

which coincides with the expression for m_1 from (68).

Note also that in the case under discussion here, the mean-square fluctuations of n_{k_1} and n_{k_2} are determined by the expression

$$[(\Delta n_{k_1})^2]^{1/2}=[(\Delta n_{k_2})^2]^{1/2}=\frac{A}{2K}. \tag{88}$$

It is clear from (88) that in the absence of correlations, i.e., for $A=0$, there are no fluctuations in n_{k_1} and n_{k_2}. For a given A, as $|L|$ increases the fluctuations decrease, while for a given value of $|L|$ the fluctuations of n_{k_1} and n_{k_2} increase with increasing A. As $A/|L|\to\infty$, the mean-square fluctuations $[(\Delta n_{k_1})^2]^{1/2}=[(\Delta n_{k_2})^2]^{1/2}$ go to 1.

An analogous discussion can be carried out for the effective mass m_2 in the state ψ_4.

APPENDIX 2

EFFECTIVE MASS IN THE CASE OF AN ENERGY SPECTRUM OBTAINED IN THE QUASI-CLASSICAL APPROXIMATION AND BY THE VARIATIONAL METHOD

The energy spectrum of the polar model has the form

$$E=ANh+8N|L|(1/2-h)h\sin k_1a\cdot\sin k_2a, \tag{89}$$

where

$$h_{\rm gr}=\frac{1}{4}\left(1-\frac{A}{4|L|}\right),$$
$$h_{\rm h.ex.}=\frac{1}{4}\left(1+\frac{A}{4|L|}\right). \tag{90}$$

This spectrum is obtained by using the quasiclassical approximation described in Ref. 1 and the variational method from Ref. 10. According to (89), the average value $\varepsilon=E/N$ for a single electron near the minimum of E (where $\sin k_1a\cdot\sin k_2a\approx -1$ and we can set $k_2a=-\pi/2$ and $k_1a=\pi/2+\delta$, $\delta\ll 1$) is determined by the expression

$$\varepsilon=Ah-8|L|(1/2-h)h+4|L|h(1/2-h)\left(k_1a-\frac{\pi}{2}\right)^2. \tag{91}$$

Taking (10) into account, we find from (91) that

$$m_{\rm gr}=\frac{\hbar^2}{8|L|h(1/2-h)a^2}. \tag{92}$$

By introducing value $h_{\rm gr}$ from (90) in (92) we find

$$m_{\rm gr}=\frac{2\hbar^2}{a^2|L|[1-(A/4L)^2]}. \tag{93}$$

On the other hand, according to (89) and the first of the equations (90),

$$\langle 0|H_L|0\rangle=-\frac{1}{2}N|L|\left[1-\left(\frac{A}{4L}\right)^2\right]. \tag{94}$$

We again obtain (93) from (94) and (16).

Thus, in the ground state, the effective mass (16) determined in this paper coincides with the effective mass determined from the energy spectrum. Analogously, it can be shown that in the highest excited state

$$m_{\rm h.ex.}=-\frac{2\hbar^2}{a^2|L|[1-(A/4L)^2]}. \tag{95}$$

The same equation is obtained from (16) by taking into account the equation

$$\langle F|H_L|F\rangle=-\langle 0|H_L|0\rangle.$$

Thus, in the highest excited state the effective mass (16) also coincides with the effective mass determined from the energy spectrum.

APPENDIX 3

ELECTRONIC SPECIFIC HEAT OF A SYSTEM WITH TWO LATTICE SITES AND TWO ELECTRONS

For a nonzero temperature T the average value of the system energy has the form

$$\bar{E}=E_1+\frac{K+A/2+3(K-A/2)\exp(A/k_BT)+2K\exp[-(K-A/2)/k_BT]}{1+3\exp(A/k_BT)+\exp[(K+A/2)/k_BT]+\exp[-(K-A/2)/k_BT]} \tag{96}$$

where k_B is Boltzmann's constant.

In the region of relatively low temperature ($k_BT \ll K - A/2$) is follows from (6) that

$$\bar{E}=\frac{E_1}{1+3\exp(E_1/k_BT)}. \tag{97}$$

In this case the heat capacity is determined by the expression

$$C=\frac{3E_1^2}{k_BT^2}\exp\left(\frac{E_1}{k_BT}\right). \tag{98}$$

For the case $A \gg |L|$, according to (65), $E_1 \approx -4L^2/A$ and, according to (68), $m_1 \approx \hbar^2 A/4a^2L^2$. Therefore,

$$E_1 \approx -\frac{\hbar^2}{m_1a^2}. \tag{99}$$

It follows from (99) and (98) that

$$C=\frac{3}{k_BT^2}\left(\frac{\hbar^2}{m_1a^2}\right)^2\exp\left(-\frac{\hbar^2}{m_1a^2k_BT}\right). \tag{100}$$

It is clear from (100) that the effective mass introduced in (16) also determines the heat capacity of the electron system. According to (68), as A increases the effective mass m_1 increases. Therefore it follows from (100) that as A increases the low-temperature heat capacity of the electronic system increases.

APPENDIX 4

PARAMAGNETIC SUSCEPTIBILITY OF A SYSTEM WITH TWO LATTICE SITES AND TWO ELECTRONS

In a uniform magnetic field of intensity H, the level E_2 from (65) splits into two levels of 0 and $\pm 2\mu H$, where μ is the Bohr magneton.

Correspondingly, the partition function Z is determined by the equation

$$Z=1+\exp\left(-\frac{A}{k_BT}\right)+2\exp\left(-\frac{A}{2k_BT}\right)\operatorname{ch}\frac{K}{k_BT}+2\operatorname{ch}\frac{\mu H}{k_BT}. \tag{101}$$

Using the fact that the free energy equals $F = k_BT\ln Z$, we find the following expression for the magnetic moment:

$$\mathcal{M}=-\frac{\partial F}{\partial H}=4\mu\frac{\operatorname{sh}(2\mu H/k_BT)}{1+\exp(-A/k_BT)+2\exp(-A/2k_BT)\operatorname{ch}(K/k_BT)+2\operatorname{ch}(2\mu H/k_BT)}. \tag{102}$$

For $\mu M/k_BT \ll 1$, we obtain from (102) an expression for the paramagnetic susceptibility:

$$\chi=\frac{8\mu^2}{k_BT}\frac{1}{3+\exp(-A/k_BT)+2\exp(-A/2k_BT)\operatorname{ch}(K/k_BT)}. \tag{103}$$

In the region $k_BT \ll K - A/2$, it follows from (103) that

$$\chi=\frac{8\mu^2}{k_BT}\frac{1}{3+\exp(-E_1/k_BT)}. \tag{104}$$

Taking into account (86), we obtain from (104)

$$\chi=\frac{8\mu^2}{k_BT}\frac{1}{3+\exp(\hbar^2/m_1a^2k_BT)}. \tag{105}$$

It is clear from (105) that the effective mass (16) introduced in this paper also determines the paramagnetic susceptibility of the electron system. As A grows, the increase in the effective mass [see (68)] also leads to an increase in the paramagnetic susceptibility.

In the case we have discussed here, with $A \gg |L|$, the enhancement of the effective mass $m_{A\neq 0}/m_{A=0} \approx A/4|L|$ can turn out to be significant. This shows that the results obtained here are valuable in interpreting the properties of heavy-fermion systems from the point of view of effective mass increases caused by electron correlations.

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