Electron exchange of an atomic particle with a bounded band of electron surface states

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Using the time-dependent Anderson–Newns model, a study is made of charge exchange in connection with the scattering of an atomic particle from the surface of a solid in the limit of slow collisions. Asymptotically exact solutions of this problem are obtained for different models of the time dependence of the hybridization of the atomic and band states. It is shown that in the case of a real-finite energy band of electron surface states the charge state of the scattered atomic particle can be nonmonotonic as a function of its energy only if there is an interval on which the variation of the hybridization is adiabatically slow. The role of Coulomb correlations in the charge-exchange process is also discussed. © *1996 American Institute of Physics*. [S1063-7761(96)01702-8]

1. INTRODUCTION

In recent years, much attention has been devoted to the theory of charge exchange in processes in which atomic particles interact with a crystal surface.[1,2] To a large degree, the interest in this problem is due to the requirements of the investigations into the diagnostics of surfaces by ion beams and the ion stimulation of phase transitions on surfaces. This is a field that has recently been growing rapidly. The experimental study of these processes has revealed some general properties. First, it has been established that there is an intimate connection between the efficiency of ion bombardment and the details of the process of charge exchange between the bombarding ions and the surface.[3] Second, it has been shown that the intensity of the charge exchange depends strongly on the energy of the incident ions; moreover, in a number of cases this dependence is nonmonotonic (oscillatory).[4,5] Precisely this last circumstance has been the subject of numerous recent theoretical discussions.

The simplest model used to describe the probability of charge exchange of ions when they are scattered by the surface of a solid is the time-dependent Anderson–Newns models.[6,7] In accordance with this model, the incident ion is modeled by a single-level system (the excited intra-atomic states are not taken into account) that interacts with Bloch states of the crystal.

The Hamiltonian of the model (without allowance for the intraatomic Coulomb interaction between the valence electrons) has the form

$$\hat{H}(R(t))=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})\hat{c}^{+}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma}+\varepsilon_a(R(t))\sum_{\mathbf{k},\sigma}\hat{a}^{+}_{\sigma}\hat{a}_{\sigma}+\frac{\lambda(R(t))}{\sqrt{V}}\sum_{\mathbf{k},\sigma}(V^{*}_{\mathbf{k},\sigma}\hat{a}^{+}_{\sigma}\hat{c}_{\mathbf{k},\sigma}+V_{\mathbf{k},\sigma}\hat{c}^{+}_{\mathbf{k},\sigma}\hat{a}_{\sigma}), \tag{1}$$

where $\hat{c}^{+}_{\mathbf{k},\sigma},\hat{c}^{+}_{\sigma}(\hat{a}_{\mathbf{k},\sigma},\hat{a}_{\sigma})$ are the creation (and annihilation) operators of electrons with spin σ in the Bloch state $|\mathbf{k}\rangle$ and in the nondegenerate atomic state $|a\rangle$, respectively, $R(t)$ is the distance between the atom and the surface at the time t (the motion of the atom is assumed to be classical), $\varepsilon_a(R(t))$ is the position of the atomic energy level at the time t, and $\lambda(R(t))V_{\mathbf{k}}/\sqrt{V}$ is the matrix element for the hybridization of the atomic state and a band state normalized by the volume V of the system. It is also assumed that $R=v_{\perp}|t|$, where $v_{\perp}$ is the component of the velocity perpendicular to the surface of the crystal. Then the charge state is determined by the mean number of electrons in the state $|a\rangle$: $n(t)=\Sigma_{\sigma}(\hat{a}^{+}_{\sigma}(t)\hat{a}_{\sigma}(t))$.

Thus, the time-dependent Anderson—Newns model allowed the final occupancy $n(+\infty)$ of the atomic state to be determined as a function of the component $v_{\perp}$ of the velocity normal to the surface, which occurs as a parameter in $\lambda(t)$, and as a functional of the initial occupancies $n(-\infty)$ and $n_{\mathbf{k}}(-\infty)$. Note that the time t occurs in the electron Hamiltonian (1) only through the ion coordinate $R(t)$ at the same time. This means that, essentially, we consider only "slow" collisions,[8] i.e., collisions in which the characteristic ion velocities are much less than the characteristic electron velocities. In practice, this reduces to the condition that, for example, the energy of Ar^{+} ions in the beam must not exceed 20 keV.

Despite the relative simplicity of the Hamiltonian (1), a consistent calculation of the charge-exchange probability has hitherto been made only in two limiting cases, namely, under the assumptions that the states of the continuous spectrum form either an infinitesimally narrow or an infinitely wide energy band.[9,10] In the first case, the problem reduces to the investigation of charge exchange in a two-level system. The properties of this model have been studied in detail in the theory of atomic collisions.[11,12] It was shown that resonant charge exchange is indeed characterized by an oscillatory dependence of the charge-exchange probability on the velocity of approach v.

However, it should be noted that the region of applicability in which the band of the final particle can be replaced by an infinitesimally narrow band is very restricted. Indeed,

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such an approximation is possible in the case of a large "resonance deficit": $E_2-E_1 \ll |\varepsilon_a-\varepsilon(\mathbf{k})|$, where E_2 and E_1 are, respectively, the top and bottom of the band, and the inequality is satisfied for any $\mathbf{k}$. As a rule, the following relation holds then in real systems in terms of our model:

$$|\varepsilon_a-\varepsilon(\mathbf{k})| \gg \left|\lambda(R=0)\sqrt{\frac{1}{V}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2}\right|.$$

For the two-level model, this relation means the absence of quasiresonance and, as a consequence, an exponential law for the charge-exchange probability as a function of the velocity v. Generally speaking, this is inconsistent with the existing experimental data. The experimentally obtained oscillations indicate, rather, that the charge exchange has a "quasiresonant" nature, but in this case band-structure effects are already important and the simple two-level model is invalid.

The region of applicability of the other approximation, in accordance with which the states of the band spectrum form an infinitely broad band with energy-independent density of states, is also very restricted. In particular, it does not describe the situation in which the atomic level is near the bottom or top of the valence band or anywhere in the band gap.

Thus, great interest attaches to an investigation of the charge-exchange problem in the general case, i.e., without any restrictions on the form of the band spectrum and the position of the "atomic" energy ε_a.

To understand the possible consequences of allowing for a finite band spectrum, it is helpful to go over in the Hamiltonian (1) from the quasimomentum representation to the site representation (Wannier representation). Then the atomic state there corresponds to the site with $n=0$, which is coupled by means of the matrix element $\lambda(R)V_{0i}$ to the ith site of the crystal lattice. In their turn, the lattice sites are coupled to each other by the hopping matrix element t_{ij}, the form of which determines the structure of the electron spectrum $\varepsilon(\mathbf{k})$.

In the Wannier representation, the approximation of an infinitely broad band corresponds to the limit $zt_{i,i+1}\to\infty$, where z is the first coordination number of the crystal lattice, and $t_{i,i+1}$ is the matrix element of hops between nearest neighbors. Using this approximation, let us consider the decay of the atomic state $|a\rangle$. Suppose that at the initial time the electron is localized in the atomic state. Because the transition probability $|V_{0i}|^2$ is finite, the electron can "hop" to the ith lattice site. At subsequent times, there exist two possibilities for the electron: either to return to the original atomic state or to go over to the nearest sites of the lattice. However, by virtue of the condition specified above, it is the second possibility that will be realized with overwhelming probability. The same thing will also happen at later times. In other words, in the approximation of an infinitely broad band the electron, having once gone over to a site state of the lattice, will never return to the original state. Essentially this means that the electron wave function is a centered, purely outgoing wave, in connection with which the situation becomes analogous to the α decay of nuclei in the Gamow theory. Then the probability of finding the electron in the state $|a\rangle$ will decrease exponentially with the time.

If an electron that has gone over to a site state of the lattice has a finite band, there is a finite probability of return to the original atomic state. In wave-function language, this means that in addition to an outgoing wave there will also be a wave converging on the center (Bragg reflection). The interference of these waves at the atomic center can lead to nonexponential and even nonmonotonic dependence of the atomic state on the time.

The effect of a finite band spectrum on the probability of ion charge exchange was investigated in detail in our paper Ref. (13) under the assumption that the hybridization matrix element switches on and off instantaneously. The results of this study confirmed that the decay of the atomic state is essentially nonexponential and made it possible to explain the oscillatory behavior of the charge-exchange probability as a function of the ion energy. However, it was not clear to what extent this model of the time dependence of the hybridization could be applied to the case of "slow" scattering in which the atom—surface interaction is switched on and off smoothly through sections of exponential growth and decay of the hybridization. The aim of the present paper is to investigate the effect of the exponential "tails" of the switching on and off of the hybridization matrix element on the charge state of the ion. We begin by discussing an asymptotically exact solution for the "exponential model" of interaction. In Sec. 2, we consider a combined model of the time behavior of $\lambda(R)$, including allowance for exponential growth and decay and also a section on which the variation of the hybridization is relative smooth. In Sec. 3, we make a brief qualitative analysis of the results obtained in Sec. 2. In Sec. 4, we give some known experimental results and discuss them from the point of view of the model solutions obtained earlier. In Sec. 5, we discuss the role of Coulomb correlations in charge-exchange problems.

2. ASYMPTOTICALLY EXACT SOLUTION FOR THE "EXPONENTIAL MODEL" OF INTERACTION

In the case of an arbitrary law $\lambda(t)$, it is easy to express the charge state of the atomic particle in terms of the retarded form of the Green–Keldysh function. If at an initial time t_0 such that $\lambda(t_0)=0$ the occupancy of the electron states of the solid was specified by the occupation numbers $n_{\mathbf{k}}(t_0)$ and that of the electron states of the atomic center by the numbers $n_\sigma(t_0)$, then for $n(t)$ we obtain

$$n(t)=n(t_0)|G^{\rm ret}_{aa}(t,t_0)|^2+\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2 G^{\rm ret}_{aa}(t,t_1)$$
$$\times G^{\rm ret*}_{aa}(t,t_2)\lambda(t_1)\lambda(t_2)\frac{2}{V}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2 n_{\mathbf{k}}(t_0)$$
$$\times\exp(-i\varepsilon(\mathbf{k})(t_1-t_2)), \qquad (2)$$

where $G^{\rm ret}_{aa}(t,t_0)$ satisfies the equation

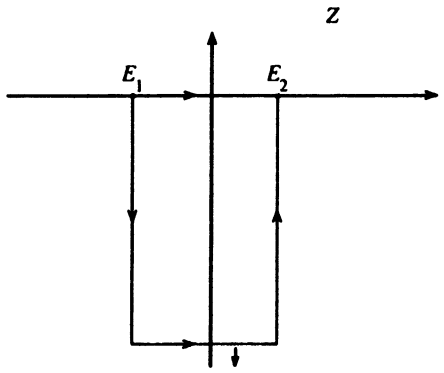

FIG. 1. Modification of the contour of integration.

$$\begin{cases} iv\dfrac{\partial}{\partial R}G_{aa}^{\rm ret}(R,R_0)-\varepsilon_a(R)G_{aa}^{\rm ret}(R,R_0) \\ \quad=-i\lambda(R)\displaystyle\int_{R_0}^{R}\frac{dR_1}{v}\lambda(R_1)\int_{E_1}^{E_2}d\varepsilon\Delta(\varepsilon) \\ \quad\times\exp\left(-\dfrac{i}{v}\varepsilon(R-R_1)\right)G_{aa}^{\rm ret}(R_1,R_0), \\ G_{aa}^{\rm ret}(R_0+\delta,R_0)=-i, \end{cases} \tag{3}$$

where

$$R=vt \quad (R_0=vt_0) \quad (R>R_0). \tag{4}$$

$$\Delta(\omega)=\frac{1}{V_{\mathbf{k}}}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\delta(\omega-\varepsilon(\mathbf{k})). \tag{5}$$

Note that Eq. (3) can be rewritten in the form

$$\begin{aligned} &iv\frac{\partial}{\partial R}G_{aa}^{\rm ret}(R,R_0)-\varepsilon_a(R)G_{aa}^{\rm ret}(R,R_0) \\ &=-\frac{i}{v}\lambda(R)\int_{E_1}^{E_2}d\varepsilon\Delta(\varepsilon)\int_{R_0}^{R}dR_1\lambda(R_1) \\ &\quad\times\left[\exp\left(-\frac{i}{v}\varepsilon(x-R_1)\right)\right. \\ &\quad\left.\times\exp\left(-(x-R_1)\frac{\partial}{\partial R}\right)G_{aa}^{\rm ret}(R,R_0)\right]_{x=R}. \end{aligned} \tag{6}$$

Further, we shall assume that

$$\lambda(R)=\exp(-\gamma|R|). \tag{7}$$

We consider the case $R<0$. Then the integration over R_1 on the right-hand side of Eq. (6) can be performed. Representing the Green's function on the right-hand side of (6) in the form of an expansion in a Fourier integral with respect to the first coordinate and assuming analyticity of $\Delta(\varepsilon)$ in the lower half-plane of the complex plane of Z and boundedness at infinity, we can modify the contour of integration with respect to ε, since the possible singularities cancel out (Fig. 1). The interval $[E_1-i\infty,E_2-i\infty]$ does not contribute to the integral. As a result, returning to the operator expression and going to the limit $R_0\to-\infty$, we obtain instead of (6)

$$\begin{aligned} &iv\frac{\partial}{\partial R}G_{aa}^{\rm ret}(R)-\varepsilon_a(R)G_{aa}^{\rm ret}(R) \\ &=-\exp(2\gamma R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\} \\ &\times\frac{\Delta(\varepsilon)}{\varepsilon-iv\dfrac{\partial}{\partial R}-iv\gamma}G_{aa}^{\rm ret}(R). \end{aligned} \tag{8}$$

where $G_{aa}^{\rm ret}(R)=\lim\limits_{R_0\to-\infty}G_{aa}^{\rm ret}(R,R_0)$. We shall seek $G_{aa}^{\rm ret}(R,R_0)$ in the form

$$G_{aa}^{\rm ret}(R,R_0)=\exp\left\{-\frac{i}{v}\int_{R_0}^{R}\varphi(\xi,R_0)d\xi\right\}. \tag{9}$$

We denote $\varphi(R)=\lim\limits_{R_0\to-\infty}\varphi(R,R_0)$. Then

$$G_{aa}^{\rm ret}(R)=\exp\left\{\frac{i}{v}\int_{-\infty}^{R}d\xi\varphi(\xi)\right\}. \tag{10}$$

We consider the action of the operator on the right-hand side of (8) on $G_{aa}^{\rm ret}(R)$:

$$\frac{1}{(\varepsilon-iv\gamma)-iv\dfrac{\partial}{\partial R}}G_{aa}^{\rm ret}(R). \tag{11}$$

Applying the operator to $G_{aa}^{\rm ret}(R)$ in the form (10), we obtain

$$\begin{aligned} &\frac{1}{\varepsilon-iv\gamma}\left(1+\frac{1}{\varepsilon-iv\gamma}\varphi(R)+\frac{1}{(\varepsilon-iv\gamma)^2}\varphi^2(R)\right. \\ &+\frac{1}{(\varepsilon-iv\gamma)^3}\varphi^3(R)+\ldots+\frac{1}{(\varepsilon-iv\gamma)^2} \\ &\left.\times(iv)\frac{\partial\varphi(R)}{\partial R}+\ldots\right)G_{aa}^{\rm ret}(R). \end{aligned} \tag{12}$$

Further, we can assume that

$$\left|v\frac{\partial\ln\varphi}{\partial R}\right|\ll|\varphi(R)|. \tag{13}$$

The requirement (13) is actually equivalent to the semiclassical approximation. In this case, we can write

$$\frac{1}{(\varepsilon-iv\gamma)-iv\dfrac{\partial}{\partial R}}G_{aa}^{\rm ret}(R)\approx\frac{1}{\varepsilon-iv\gamma-\varphi(R)}G_{aa}^{\rm ret}(R). \tag{14}$$

Alternatively, returning to Eq. (8), we obtain

$$\begin{aligned} \varphi(R)-\varepsilon_a(R)=-\lambda^2(R)&\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\} \\ &\times\frac{\Delta(\varepsilon)}{\varepsilon-\varphi(R)-iv\gamma} \quad (R<0). \end{aligned} \tag{15}$$

In a number of studies (see, for example Ref. 14), a solution has been sought in a form analogous to (10). However, because of an incorrect asymptotic expansion, this led to the result[14,15]

$$\varphi(R)-\varepsilon_a(R)=-\lambda^2(R)\int_{E_1}^{E_2}\frac{d\varepsilon\Delta(\varepsilon)}{\varepsilon-\varphi(R)}. \tag{16}$$

Despite the apparent identity with (15), these equations are different. Even if in (15) we ignore the term $-iv\gamma$ describing nonadiabatic transitions in the denominator, the difference between (15) and (16) will be significant. The difference is that Eq. (16), in contrast to (15), cannot have solutions with nonzero imaginary part. This can be readily verified by direct substitution of $\varphi(R)$ in the form $\Omega(R)-i\Gamma(R)$, which gives

$$-\Gamma(R)=\Gamma(R)\lambda^2(R)\int_{E_1}^{E_2}\frac{d\varepsilon\Delta(\varepsilon)}{(\varepsilon-\Omega(R))^2+\Gamma^2(R)}. \tag{17}$$

It is readily seen that the only possible solution of (17) is $\Gamma(R)=0$.

Thus, the incorrect asymptotic expansion in Refs. 14 and 15 simply violated the theory of quasiresonance.

It is now necessary for us to solve Eq. (6) in the region $R>0$. In this case, after similar manipulations, we obtain

$$\begin{aligned}iv\frac{\partial}{\partial R}G_{aa}^{\rm ret}(R)-\varepsilon_a(R)G_{aa}^{\rm ret}(R)&\\ =-\lambda^2(R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}&\\ \times\frac{\Delta(\varepsilon)}{\varepsilon-\varphi(R)+iv\gamma}G_{aa}^{\rm ret}(R)-2iv\gamma\lambda(R)&\\ \times\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}&\\ \times\exp\left(-\frac{i}{v}R\varepsilon\right)\frac{\Delta(\varepsilon)}{(\varepsilon-\varphi(0))^2+v^2\gamma^2}G_{aa}^{\rm ret}(0).&\end{aligned} \tag{18}$$

For the subsequent considerations, the following property of the Green's function is important:

$$\begin{aligned}G_{aa}^{\rm ret}(R,R_0)&=\exp\left\{-\frac{i}{v}\int_{R_0}^{R}d\xi\varphi(\xi,R_0)\right\}\\ &=\exp\left\{-\frac{i}{v}\int_{R_0}^{x}d\xi\varphi(\xi,R_0)\right\}\\ &\quad\times\exp\left\{-\frac{i}{v}\int_{x}^{R}d\xi\varphi(\xi,R_0)\right\}\\ &=G_{aa}^{\rm ret}(x,R_0)\tilde{G}_{R_0}(R,x),\end{aligned} \tag{19}$$

where

$$\tilde{G}_{R_0}(R,x)=\exp\left\{-\frac{i}{v}\int_{x}^{R}d\xi\varphi(\xi,R_0)\right\}$$

is actually the S matrix.

We denote

$$\tilde{G}(R,x)=\lim_{R_0\to-\infty}\tilde{G}_{R_0}(R,x). \tag{20}$$

Then, dividing the left- and right-hand sides of (18) by $G_{aa}^{\rm ret}(R)$, we obtain

$$\begin{aligned}iv\frac{1}{\tilde{G}(R,0)}\frac{\partial\tilde{G}(R,0)}{\partial R}-\varepsilon_a(R)&\\ =J(\varphi(R),R)+\frac{1}{\tilde{G}(R,0)}f(\varphi(0),R),&\end{aligned} \tag{21}$$

where

$$\begin{aligned}J(\varphi(R),R)=-\lambda^2(R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon\right.&\\ \left.+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}\frac{\Delta(\varepsilon)}{\varepsilon-\varphi(R)+iv\gamma},&\end{aligned} \tag{22}$$

$$\begin{aligned}f(\varphi(0),R)=-2iv\gamma\lambda(R)\frac{1}{\tilde{G}(R,0)}\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon\right.&\\ \left.+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}\exp\left(-\frac{i}{v}R\varepsilon\right)&\\ \times\frac{\Delta(\varepsilon)}{(\varepsilon-\varphi(0))^2+v^2\gamma^2}.&\end{aligned} \tag{23}$$

We consider the structure of this equation: $\varepsilon_a(R)$ and $J(\varphi(R),R)$ are slowly varying functions compared with $(1/\tilde{G}(R,0))f(\varphi(0),R)$, which contains rapidly oscillating factors. In addition, $(1/\tilde{G}(R,0))f(\varphi(0),R)$ is small. It is then sensible to seek a solution of (21) in the form

$$\tilde{G}(R,0)=\tilde{G}_1(R,0)+\tilde{G}_2(R,0), \tag{24}$$

where $\tilde{G}_1(R,0)$ again owes its appearance to the slow term and $\tilde{G}_2(R,0)$ to the fast one. In addition, $|\tilde{G}_2(R,0)|\ll|\tilde{G}_1(R,0)|$ because f is small. Then

$$\frac{1}{\tilde{G}_1(R,0)+\tilde{G}_2(R,0)}\approx\frac{1}{\tilde{G}_1(R,0)}. \tag{25}$$

As a result, we have

$$\begin{aligned}iv\frac{1}{\tilde{G}_1(R,0)}\left(\frac{\partial\tilde{G}_1(R,0)}{\partial R}+\frac{\partial\tilde{G}_2(R,0)}{\partial R}\right)-\varepsilon_a(R)&\\ =J(\varphi(R),R)+\frac{1}{\tilde{G}_1(R,0)}f(\varphi(0),R).&\end{aligned} \tag{26}$$

Thus, we assume that the function $iv(1/\tilde{G}_1(R,0))(\partial\tilde{G}_1(R,0)/\partial R)$ is slow and that $iv(1/\tilde{G}_1(R,0))(\partial\tilde{G}_2(R,0)/\partial R)$ is a fast function. Assuming mutual cancellation of the fast and slow terms of Eq. (26), we obtain

$$\begin{cases}\dfrac{\partial\tilde{G}_2(R,0)}{\partial R}=-\dfrac{i}{v}f(\varphi(0),R),\\ iv\dfrac{\partial\ln\tilde{G}_1(R,0)}{\partial R}-\varepsilon_a(R)=J(\varphi(R),R).\end{cases} \tag{27}$$

We shall seek $\tilde{G}_1(R,0)$ in the form

$$\tilde{G}_1(R,0)=C\exp\left\{-\frac{i}{v}\int_0^R d\xi\varphi_0(\xi)\right\}, \tag{28}$$

where $C=\text{const}_R$. Then in place of (27) we can write to asymptotic accuracy

$$\begin{cases}\varphi_0(R)-\varepsilon_a(R)=J(\varphi_0(R),R),\\ \tilde{G}_2(R,0)=-\dfrac{i}{v}\displaystyle\int_0^R d\xi f(\varphi_0(0),\xi)+B,\end{cases} \tag{29}$$

where $B=\text{const}_R$. As a result,

$$\tilde{G}(R,0)=C\exp\left\{-\frac{i}{v}\int_0^R d\xi\varphi_0(\xi)\right\}$$
$$-\frac{i}{v}\int_0^R d\xi f(\varphi_0(0),\xi)+B. \tag{30}$$

The constants C and B can be determined from the equation $C+B=1$. The second equation for C and B is replaced by the condition $|\tilde{G}_2(R,0)|\ll|\tilde{G}_1(R,0)|$, which we used in the derivation of (30).

As a result, we obtain for $R>0$, remembering that $G_{aa}^{\text{ret}}(R)=\tilde{G}(R,0)G_{aa}^{\text{ret}}(0)$,

$$G_{aa}^{\text{ret}}(R)$$
$$=-i\exp\left\{-\frac{i}{v}\int_{-\infty}^0 d\xi\varphi(\xi)\right\}$$
$$\times\left\{C\exp\left(-\frac{i}{v}\int_{-\infty}^R d\xi\varphi_0(\xi)\right)-2iv\gamma\lambda(R)\right.$$
$$\times\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}\exp\left(-\frac{i}{v}R\varepsilon\right)$$
$$\left.\times\frac{\Delta(\varepsilon)}{((\varepsilon-\varphi_0(0))^2+v^2\gamma^2)(\varepsilon-iv\gamma)}\right\}, \tag{31}$$

where

$$C=1+2iv\gamma\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}$$
$$\times\frac{\Delta(\varepsilon)}{((\varepsilon-\varphi_0(0))^2+v^2\gamma^2)(\varepsilon-iv\gamma)}.$$

We see that the expression (31) contains a term describing the effect of the "Bragg-reflected wave" (the second term in the braces).

To describe the effects due explicitly to the fact that the band is finite, we consider the case when the band is empty. In this case,

$$n(+\infty)=n(-\infty)|G_{aa}^{\text{ret}}(+\infty)|^2. \tag{32}$$

In the limit $R\to+\infty$, the second term in the braces in (31) vanishes:

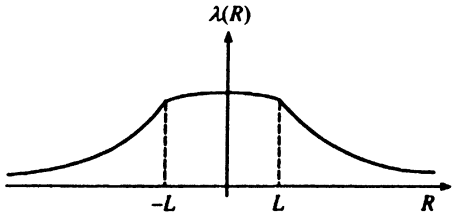

FIG. 2. The dependence $\lambda(R)$.

$$G_{aa}^{\text{ret}}(+\infty)=-iC\exp\left\{-\frac{i}{v}\int_{-\infty}^0 d\xi\varphi(\xi)\right.$$
$$\left.-\frac{i}{v}\int_0^{+\infty}d\xi\varphi_0(\xi)\right\}. \tag{33}$$

Thus, we will not observe any qualitative contributions to the final charge state from interference effects. This is due to the absence of an interval on which the system evolves adiabatically and, as a consequence, to instability of the phase relationships. As a result, the picture of the formation of the final charge state will be the same as if the state decayed exponentially in all intervals.

Thus, in the case $\lambda(R)=\exp(-\gamma|R|)$ considered above we have not obtained the nonmonotonic (in the general case oscillatory) dependence of $n(+\infty)$ on $1/v$ characteristic of the experimental data. This failure can be attributed to the absence of intervals of adiabatic evolution for the system. It is therefore most probable that in practice a different case is realized, a model of which we consider in the following section.

3. ASYMPTOTICALLY EXACT SOLUTION FOR THE CASE OF AN INTERACTION HAVING AN INTERVAL OF ADIABATIC EVOLUTION

We shall be interested in the case in which $\lambda(R)$ has the following form (Fig. 2). In the general case, a dependence of this type can be expressed as follows: $\lambda(R)$ decreases exponentially from the points $-L$ and L, while on the interval $[-L,L]$ we have a function that varies slowly compared with the characteristic time of the problem. Thus, we wish to consider a problem that differs from the one considered in Ref. 13 through the presence of exponential decays in the switching on and off of the hybridization. In other words, we shall be interested in the consequences of taking into account exponential intervals in which the hybridization is switched on and off possessing a portion whose characteristic time of variation is much greater than the characteristic times of the system. To consider such a system, we adopt the following model dependence of the hybridization behavior, namely, that on the interval $(-\infty, L)$ the exponential switching-on law is $\exp(\gamma(R+L))$, on the interval $(L, +\infty)$ the switching-off law is $\exp(-\gamma(R-L))$, while on the section $[-L, L]$ we have a certain $\lambda_0(R)$ that can be regarded as slow compared with the characteristic times of the problem, i.e.,

$$\left|\frac{d\lambda_0(R)}{\partial R}\frac{v}{\Delta E}\right|<|\lambda_0(R)|,$$

where $\Delta E=E_2-E_1$:

$$\lambda(R)=\begin{cases}\exp(\gamma(R+L)), & R<-L\\ \lambda_0(R), & -L<R<L.\\ \exp(-\gamma(R-L)), & R>L\end{cases} \tag{34}$$

In this case, the solution to the problem is similar in its general features to the one given in Sec. 1. As a result, we obtain for the function the expression

$$G_{aa}^{\rm ret}(+\infty)=A\exp\left\{-\frac{i}{v}\int_{-\infty}^{+\infty}d\xi\varphi_0(\xi)\right\}$$
$$+i(v\gamma)^2\exp\left\{-\frac{i}{v}\int_{-\infty}^{-L}d\xi\varphi_0(\xi)\right\}$$
$$\times\exp\left\{-\frac{i}{v}\int_{L}^{+\infty}d\xi\varphi_0(\xi)\right\}$$
$$\times\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_1}^{E_1-i\infty}d\varepsilon\right\}\exp\left\{-\frac{i}{v}\varepsilon 2L\right\}\Delta(\varepsilon)$$
$$\times\left\{\frac{1}{\varepsilon(\varepsilon-iv\gamma)(\varepsilon-\varphi_0(-L))(\varepsilon-\varphi_0(-L)-iv\gamma)}\right.$$
$$\left.-\frac{K}{\varepsilon(\varepsilon-\varphi_0(-L))(\varepsilon-\varphi_0(-L)-iv\gamma)}\right\}. \tag{35}$$

where

$$A=-i(1+iv\gamma K)\left(1+iv\gamma\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon\right.\right.$$
$$\left.\left.+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}\frac{\Delta(\varepsilon)}{\varepsilon(\varepsilon-\varphi_0(-L))(\varepsilon-\varphi_0(-L)-iv\gamma)}\right).$$
$$K=\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}$$
$$\times\frac{\Delta(\varepsilon)}{(\varepsilon-iv\gamma)(\varepsilon-\varphi_0(-L))(\varepsilon-\varphi_0(L)-iv\gamma)},$$

while φ_0 satisfies the equations

$$\varphi_0(R)-\varepsilon_a(R)=-\lambda^2(R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}$$
$$\times\frac{\Delta(\varepsilon)}{\varepsilon-\varphi_0(R)-iv\gamma},\quad R<L,$$
$$\varphi_0(R)-\varepsilon_a(R)=-\lambda^2(R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}$$
$$\times\frac{\Delta(\varepsilon)}{\varepsilon-\varphi_0(R)},\quad -L<R<L,$$
$$\varphi_0(R)-\varepsilon_a(R)=-\lambda^2(R)\left\{\int_{E_1}^{E_1-i\infty}d\varepsilon+\int_{E_2-i\infty}^{E_2}d\varepsilon\right\}$$
$$\times\frac{\Delta(\varepsilon)}{\varepsilon-\varphi_0(R)+iv\gamma},\quad R>L. \tag{36}$$

The result (35) can be represented in the form

$$G_{aa}^{\rm ret}(+\infty)=A(v)\exp\left\{-\frac{i}{v}\int_{-\infty}^{+\infty}d\xi\varphi_0(\xi)\right\}+i(v\gamma)^2f_1(v)$$
$$\times\exp\left\{-\frac{i}{v}\int_{-\infty}^{-L}d\xi\varphi_0(\xi)\right\}\exp\left\{-\frac{i}{v}E_1 2L\right\}$$
$$\times\exp\left\{-\frac{i}{v}\int_{L}^{+\infty}d\xi\varphi_0(\xi)\right\}+i(v\gamma)^2f_2(v)$$
$$\times\exp\left\{-\frac{i}{v}\int_{-\infty}^{-L}d\xi\varphi_0(\xi)\right\}\exp\left\{-\frac{i}{v}E_2 2L\right\}$$
$$\times\exp\left\{-\frac{i}{v}\int_{L}^{+\infty}d\xi\varphi_0(\xi)\right\}. \tag{37}$$

The difference between (37) and (33) consists in the appearance of the two additional terms describing the contribution of the reflected wave. They owe their appearance to the presence of the interval of length $2L$ on which the hybridization varies adiabatically.

Thus, the final charge state in the case of interaction with the unfilled band of surface states (32) will be the result of the interference of two waves, one spreading out from the atomic center and the other converging on the center, corresponding to the different terms of the expression (37).

4. QUALITATIVE ANALYSIS OF THE RESULTS

We discuss the result (37). We shall continue to consider charge exchange for the case of an empty (or completely filled) band of electron surface states. We consider qualitatively the two most instructive cases.

The first case we consider arises when the atomic level is either originally opposite the band of forbidden surface states or, as a result of interaction, is expelled outside the band limits and becomes infinitesimally narrow (we assume, for simplicity, that there exists a unique solution φ_0 describing the state genetically related to ε_a). In this case, the first term in the expression (37) is large compared with the two other terms because it describes a stationary state. As a result, we obtain for $n(+\infty)$ as a function of $1/v$ an expression that contains terms oscillating at all possible frequency combinations $2LE_1$, $2LE_2$, and $2L\varphi_0(R\in 2L)$; the terms containing $2L\varphi_0(R\in 2L)$ will, in accordance with what was said above, have the greatest amplitude. If $\varphi_0(R\in 2L)$ is near one of the band edges, for example, $E_1(E_1-\varphi_0(R\in 2L)\ll E_2-E_1)$, then we shall observe in the dependence of $n(+\infty)$ on $1/v$ the presence of components with two different frequencies: a low-frequency component $2L(E_1-\varphi_0(R\in 2L))$ with large amplitude and a high-frequency component $2L(E_2-\varphi_0(R\in 2L))$ with small amplitude (Fig. 3) [the term oscillating at the frequency $2L(E_2-E_1)$ is much smaller than the first two and differs little in frequency from the second].

The next characteristic case that we consider arises when the atomic level lies opposite the band of electron surface states. We shall assume that for all R it is very far from its edges. In this case, the amplitudes $f_1(v)$ and $f_2(v)$ of the second and third terms in the expression (37) are extremely small, and so we can ignore in (37) all the terms except for

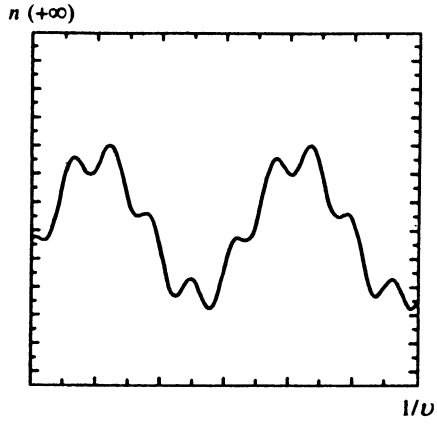

FIG. 3.

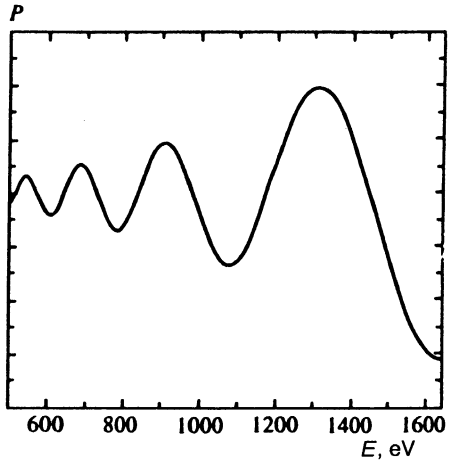

FIG. 5. Theoretical energy dependence of the probability of preserving the $^4He^+$ charge state in the scattering of $^4He^+$ ions by Ge.

the first. As a result we obtain a purely exponential dependence of $n(+\infty)$ on $1/v$ (Fig. 4), as indeed is typical for the case of a broad band.

Note that, in the qualitative analysis of the result given above, we have for simplicity effectively ignored the dependence of the amplitudes of the terms that occur in the expression (37) on v. We shall consider the exact results that follow from the expression (37) for a number of cases in the following section.

5. ANALYSIS OF EXPERIMENTAL DATA

Our results enable us to explain a broad range of experimental data. We consider the two most striking examples. The first is the experiment on the scattering of $^4He^+$ ions by Ge.[16] In this case, we have interaction with a very narrow filled $3d$ band of Ge (33 eV from the vacuum level). The vacant $1s$ level of He^+ is at a depth 24.5 eV. The dependence of the probability preserving of the charge state of the $^4He^+$ ions as a function of the energy of the projectile particles that follows from the asymptotically exact solution obtained in Sec. 2 is shown in Fig. 5. As follows from the results of the qualitative discussion in Sec. 3, in this case we observe oscillations at frequencies proportional to the distance between the state into which the $1s$ state of He^+ is transformed as a result of the interaction (with energy $\alpha \approx 25$ eV) and the edges E_1 and E_2 of the $3d$ band of Ge. However, these frequencies, proportional to $|\alpha - E_1|$ and $|\alpha - E_2|$, are very close to each other because of the narrowness of the $3d$ band, and they are indistinguishable in the experiment. The oscillations at the lower frequency, proportional to $|E_1 - E_2|$, have a very small amplitude and are therefore effectively unobservable. In the following figure, we give experimental data that, besides the charge-exchange probability, are proportional to the scattering cross section, which is the reason for the suppression at high energies (Fig. 6).

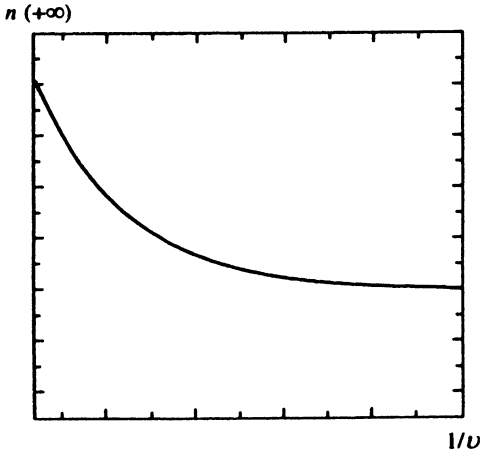

FIG. 4.

The next example is associated with Ref. 5, in which a study was made of the change in the charge state of N^+ ions in the case of scattering from the surface of NaCl crystals. The vacant $2p$ level (14.7 eV) lies opposite the filled $3p$ surface band of Cl near its lower edge E_1 ($E_1 - \varepsilon_a \approx 1$ eV). The band width is $E_1 - E_2 \approx 7$ eV. The theoretical calculation and the experimental results are shown in Fig. 7. In this case, we observe in the dependence of the yield of N^+ ions oscillations that differ appreciably in both frequency and amplitude (the high-frequency oscillations have smaller amplitude). This picture can be explained as follows: The level α, which is genetically related to ε_a is expelled as a result of the interaction outside the band (at the instant of saturation of the hybridization, by an amount of order 0.6 eV. As a result of this, we obtain low-frequency oscillations at the frequency $|\alpha - E_1|$ with large amplitude. The high-frequency contributions at the frequencies proportional to $|\alpha - E_2|$ and $|E_1 - E_2|$ are practically indistinguishable in their frequencies and have a small amplitude; however, in this case they have the same order of magnitude as the low-frequency contribution. It is just such a picture that we observe (Fig. 7).

In a similar way we can explain different experimental data on charge exchange in the case of the scattering of atomic particles by surfaces.

6. THE ROLE OF COULOMB CORRELATIONS IN THE CHARGE-EXCHANGE PROBLEM

The analysis made above of the time dependence of the occupancy of the atomic state is based on the assumption of

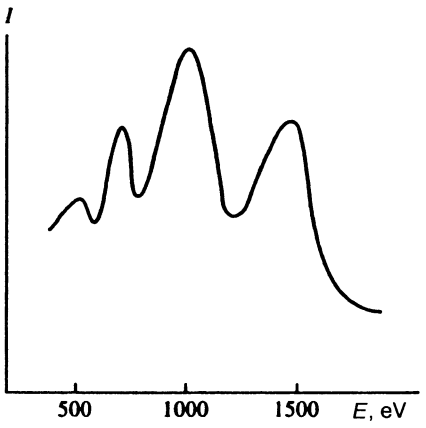

FIG. 6. Experimental dependence of the relative yield of $^4He^+$ ions on the energy of the initial beam.[16]

complete independence of the motion of electrons with different spin projections. It would appear that allowance within the framework of the Anderson–Newns model for the intra-atomic Coulomb interaction between valence electrons must significantly change the entire picture of electron transitions between the atomic and band states. In fact, the strong Coulomb repulsion at the atomic center, which is manifested in practice as a significant deviation of the electron affinity energy from the ionization energy of the atom, essentially implies that two electrons with opposite spin projections cannot be present simultaneously. Therefore, the motion of the electrons must be correlated in such a way that at each instant of time there is at the atomic center an electron either with spin up or spin down, or else there is no electron at all.

The extent to which these correlations affect the dynamics of the atomic occupancy in the process of charge exchange depends on several factors such as the relative position of the atomic level ε_a and the Fermi level of the band electrons, the characteristic time of the atom–surface interaction, the surface temperature, etc.

Thus, if the level ε_a is higher in energy than ε_F, then the role played by the Coulomb correlations is very weak. For in this case electron transitions from the band to the atomic level are relatively rare, and the appearance of two electrons at the center has a low probability even in the absence of interaction.

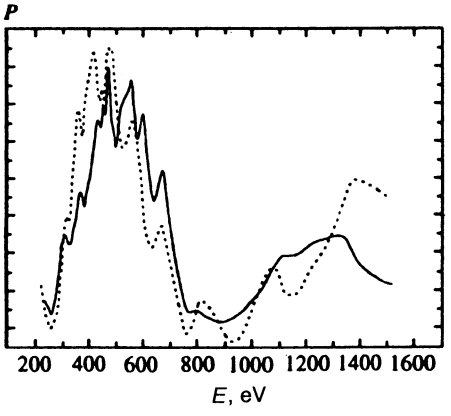

FIG. 7. Energy dependence of the relative yield of N^+ ions in the case of scattering by the surface of an NaCl crystal (the dashed curve is the result of the calculation, and the solid curve the result of the experiment of Ref. 5).

In the opposite case, when ε_a lies below the Fermi level of the system, the influence of the Coulomb correlations is appreciable. In this case, the impossibility of double occupation of the atomic center generates a strong rearrangement in the energy distribution of the band electrons, leading in the limit of a sufficiently long atom–surface interaction time to the formation of a narrow peak in the single-particle density of states at the energy corresponding to the Fermi energy of the system (Kondo resonance). As follows from the previous consideration, a narrow peak like this in the density of states could be an additional source of nonadiabaticity for charge exchange in the atomic-level–band system and, as a result of this, significantly change the nature of the time behavior of the atomic-state occupancy. Quantitative allowance for the effect of the Kondo resonance on the final occupancy of the scattered ion must be complicated and up to now has been done only by numerical methods for some limiting situations.[17] However, it should be noted that thermal fluctuations strongly disturb the correlated motion of the electrons, as a result of which the Kondo resonance disappears. Therefore, the effect of the Kondo resonance on the charge exchange is important only if the temperature of the target (in energy units) is less than the width of the Kondo peak; this is very difficult to achieve under the conditions of a real experiment.

At the same time, the effect of the strong intra-atomic repulsion does not reduce solely to the Kondo effect. To justify this statement, we consider a situation in which Kondo resonance does not occur at all because the Fermi level lies in the forbidden band of the spectrum, i.e., we consider the case when the atomic level interacts with a completely filled surface band.

In the approximation of an infinite Coulomb interaction at the atomic center, the Anderson–Newns Hamiltonian has the form

$$\hat{H}_\infty(R(t))=\hat{P}\hat{H}(R(t))\hat{P}, \tag{38}$$

where $\hat{H}(R(t))$ is the Hamiltonian of the noninteracting electrons (1), and $\hat{P}=1-\hat{n}_\uparrow\hat{n}_\downarrow$ is the projection operator onto the subspace of states with at most one electron per atom.

Note that when all the surface band states are occupied and it is impossible for there to be two electrons at the atomic center charge, exchange is possible only when the initial atomic state is empty. Under this assumption, we shall now calculate the probability that the final atomic state will be the empty state (P_0) or the single-electron state (P_1).

In our case, the wave function will have the simple form

$$\Psi(t)=b_0(t)|0\rangle|\Psi_b\rangle+\sum_{\mathbf{k},\sigma} b_{\mathbf{k},\sigma}(t)\hat{a}_\sigma^+\hat{c}_{\mathbf{k},\sigma}|0\rangle|\Psi_b\rangle, \tag{39}$$

where $|0\rangle$ is the vacuum state of the atomic electrons, and $|\Psi_b\rangle$ is the Slater determinant corresponding to a completely filled band of surface electron states.

Then the required probabilities are given by

$$P_0(+\infty)=|b_0(+\infty)|^2,$$

$$P_1(+\infty)=\sum_{\mathbf{k},\sigma}|b_{\mathbf{k},\sigma}(+\infty)|^2 \tag{40}$$

subject to the conditions $P_0(-\infty)=1$, $P_1(-\infty)=0$. Substitution of the wave function (39) in the Schrödinger equation leads to the following system of equations for the amplitudes b_0 and $b_{\mathbf{k}}$:

$$\begin{cases} i\dfrac{\partial b_0(t)}{\partial t}=\dfrac{\lambda(t)}{\sqrt{V}}\displaystyle\sum_{\mathbf{k},\sigma}V_{\mathbf{k}}b_{\mathbf{k},\sigma}(t), \\ i\dfrac{\partial b_{\mathbf{k},\sigma}(t)}{\partial t}=(\varepsilon_a-\varepsilon(\mathbf{k}))b_{\mathbf{k},\sigma}(t)+\dfrac{\lambda(t)}{\sqrt{V}}V_{\mathbf{k}}^*b_0(t). \end{cases} \tag{41}$$

Note that for our purposes there is no need to calculate all the amplitudes $b_{\mathbf{k},\sigma}$—it is sufficient to calculate just the amplitude b_0; then the probability P_1 of single-electron occupancy will be $1-|b_0|^2$. Expressing $b_{\mathbf{k},\sigma}$ in terms of b_0 in the system (41), we obtain the equation

$$i\frac{\partial b_0(t)}{\partial t}=-i2\lambda(t)\int_{-\infty}^{t}dt_1\lambda(t_1)\exp(-i\varepsilon_a(t-t_1)) \times\frac{1}{V}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\exp(i\varepsilon(\mathbf{k})(t-t_1))b_0(t_1). \tag{42}$$

Since at the moment we are not interested in the effects of the finiteness of the band spectrum, to solve Eq. (42) we can use the wide-band approximation. As a result, we obtain for the probabilities P_0 and P_1

$$P_0(+\infty)=\exp\left(-4\int_{-\infty}^{+\infty}dt_1\Gamma(t_1)\right),$$

$$P_1(+\infty)=1-\exp\left(-4\int_{-\infty}^{+\infty}dt_1\Gamma(t_1)\right), \tag{43}$$

where $\Gamma(t)=\pi N_0V_0^2\lambda^2(t)$ is the half-width of the resonance. The factor 4 in the argument of the exponential arises from the summation over the spins [the factor 2 in Eq. (42)] and the subsequent squaring of the amplitude. We now compare the expression (43) with the expression obtained in the case of noninteracting electrons. Using the same approximations, one can easily show that the probabilities P_0 and P_1 will have the form

$$P_0(+\infty)=\exp\left(-4\int_{-\infty}^{+\infty}dt_1\Gamma(t_1)\right),$$

$$P_1(+\infty)=2\exp\left(-2\int_{-\infty}^{+\infty}dt_1\Gamma(t_1)\right) \times\left(1-\exp\left(-2\int_{-\infty}^{+\infty}dt_1\Gamma(t_1)\right)\right). \tag{44}$$

It can be seen from this that the probability P_0 for the cases of infinitely strong interaction and the absence of interaction are the same, while the probabilities for P_1 for these cases are very different. The reason for this difference is essentially that the possibility of pair occupation of the center means that the noninteracting electrons "live" in a larger Hilbert state space than the strongly interacting electrons. Therefore, the probability P_1 is no longer equal to $1-P_0$.

To explain this circumstance, we return to the determination of the probabilities in terms of the electron-number operators at the center:

$$P_0=\langle(1-\hat{n}_\uparrow)(1-\hat{n}_\downarrow)\rangle,$$

$$P_1=\langle\hat{n}_\uparrow(1-\hat{n}_\downarrow)+\hat{n}_\downarrow(1-\hat{n}_\uparrow)\rangle,$$

$$P_2=(\hat{n}_\uparrow\hat{n}_\downarrow). \tag{45}$$

The impossibility of pair occupation of the center has the consequence that $P_2\equiv0$ holds at all times t. Therefore, the probabilities P_0 and P_1 depend linearly on the atomic occupancies $\langle\hat{n}_\uparrow\rangle$ and $\langle\hat{n}_\downarrow\rangle$:

$$P_0=1-(\langle\hat{n}_\downarrow\rangle+\langle\hat{n}_\uparrow\rangle),\quad P_1=\langle\hat{n}_\downarrow\rangle+\langle\hat{n}_\uparrow\rangle. \tag{46}$$

In the case of noninteracting electrons, the probability of pair occupation is no longer equal to zero; moreover, by virtue of the independence of the motion of electrons with different spin projections we have $P_2=\langle\hat{n}_\downarrow\hat{n}_\uparrow\rangle=\langle\hat{n}_\downarrow\rangle\langle\hat{n}_\uparrow\rangle$. Then for the probabilities P_0 and P_1 we have ($\langle\hat{n}_\uparrow\rangle=\langle\hat{n}_\downarrow\rangle=\langle\hat{n}_\sigma\rangle$):

$$P_0=(1-\langle\hat{n}_\sigma\rangle)^2,\quad P_1=2\langle\hat{n}_\sigma\rangle(1-\langle\hat{n}_\sigma\rangle). \tag{47}$$

Thus, $P_0+P_1\neq1$ holds, although the sum of the probabilities over the complete set of states is, as before, equal to unity ($P_0+P_1+P_2=1$).

It also follows from the expressions (43), (44), (46), and (47) that the time dependence of the occupancies $\langle\hat{n}_\sigma\rangle$ in these two limiting cases is different:

$$\langle\hat{n}_\sigma\rangle_{\text{int}}=\frac{1-\exp(-4\int_{-\infty}^{t}dt_1\Gamma(t_1))}{2},$$

$$\langle\hat{n}_\sigma\rangle_{\text{free}}=1-\exp\left(-2\int_{-\infty}^{t}dt_1\Gamma(t_1)\right). \tag{48}$$

Therefore, the strong interaction leads to a change in the rate of exponential decay of the atomic state.

In the case of a finite band spectrum, the effect of correlations on the behavior in time of the charge-exchange probability is not so obvious. In particular, one can no longer assert that the probability P_0 will have the same form for interacting and noninteracting electrons. Detailed understanding of this question requires further investigations.

7. CONCLUSIONS

This paper contains asymptotically exact solutions to the problem of charge exchange between a local level corresponding to a projectile atom and a finite continuous spectrum corresponding to a band of allowed crystal states. It is clear from our analysis that if oscillations are to appear in the energy distribution of the scattered atomic particles there must be an interval on which the hybridization of the local state and the band states varies adiabatically. In this case, during the interval on which the hybridization varies adiabtically stable phase relationships between the electron wave function at the atomic level and the Bragg-reflected wave arise, and this allows a stable interference picture to develop.

The subsequent nonadiabatic switching off of the hybridization leads to conservation of the interference contribution to the amplitude of the final electron state at the local atomic level. This is the reason for the nonmonotonicity of the energy dependence of the charge-exchange probability of the scattered atomic particles. Moreover, one observes in the spectrum all possible combinations of the frequencies proportional to the difference of the energies of the band energies and the energy of the quasistationary state in the section of adiabatic variation. The amplitudes of the corresponding oscillatory contributions are greater the higher the degree of nonadiabaticity of the switching-on and switching-off processes. The amplitudes of the oscillating contributions are also related to the form of the Van Hove singularities at the band edges and the distance from the quasistationary state to the band edges.

Thus, only the model time dependence of the hybridization with an interval of adiabatic variation and nonadiabatic switching-on and switching-off tails makes it possible to describe adequately the oscillatory energy spectrum of the scattered atomic particles.

The investigation of the effect of the intraatomic Coulomb interaction of the electrons on the charge exchange showed that this interaction leads in general to a change in the rate of charge exchange. However, detailed understanding of the role of Coulomb correlations in charge-exchange processes requires further investigations.

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