Electronic states of variable-valence impurity centers in crystals with charge- and spin-density waves

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The matrix for the scattering of band electrons by a variable-valence impurity center in a crystal with a charge-density wave (CDW) or a spin-density wave (SDW) has been found. The calculations have been performed by the $1/N$ expansion method in the Anderson model with infinite Hubbard repulsion at the impurity center. The energies of the localized impurity states within an CDW or SDW target have been calculated. In the case of a CDW, the level remains N-fold degenerate, but its energy depends on the type of sublattice (with a charge-density maximum or minimum). In the case of an SDW, the degeneracy of the level is removed, but its energy does not depend on the type of sublattice (with a spin-density maximum or minimum).

1. INTRODUCTION

The behavior of impurities in crystals with charge- and spin-density waves (CDW's and SDW's) has been studied off and on for the last 20 years. Since the early studies (for example, Ref. 1), the most popular model has been the nonself-consistent point-defect potential, which in some cases provides a qualitatively correct description of the electronic structure of impurity states, the redistribution of the electron and spin density in the vicinity of an impurity center, and the renormalization of the amplitude (and, in some cases, the spatial structure) of a CDW and an SDW. One common property of all the models of systems with a CDW and an SDW that have been considered for both nonmagnetic and magnetic impurity centers is the appearance of localized states within the gap in the spectrum of one-particle excitations even when the potential of the electron-impurity interaction is as weak as desired (see, for example, the discussion and references in Ref. 2). The radius and energy of these states are strongly dependent on the parameters of the CDW (SDW), and their genesis is governed by the special features of the density of states of the band electrons near the edges of the dielectric gap. A more detailed discussion of the situation for specific structures was given in Refs. 3 and 4, and there is no need to repeat it here.

We recently[5] turned to an investigation of complex centers in systems with a CDW and an SDW, which, in principle, cannot be described by the nonself-consistent point-defect scattering potential model.

More specifically, we examined the Anderson impurity model in the Kondo regime. The problem of the electronic spectrum of impurity states was reduced by the $1/N$ expansion method to the solution of a system of equations for the poles of the one-particle Green's function of the band electrons in a self-consistent (with respect to the occupancies of the states) frequency-dependent pseudopotential $U(\omega)$. The situation formally treated in Ref. 5 corresponds to a range of parameters of the model which are such that $T_{s,t} \ll T_k$, where $T_{s,t}$ is the temperature of the transition to the CDW (SDW) phase and T_k is the Kondo temperature.

In this paper we study another limiting case, viz., a variable-valence impurity center with model parameters obeying the relationship $T_{s,t} \gg T_k$. We note that T_k should be understood to be the Kondo temperature renormalized under the influence of a CDW (or SDW) (which is generally lower than in a normal metallic phase). Under these conditions a calculation scheme like the mean-field approximation,[6] which was used in Ref. 5, is inapplicable. As before, we consider the N-fold degenerate Anderson impurity model in the limit $U \to \infty$ (U is the Hubbard repulsion energy at the center), and the analytic calculation will be performed by the $1/N$ expansion method in the limit $N \to \infty$.

2. MODEL HAMILTONIAN AND METHOD FOR CALCULATING PHYSICAL MEDIA

A system that is unstable with respect to a transition to a CDW or SDW state can be described using the standard model of a metal with congruent regions on the Fermi surface separated by half the reciprocal lattice vector $\mathbf{Q}=\mathbf{G}/2$ (Ref. 7). An impurity center is described in a two-configuration model, in which it fluctuates between the states $f^0=|0\rangle$ and $f^1=|m\rangle$, where $m=(J,\ldots,-J)$, $N=2J+1$, and N is the multiplicity of the degeneracy of the f^1 state (the Anderson impurity model with N-fold degeneracy in the limit of infinite one-center repulsion). The interaction of the band states with states localized on the impurity center is specified in the form of one-particle hybridization. Thus, the Hamiltonian of the system under investigation is

$$H=H_1+H_2+H_3-\mu n. \tag{1}$$

Here μ is the chemical potential, and n is the operator of the total number of particles. The Hamiltonian H_1 describes the band electrons in the CDW or SDW phase:

$$H_1=\sum_{\mathbf{k},\alpha}\varepsilon(\mathbf{k})a^+_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}-\sum_{\mathbf{k},\alpha,\beta}[\Delta_{\beta\alpha}a^+_{\mathbf{k}\alpha}a_{\mathbf{k}+Q\beta}+\text{k.c.}]. \tag{2}$$

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Here $\Delta_{\beta\alpha}=(\Delta_t\boldsymbol{\sigma})_{\beta\alpha}$ in the case of an SDW, and $\Delta_{\beta\alpha}=\Delta_s\delta_{\beta\alpha}$ in the case of a CDW, where Δ_t and Δ_s are the corresponding order parameters. The dispersion law of the band electrons satisfies the "nesting" condition $\varepsilon(\mathbf{k})=-\varepsilon(\mathbf{k}+\mathbf{Q})$, α and β are the spin indices, and $\boldsymbol{\sigma}$ is the vector consisting of the Pauli spin matrices. The chemical potential is measured from the middle of the band gap.

We write Hamiltonians H_2 and H_3 with the aid of auxiliary pseudofermion (f_m) and pseudoboson (b) fields, following Ref. 8:

$$H_2=\sum_m E_f f_m^+ f_m+E_0\, b^+ b, \tag{3}$$

$$H_3=\sum_{\mathbf{k},m,\alpha}[V_{m\alpha}(\mathbf{k})f_m^+ b a_\alpha(\mathbf{k})+\text{k.c.}]. \tag{4}$$

The operator of the total number of pseudofermions and pseudobosons on the impurity commutes with H:

$$Q=b^+b+\sum_m f_m^+ f_m\,. \tag{5}$$

Strict fulfillment of the requirement $Q=1$ is necessary in our problem. Nonphysical states can be formally eliminated by adding the term $\lambda(Q-1)$ to H and making the transition to the limit $\lambda\to\infty$ in the expressions for the physical expected values.[9]

We write several general relations needed for subsequent calculations. The partition function of the model with Hamiltonian (1) is

$$\begin{aligned}Z&=\exp[-\beta\Omega]\\&=\lim_{\lambda\to\infty}\text{Sp}[\exp[-\beta H(\lambda)]]\\&=Z_{\text{band}}\lim_{\lambda\to\infty}(\exp[\beta\lambda]\,\langle Q\rangle_\lambda),\end{aligned} \tag{6}$$

$$\langle Q\rangle_\lambda=\int d\omega\left\{\sum_m A_m(\omega+\lambda,\lambda)f(\omega+\lambda)+B(\omega+\lambda,\lambda)n(\omega+\lambda)\right\}, \tag{7}$$

$$D(i\nu_n,\lambda)=\int_{-\infty}^{\infty}d\omega\,\frac{B(\omega,\lambda)}{i\nu_n-\omega},$$

$$G_m(i\omega_n,\lambda)=\int_{-\infty}^{\infty}d\omega\,\frac{A_m(\omega,\lambda)}{i\omega_n-\omega}, \tag{8}$$

where $n(\omega)$ is the Bose–Einstein function, $\nu_n=2\pi nT$, $f(\omega)$ is the Fermi–Dirac function, $\omega_n=\pi T(2n+1)$, $n=0,\pm1,\pm2,\ldots$, Z_{band} is the partition function for the band electrons, and $B(\omega,\lambda)$ and $A_m(\omega,\lambda)$ are the spectral functions of the pseudoboson Green's function $D(i\nu_n,\lambda)$ and the pseudofermion Green's function $G_m(i\omega_n,\lambda)$, respectively.

The scattering matrix $\hat{\Sigma}$ of the band electrons on an impurity center can be written as the projection of the scattering matrix $\hat{\Sigma}(\lambda)$ onto the subspace with $Q\equiv1$.

$$\Sigma_{ij}^{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega)=\lim_{\lambda\to\infty}[\Sigma_{ij}^{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega,\lambda)/\langle Q\rangle_\lambda]. \tag{9}$$

Similarly, the corrections to the self-energies of a pseudoboson (Π) and a pseudofermion (Σ_m) can be expressed by the relations

$$\Pi(\nu)=\lim_{\lambda\to\infty}\Pi(\nu+\lambda,\lambda), \tag{10}$$

$$\Sigma_m(\omega)=\lim_{\lambda\to\infty}\Sigma_m(\omega+\lambda,\lambda). \tag{11}$$

In the noncrossing approximation (NCA) the functions $\hat{\Sigma}(\lambda)$, $\Pi(\lambda)$, and $\Sigma_m(\lambda)$ satisfy the equations

$$\Sigma_{ij}^{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega_n,\lambda)=-T\Sigma[V_{m\alpha}^i(\mathbf{k})G_m(\omega_n+\nu_n,\lambda)D(\nu_n,\lambda)V_{m\beta}^{j*}(\mathbf{k}')], \tag{12}$$

$$\Sigma_m(\omega_n,\lambda)=-T\Sigma[V_{m\alpha_1}^{i_1}(\mathbf{k})D(\nu_n,\lambda)G_{i_1i_2}^{\alpha_1\alpha_2}(\mathbf{k},\omega_n-\nu_n)V_{m\alpha_2}^{i_2*}(\mathbf{k})]\delta_{mm_1}, \tag{13}$$

$$\Pi(\nu_n,\lambda)=T\Sigma[V_{m\alpha_1}^{i_1}(\mathbf{k})G_m(\omega_n,\lambda)G_{i_1i_2}^{\alpha_1\alpha_2}(\mathbf{k},\omega_n-\nu_n)V_{m\alpha_2}^{i_2*}(\mathbf{k})]. \tag{14}$$

The Green's functions of the band electrons, pseudofermions, and pseudobosons are, respectively,

$$G_{ij}^{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega_n,\lambda)=\mathring{G}_{ij}^{\alpha\beta}(\mathbf{k},\omega_n)\delta_{\mathbf{k}\mathbf{k}'}+\Sigma[\mathring{G}_{ii_1}^{\alpha\alpha_1}(\mathbf{k},\omega_n)\Sigma_{i_1i_2}^{\alpha_1\alpha_2}(\mathbf{k},\mathbf{k}_1,\omega_n,\lambda)\times G_{i_2j}^{\alpha_2\beta}(\mathbf{k}_1,\mathbf{k}',\omega_n,\lambda)], \tag{15}$$

$$G_m(\omega_n,\lambda)=[i\omega_n-E_f-\Sigma_m(\omega_n,\lambda)-\lambda]^{-1}, \tag{16}$$

$$D(\nu_n,\lambda)=[i\nu_n-E_0-\Pi(\nu_n,\lambda)-\lambda]^{-1}, \tag{17}$$

$$\mathring{G}_{ii}^{\alpha_1\alpha_2}(\mathbf{k},\omega_n)=\mathring{G}^{\alpha_1\alpha_2}(\mathbf{k},\mathbf{k},\omega_n)=\frac{i\omega_n+\varepsilon(\mathbf{k})}{(i\omega_n)^2-\varepsilon^2(\mathbf{k})-|\Delta|^2}, \tag{18}$$

$$\mathring{G}_{ij}^{\alpha_1\alpha_2}(\mathbf{k},\omega_n)=\mathring{G}^{\alpha_1\alpha_2}(\mathbf{k},\mathbf{k}+\mathbf{Q},\omega_n)=-\frac{\Delta_{\alpha_1\alpha_2}\delta_{ij\pm1}}{(i\omega_n)^2-\varepsilon^2(\mathbf{k})-|\Delta|^2}. \tag{19}$$

For values of the momentum $\mathbf{k}$ close to the Fermi values, we assume that the matrix elements $V_{m\alpha}^i(\mathbf{k})$ are independent of $\mathbf{k}$, and we use the approximation

$$V_{m\alpha}^{(1)}(\mathbf{k})=V_{m\alpha};\quad V_{m\alpha}^{(2)}(\mathbf{k})=V_{m\alpha}\exp i\mathbf{Q}\mathbf{R}_0\,. \tag{20}$$

Here $\mathbf{R}_0$ is the coordinate of the impurity center in the lattice ($\exp i\mathbf{Q}\mathbf{R}_0=\pm1$) in terms of the position of the impurity relative to a crest or valley of a CDW (or SDW). The dependence of the matrix elements $V_{m\alpha}$ on the indices (m and α) in the simple approximation of an isotropic scattering potential is specified in the form

$$V_{m\alpha}^{(i)}=V^{(i)}f_{m\alpha},\quad f_{m\alpha}=\left(\frac{J+m\alpha}{2J}\right)^{1/2}, \tag{21}$$

where the $f_{m\alpha}$ are the standard Clebsch–Gordan coefficients. As can easily be seen, they satisfy the relations

$$\sum_\alpha f_{m\alpha}^2=1, \quad \sum_\alpha \alpha f_{m\alpha}^2=\mathrm{m/J}, \tag{22}$$

which are needed below.

3. CALCULATION OF THE SPECTRUM OF LOCALIZED STATES

Deriving analytic expressions for the self-energy corrections Π and Σ_m is fairly difficult even in the NCA (without considering vertex renormalization). Here we are interested only in the situation in which the hybridization V is small ($V \ll W$, where $2W$ is the width of the allowed band) and the Kondo regime is inapplicable ($T_k \ll 2\Delta$, where T_k is the Kondo temperature and 2Δ is the width of the bond gap), and to obtain qualitative estimates it is sufficient to confine ourselves to the simpler random phase approximation (RPA) by setting the Green's functions D, G, and G_m on the right-hand sides of Eqs. (13) and (14) equal to their "zeroth" values. We also restrict ourselves to the case of low temperatures ($T \ll \Delta, |E_f - E_0|$), and we then rewrite the expressions for Π and Σ_m in the form

$$\Sigma_m(\omega)=V^2\sum_{\mathbf{k}} \frac{1}{\omega-E_0-E_{\mathbf{k}}}\left[1+\frac{\tilde{m}_{s,t}\Delta\cos\mathbf{QR}_0}{E_{\mathbf{k}}}\right], \tag{23}$$

$$\Pi(\nu)=V^2N\sum_{\mathbf{k}} \frac{1}{\nu-E_f-E_{\mathbf{k}}}\left[1-\frac{A_{s,t}\Delta\cos\mathbf{QR}_0}{E_{\mathbf{k}}}\right], \tag{24}$$

$$\tilde{m}_s=-1 \ \text{(CDW)}, \quad \tilde{m}_t=-\mathrm{m/J} \ \text{(SDW)}, \tag{25}$$

$$A_s=1 \ \text{(CDW)}, \quad A_t=0 \ \text{(SDW)}. \tag{26}$$

After summation with respect to the quasimomentum $\mathbf{k}$, we can obtain explicit expressions for Σ_m and Π as functions of ω and ν (see Appendix). In Eqs. (23)–(24) the frequency of the pseudofermions ω is calculated relative to the level of the chemical potential μ, and the latter is assumed to lie within the band gap 2Δ ($\mu < \Delta$). The energy of a one-particle pseudofermion excitation $E_f - E_0$ is calculated relative to the middle of the gap, so that $E_f - E_0$ can be either positive or negative, and the filling of the E_f level is determined by the sign of the expression $E_f - E_0 - \mu$.

Calculating scattering matrix (6), we should recall that upon projection onto the subspace of states with $Q \equiv 1$ (i.e., upon the transition to the limit $\lambda \to \infty$) all the diagrams containing two or more closed loops from the pseudofermion and pseudoboson Green's functions vanish.[9] After some simple substitutions we write

$$\Sigma_{ij}^{\alpha\beta}=V^2\sum_m [\delta_{ij}+(1-\delta_{ij})\cos\mathbf{QR}_0] f_{m\alpha}f_{m\beta}\Gamma_m(\omega), \tag{27}$$

$$\Gamma_m(\omega)=\lim_{\lambda\to\infty}\frac{\Gamma_m(\omega,\lambda)}{\langle Q\rangle_\lambda}, \tag{28}$$

$$\Gamma_m(\omega,\lambda)=\int D(\nu,\lambda)G_m(\omega+\nu,\lambda)\frac{d\omega}{(2\pi i)}. \tag{29}$$

The calculation of $\Gamma_m(\omega)$ is performed in the polar (quasiparticle) approximation, which was discussed in detail in Refs. 8 and 9 and is valid in our situation, in which the Kondo regime is not realized. Calculating integral (29) and making the transition in (28) to the limit $\lambda \to \infty$, we have

$$\Gamma_m(\omega)\approx\frac{\gamma_m(\omega_m^*)}{\omega-\omega_m^*}, \tag{30}$$

$$\gamma_m(\omega_m^*)=\Theta(\eta_m^*-\nu^*)\gamma_m^>+\Theta(\nu^*-\eta_m^*)\gamma_m^<, \tag{31}$$

$$\gamma_m^>=\left(1-\frac{\partial\Sigma_m}{\partial\omega}\bigg|_{\omega=\eta_m^*+E_f}\right)^{-1}, \tag{32}$$

$$\gamma_m^<=\left(1-\frac{\partial\Pi}{\partial\omega}\bigg|_{\omega=\nu^*+E_f}\right)^{-1}, \tag{33}$$

$$\omega_m^*=\eta_m^*-\nu^*. \tag{34}$$

The values of η_m^* and ν^* are found from the self-consistency equations

$$\eta_m^*=\Sigma_m(\eta_m^*+E_f), \tag{35}$$

$$\nu^*+\varepsilon_f=\Pi(\nu^*+E_f), \tag{36}$$

$$\varepsilon_f=E_f-E_0. \tag{37}$$

An actual calculation is completed in the limit $N \to \infty$, at which the $1/N$ expansion technique is applicable. In the zeroth order with respect to $1/N$, the self-energy correction (Σ_m) to the pseudofermion Green's function ($\Sigma_m \sim 1/N \to 0$) is negligible compared with the correction (Π) to the pseudoboson Green's function (we recall that V^2N remains finite in the limit $N \to \infty$ when the $1/N$ expansion technique is used). After this we write a closed equation for the energy $\omega_m^* = -\nu^*$

$$\omega_m^*=\varepsilon_f-\Pi(-\omega_m^*+E_f), \tag{38}$$

where $\Pi(\nu)$ is given by Eqs. (A3), (A4), (A7), and (A8). The restrictions on the applicability of Eq. (38) will be described below.

Real solutions of Eq. (38), which will be discussed below, exist in the energy range $|\omega_m^*| < \Delta$ and describe localized states on a defect. Complex solutions in the ranges $\omega_m^* > \Delta$ and $\omega_m^* < -\Delta$ describe resonances, and we are not interested in them here.

A. Systems with an SDW (Fig. 1)

A solution exists in a semirestricted range of values of ε_f ($-\infty < \varepsilon_f < \varepsilon_f'$):

$$\varepsilon_f'=\Delta+U\left\{\ln\frac{\Delta}{2W}+\frac{1}{2}\right\}, \tag{39}$$

$$U=2V^2N\cdot N(0). \tag{40}$$

As $\varepsilon_f \to -\infty$, $\omega_m^*(\varepsilon_f) \to -\Delta$, and as $\varepsilon_f \to \varepsilon_f'$, $\omega_m^*(\varepsilon_f') \to \Delta$. The asymptotic behavior at large negative values of ε_f ($|\varepsilon_f| \gg \Delta$, $U \ln 2W/\Delta$) is given by

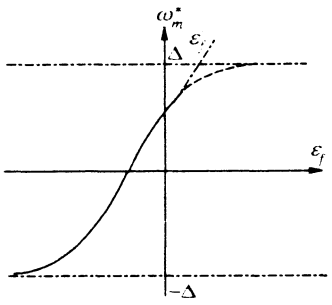

FIG. 1.

$$\omega_m^* \approx -\Delta\left[1-\frac{1}{2}\left(\frac{U\pi}{2|\varepsilon_f|}\right)^2\right]. \tag{41}$$

B. Systems with a CDW (the "positive" half-wave cos $\mathbf{QR}_0=1$, Fig. 2)

A solution exists in a semirestricted range of values of ε_f $(-\infty<\varepsilon_f<\varepsilon_f^+)$. Here $\omega_m^*(-\infty)=-\Delta$ and $\omega_m^*(\varepsilon_f^+)=\Delta$:

$$\omega_m^*(\varepsilon_f\to\varepsilon_f^+)\to\Delta[1+(\varepsilon_f-\varepsilon_f^+)/\Delta], \quad \varepsilon_f\leqslant\varepsilon_f^+,$$

$$\varepsilon_f^+=\Delta+U\ln\frac{\Delta}{2W}. \tag{42}$$

As $\varepsilon_f\to-\infty$ $(|\varepsilon_f|\gg\Delta,\ U\ln 2W/\Delta)$ the asymptotic behavior of $\omega_m^*(\varepsilon_f)$ is similar to (38):

$$\omega_m^* \approx -\Delta\left[1-\frac{1}{2}\left(\frac{U\pi}{|\varepsilon_f|}\right)^2\right]. \tag{43}$$

C. Systems with a CDW (the "negative" half-wave cos $\mathbf{QR}_0=-1$, Fig. 3)

A solution exists in a restricted range of values of ε_f $(\varepsilon_f^- < \varepsilon_f < \varepsilon_f^-)$. Here $\omega_m^*(\varepsilon_f^-) = -\Delta$ and $\omega_m^*(\varepsilon_f'') = \Delta$:

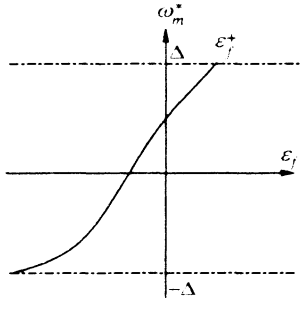

FIG. 2.

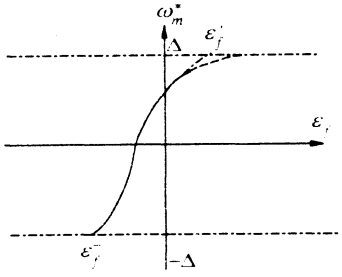

FIG. 3.

$$\omega_m^*(\varepsilon_f\to\varepsilon_f^-) = \begin{cases} -\Delta[1-8(\varepsilon_f-\varepsilon_f^-)^2/\pi^2U^2], & 0\leqslant\varepsilon_f-\varepsilon_f^-\ll U^2/\Delta \\ -\Delta[1-(\varepsilon_f-\varepsilon_f^-)/\Delta, & \varepsilon_f-\varepsilon_f^-\gg U^2/\Delta, \end{cases} \tag{44}$$

$$\varepsilon_f^-=-\Delta+U\ln\frac{\Delta}{2W},$$

$$\varepsilon_f''=\Delta+U\left(\ln\frac{\Delta}{2W}+1\right). \tag{45}$$

Let us now turn to Eqs. (34)–(37) and more attentively discuss the derivation of relation (38) from them by the $1/N$ expansion method. Discarding the term Σ_m, which has a small factor $\sim(1/N)$ compared with Π, is justified in the limit of large N only if Σ_m does not diverge. It is easily seen that as $\eta_m^* + E_f \to E_0 + \Delta$ this requirement is violated for systems with an SDW and for the "negative" half-wave of systems with a CDW [see Eqs. (A2) and (A6)]. At any finite N the correction to the self-energy part of the pseudofermions for the indicated values of η_m^* diverges. It is not difficult to understand that we are dealing here with the ranges of values $\varepsilon_f \gg \varepsilon_f'$ (in systems with an SDW) and $\varepsilon_f \gg \varepsilon_f''$ (in systems with the "negative" half-wave of a CDW), where there are no real solutions for Eq. (38). Isolating the divergent contributions to $\Sigma_m(\eta_m^* + E_f)$, we can obtain asymptotic expressions for $\omega_m^*(\varepsilon_f)$ in the lowest nonvanishing order of the $1/N$ expansion by directly solving system (34)–(37) for $U\ll 1$. Omitting the simple intermediate calculations, we present only the final equations:

A. for systems with an SDW (dashed line in Fig. 1)

$$\omega_m^*(\varepsilon_f\to\infty)=\Delta\left[1-\frac{1}{2}\left(\frac{U}{N}\right)^2\frac{\pi^2}{\varepsilon_f^2}\left(1+\frac{m}{\mathscr{T}}\cos\mathbf{QR}_0\right)^2\right]. \tag{46}$$

B. for systems with a CDW (the "negative" half-wave, dashed line in Fig. 3)

$$\omega_m^*(\varepsilon_f\to\infty)=\Delta\left[1-2\left(\frac{U}{N}\right)^2\frac{\pi^2}{\varepsilon_f^2}\right]. \tag{47}$$

4. CONCLUSIONS

Our results regarding the formation of localized states within an SDW (CDW) gap can be summarized in the following manner.

A. In systems with an SDW, a localized state exists over the entire range of seeding energies $-\infty<\varepsilon_f<\infty$. In the zeroth order of the $1/N$ expansion this state is N-fold degenerate, but this degeneracy is completely removed in the next orders with respect to $(1/N)$. The plot of $\omega_m^*(\varepsilon_f)$ is strongly asymmetric at large negative and positive values of ε_f (in the latter case the level is squeezed N^2 times faster against the edge of the conduction band than against the edge of the valence band).

B. In systems with a CDW in which an impurity is found in the region of the "positive" half-wave (i.e., at a site with excess charge density), a localized state exists in a semirestricted range of values of ε_f $(-\infty<\varepsilon_f<\varepsilon_f^+)$ and is N-fold degenerate.

C. In systems with a CDW in which an impurity is found in the region of the "negative" half-wave (i.e., at a site with insufficient charge density), a localized state exists in a semirestricted range of values of ε_f $(\varepsilon_f^-<\varepsilon_f<\infty)$ and is N-fold degenerate.

We note that the energies ε_f' and ε_f'' [Eqs. (39) and (44)] thus simply mark the boundaries of applicability of the lowest approximation with respect to $(1/N)$ in our calculation and do not have any great physical meaning. The asymmetry of the behavior of $\omega_m^*(\varepsilon_f)$ at large positive values of ε_f (for the "negative" half-wave of a CDW), like the aforementioned asymmetry of $\omega_m^*(\varepsilon_f)$ for a system with an SDW, is the result of the N-fold degeneracy of the f^1 state and the nondegeneracy of the f^0 state. In the simple model of a resonant scattering center without a strong one-center correlation with nondegenerate f^1 and f^0 states, the plots of $\omega_m^*(\varepsilon_f)$ are symmetric upon the replacement $\varepsilon_f\to-\varepsilon_f$, as well as upon the replacement of the spin index $\sigma\to-\sigma$ and $\cos\mathbf{QR}_0\to-\cos\mathbf{QR}_0$ (see the discussion in [5]). The conclusions regarding the following points are fundamental and not dependent on the choice of the approximation: a) the existence and complete removal of the degeneracy of the localized state in a system with a SDW over the entire range of values of the energy of a one-particle one-center excitation ε_f; b) the restricted range of values of ε_f for the existence and maintenance of the degeneracy of this state in a system with a CDW.

The foregoing results may be useful in studying the charge and magnetic states of local centers in numerous different systems. They include impurities of rare-earth metals in A_4B_6 semiconductors, in which the "ionicity" potential plays the role of the amplitude of a CDW in the context of the p model.[2] They also include chemisorbed centers formed by metals or halogens on reconstructed W(100) and Mo(100) metallic surfaces with a CDW (Ref. 10) or a $(2x1)$ semiconductor surface for Si(111) or C(111) (in the diamond structure) which has been reconstructed by the Pendey chain mechanism.[4] Among the systems with a SDW, the group of ordered binary alloys of Mn with group-VII and group-VIII metals,[11] as well as the dilute Cr alloys with rare-earth metals,[3] should be singled out.

APPENDIX

The functions $\Sigma_m(\omega)$ and $\Pi(\nu)$ have the following forms for systems with a SDW:

$$\Sigma_m(\omega)=\frac{U}{N}\left\{\ln\frac{\Delta}{2W}-\left(\frac{\omega-E_0}{\Delta}-\frac{m}{J}\cos\mathbf{QR}_0\right)\left[\left(\frac{\omega-E_0}{\Delta}\right)^2-1\right]^{-1/2}\left[\ln\frac{1+\dfrac{\omega-E_0}{\Delta}-\left[\left(\dfrac{\omega-E_0}{\Delta}\right)^2-1\right]^{1/2}}{1+\dfrac{\omega-E_0}{\Delta}+\left[\left(\dfrac{\omega-E_0}{\Delta}\right)^2-1\right]^{1/2}}-i\pi\right]\right\},$$

$$\frac{|\omega-E_0|^2}{\Delta^2}>1. \tag{A1}$$

$$\Sigma_m(\omega)=\frac{U}{N}\left\{\ln\frac{\Delta}{2W}-\left(\frac{\omega-E_0}{\Delta}-\frac{m}{J}\cos\mathbf{QR}_0\right)\left[1-\left(\frac{\omega-E_0}{\Delta}\right)^2\right]^{-1/2}\times\arctan\frac{1+\dfrac{\omega-E_0}{\Delta}}{\left[1+\left(\dfrac{\omega-E_0}{\Delta}\right)^{1/2}\right]}\right\},$$

$$\frac{|\omega-E_0|^2}{\Delta^2}<1. \tag{A2}$$

$$\Pi(\nu)=U\left\{\ln\frac{\Delta}{2W}-\left(\frac{\nu-E_f}{\Delta}\right)\left[\left(\frac{\nu-E_f}{\Delta}\right)^2-1\right]^{-1/2}\times\left[\ln\frac{1+\dfrac{\nu-E_f}{\Delta}-\left[\left(\dfrac{\nu-E_f}{\Delta}\right)^2-1\right]^{1/2}}{1+\dfrac{\nu-E_f}{\Delta}+\left[\left(\dfrac{\nu-E_f}{\Delta}\right)^2-1\right]^{1/2}}-i\pi\right]\right\}.$$

$$\frac{|\nu-E_f|^2}{\Delta^2}>1. \tag{A3}$$

$$\Pi(\nu)=U\left\{\ln\frac{\Delta}{2W}-\left(\frac{\nu-E_f}{\Delta}\right)\left[1-\left(\frac{\nu-E_f}{\Delta}\right)^2\right]^{-1/2}\arctan\frac{1+\frac{\nu-E_f}{\Delta}}{\left[1-\left(\frac{\nu-E_f}{\Delta}\right)^2\right]^{1/2}}\right\},$$

$$\frac{|\nu-E_f|^2}{\Delta^2}<1. \tag{A4}$$

For system with SDW

$$\Sigma_m(\omega)=\frac{U}{N}\left\{\ln\frac{\Delta}{2W}-\left(\frac{\omega-E_0}{\Delta}-\cos\mathbf{QR}_0\right)\left[\left(\frac{\omega-E_0}{\Delta}\right)^2-1\right]^{-1/2}\left[\ln\frac{1+\frac{\omega-E_0}{\Delta}-\left[\left(\frac{\omega-E_0}{\Delta}\right)^2-1\right]^{1/2}}{1+\frac{\omega-E_0}{\Delta}+\left[\left(\frac{\omega-E_0}{\Delta}\right)^2-1\right]^{1/2}}-i\pi\right]\right\},$$

$$\frac{|\omega-E_0|^2}{\Delta^2}>1. \tag{A5}$$

$$\Sigma_m(\omega)=\frac{U}{N}\left\{\ln\frac{\Delta}{2W}-\left(\frac{\omega-E_0}{\Delta}-\cos\mathbf{QR}_0\right)\left[1-\left(\frac{\omega-E_0}{\Delta}\right)^2\right]^{-1/2}\arctan\frac{1+\frac{\omega-E_0}{\Delta}}{\left[1+\left(\frac{\omega-E_0}{\Delta}\right)^{1/2}\right]}\right\},$$

$$\frac{|\omega-E_0|^2}{\Delta^2}<1. \tag{A6}$$

$$\Pi(\nu)=U\left\{\ln\frac{\Delta}{2W}-\left(\frac{\nu-E_f}{\Delta}+\cos\mathbf{QR}_0\right)\left[1-\left(\frac{\nu-E_f}{\Delta}\right)^2\right]^{-1/2}\left[\ln\frac{1+\frac{\nu-E_f}{\Delta}-\left[\left(\frac{\nu-E_f}{\Delta}\right)^2-1\right]^{1/2}}{1+\frac{\nu-E_f}{\Delta}+\left[\left(\frac{\nu-E_f}{\Delta}\right)^2-1\right]^{1/2}}-i\pi\right]\right\},$$

$$\frac{|\nu-E_f|^2}{\Delta^2}>1. \tag{A7}$$

$$\Pi(\nu)=U\left\{\ln\frac{\Delta}{2W}-\left(\frac{\nu-E_f}{\Delta}+\cos\mathbf{QR}_0\right)\left[1-\left(\frac{\nu-E_f}{\Delta}\right)^2\right]^{-1/2}\arctan\frac{1+\frac{\nu-E_f}{\Delta}}{\left[1-\left(\frac{\nu-E_f}{\Delta}\right)^2\right]^{1/2}}\right\},$$

$$\frac{|\nu-E_f|^2}{\Delta^2}<1. \tag{A8}$$

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