Induced Charge Generated by Potential Well in Transition Metal Dichalcogenides

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Abstract—We investigate the asymptotic behavior of the charge density $\rho_{ind}(\mathbf{r})$ induced by an azimuthally symmetric potential well of finite radius R. The analytic expression for $\rho_{ind}(\mathbf{r})$ at the distances $r \gg R$ is obtained. It is shown that, for a wide range of potential parameters, the induced charge density can be represented as $\rho_{ind}(\mathbf{r}) = F(r)\mathcal{L}_V$, where $F(r)$ depends only on distance and $\mathcal{L}_V$ depends on the parameters of the potential. We also investigate the behavior of the induced charge density when the potential well depth close to the critical value.

1. INTRODUCTION

It is well known that the external field leads to the appearance of polarization effects in the material. For example, in the impurity field, the induced charge density $\rho_{ind}(\mathbf{r})$ arises; the external magnetic field induces the current and can also lead to the appearance of the Aharonov−Bohm effect. Such phenomena can be described as vacuum polarization effects, i.e., the polarization of the ground state of the system. Vacuum polarization effects arise in various systems. In the quantum electrodynamics, the charge density induced by the Coulomb field of the nucleus is considered [1−4]. The charge density induced by the field of the Coulomb impurity in graphene was considered in [5−16]. The induced charge density in graphene in the case of a localized potential was studied in detail in [17].

In the present paper, we study the behavior of the charge density induced by a localized potential in two-dimensional transition metal dichalcogenides (TMDs). These materials are the so-called graphene-like or Dirac materials, since the motion of charged single-particle excitations of the electron gas are described by the $(2 + 1)$-dimensional Dirac equation [18]. Note that the dimensionless coupling constant between electrons (analogous to the fine structure constant) is not small in the TMDs, so some variant of $(2+1)$-dimensional quantum electrodynamics with strong interaction is achieved in the TMDs. In addition, in experiments it is possible to create various external fields, including quite strong ones. Therefore, the study of the effects of vacuum polarization by external fields in the TMDs also allows one to study nonperturbative effects similar to the effects of quantum electrodynamics, for example, the electronpositron pair creation by a strong field and the Klein paradox.

In two-dimensional Dirac materials, the charge density induced by the Coulomb field, as well as nonperturbative effects, were considered in [19, 20]. We consider the charge density $\rho_{ind}(\mathbf{r})$ induced by an axially symmetric potential well of the depth U and the characteristic radius R. We calculate the function $\rho_{ind}(\mathbf{r})$ analytically at the distances $r \gg R$ for the various values of the band gap and potential depth. To calculate the asymptotics, we use Green's function method for the electron in the external field, developed in [21]. We show that, in the wide range of the potential parameters, the induced charge density can be represented as $\rho_{ind}(\mathbf{r}) = F(r)\mathcal{L}_V$, where the coefficient $\mathcal{L}_V$ depends on the shape of the potential and does not depend on the distance r, while the function $F(r)$ does not depend on the potential.

The paper is organized as follows. In Section 2 we derive the general expression for the induced charge density. In Section 3 we obtain the equation for Green's function. In Section 4 the wave functions and the behavior of energy levels for bound states of the electron in the potential well are considered. In Section 5 we calculate the asymptotics of the induced charge density. In the Conclusions, we discuss the results.
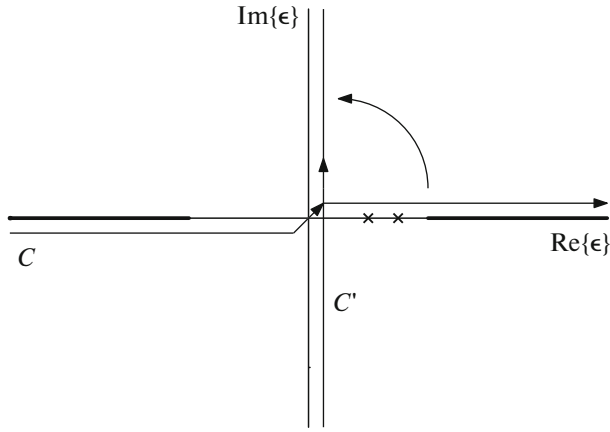
Fig. 1. Analytic properties of Green's function of ϵ and integration contour. The cuts and the poles are shown as thick lines and crosses, respectively.

2. GENERAL DISCUSSION

The charge density induced by the potential $V(r)$ can be presented in the following form:

$$\rho_{\text{ind}}(\mathbf{r}) = -ieN \int_C \frac{d\epsilon}{2\pi} \text{Tr}\{G(\mathbf{r},\mathbf{r}|\epsilon)\}, \tag{1}$$

where e is the electron charge, the coefficient $N = 4$ reflects the spin degeneracy and valley degeneracy in TMDs, and Green's function $G(\mathbf{r},\ \mathbf{r}'|\epsilon)$ satisfies the equation [18]

$$[\epsilon - V(r) - v_F \boldsymbol{\sigma} \cdot \mathbf{p} - \Delta\sigma_z]G(\mathbf{r},\mathbf{r}'|\epsilon) = \delta(\mathbf{r} - \mathbf{r}'). \tag{2}$$

Here $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$, σ_a are the Pauli sigma matrices, $\mathbf{p} = -i\hbar(\partial/\partial x, \partial/\partial y)$ is the momentum operator, and Δ is the half of the band gap, v_F is the dimensional constant of the rate. The sigma matrices correspond to the pseudospin degrees of freedom. Since the spin–orbit interaction constant is small [18], we omit the term related to it in Eq. (2). We consider the potentials $V(r)$ that go to zero fast enough at the distances R; i.e., $V(r) \approx 0$ at $r \gg R$. Below we set $\hbar = v_F = 1$. The Green's function of the electron in the field of the potential well has cuts and poles corresponding to the states of the continuous spectrum and bound states of the electron, respectively. In Fig. 1 we show schematically the cuts and the poles of Green's function. The thick lines and crosses correspond to the cuts and poles, respectively. The cuts are located on the real axis in the intervals $(-\infty, -\Delta]$ and $[\Delta, \infty)$. The poles located in the interval $(-\Delta, \Delta)$. The contour of integration over C goes below the real axis in the left half-plane and above real axis in the right half-plane; it crosses the real axis between the left cut of Green's function and the pole that corresponds to the bound state with the lowest energy (see Fig. 1). Such a choice of the integration contour means that all states with energies $\epsilon \leq -\Delta$ are occupied. Using the analytical properties of Green's

function, we deform the contour of integration over ϵ so that it coincides with the imaginary axis, perform the change of variables $\epsilon \to i\epsilon$, and obtain

$$\rho_{\text{ind}}(\mathbf{r}) = \tilde{\rho}(\mathbf{r}) - eN \sum_{\epsilon_n < 0} |\psi_n(\mathbf{r})|^2, \tag{3}$$

where

$$\tilde{\rho}(\mathbf{r}) = eN \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \text{Tr}\{G(\mathbf{r},\mathbf{r}\mid i\epsilon)\}, \tag{4}$$

$\psi_n(\mathbf{r})$ is the wave function of the electrons with the energy $\epsilon_n < 0$. Therefore, to calculate the induced charge density, it is necessary to find Green's function and the wave functions of the bound states.

To find the asymptotics of the induced charge density at distances $r \gg R$, it is convenient to represent the equation for Green's function in the following form [21]:

$$
\begin{aligned}
G(r,r' \mid i\epsilon) &= G^{(0)}(r,r' \mid i\epsilon) \\
&+ \int d\mathbf{r}_1 d\mathbf{r}_2 G^{(0)}(\mathbf{r},\mathbf{r}' \mid i\epsilon)[V(r_1)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\
&+ V(r_1)G(\mathbf{r}_1,\mathbf{r}_2 \mid i\epsilon)V(r_2)]G^{(0)}(\mathbf{r}_2,\mathbf{r}' \mid i\epsilon),
\end{aligned}
\tag{5}
$$

where $G^{(0)}(\mathbf{r}, \mathbf{r}'|i\epsilon)$ is the solution of Eq. (2) in the case $V(r) = 0$. In Eq. (5), the scales of distances r and R are separated, because on the right-hand side of the equation only the function $G^{(0)}$ depends on r, while the arguments $\mathbf{r}_1$ and $\mathbf{r}_2$ of the functions G are localized on the scale R; i.e., $r_{1,2} \sim R$, because the potential $V(r)$ is nonzero at the distances $r \sim R$. This separation of scales allows us to calculate the asymptotics of the induced charge density [21].

Using Eqs. (4), (5), we represent $\tilde{\rho}(\mathbf{r})$ in the form

$$\tilde{\rho}(\mathbf{r}) = \tilde{\rho}^{(1)}(\mathbf{r}) + \tilde{\rho}^{(2)}(\mathbf{r}). \tag{6}$$

Here, $\tilde{\rho}^{(1)}(\mathbf{r})$ is the linear in the potential $V(r)$ contribution and $\tilde{\rho}^{(2)}(\mathbf{r})$ is the contribution of higher orders in the potential:

$$
\begin{aligned}
&\tilde{\rho}^{(1)}(\mathbf{r}) \\
&= eN \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \int d\mathbf{r}_1 \text{Tr}\{G^{(0)}(\mathbf{r},\mathbf{r}_1 \mid i\epsilon)V(r_1)G^{(0)}(\mathbf{r}_1,\mathbf{r} \mid i\epsilon)\},
\end{aligned}
\tag{7}
$$

$$
\begin{aligned}
\tilde{\rho}^{(2)}(\mathbf{r}) &= eN \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \int d\mathbf{r}_1 d\mathbf{r}_2 \text{Tr}\{G^{(0)}(\mathbf{r},\mathbf{r}_1 \mid i\epsilon) \\
&\times V(r_1)G(\mathbf{r}_1,\mathbf{r}_2 \mid i\epsilon)V(r_2)G^{(0)}(\mathbf{r}_2,\mathbf{r} \mid i\epsilon)\}.
\end{aligned}
\tag{8}
$$

Thus, it is necessary to calculate the functions $G^{(0)}(\mathbf{r}, \mathbf{r}'|i\epsilon)$ and $G(\mathbf{r}, \mathbf{r}'|i\epsilon)$.

3. GREEN'S FUNCTION IN A POTENTIAL WELL

The solution of (2) in the case $V(r) = 0$ has the form

$$G^{(0)}(\mathbf{r}, \mathbf{r}' \mid \epsilon)$$
$$= -\frac{i}{2\pi}\left[(\epsilon - i\sigma_z\Delta)K_0(\kappa\rho) + \kappa\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\rho}}{\rho}K_1(\kappa\rho)\right], \quad (9)$$

where $\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}'$, $\kappa = \sqrt{\epsilon^2 + \Delta^2}$, $K_a(b)$ is the Macdonald function.

For an azimuthally symmetric potential well, it is convenient to represent Green's function in the form

$$G(\mathbf{r}, \mathbf{r}' \mid \epsilon) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}e^{im(\phi-\phi')}$$
$$\times\begin{pmatrix} \mathcal{A}_m^{(\Delta)}(r,r'\mid\epsilon) & -ie^{-i\phi'}\mathcal{B}_m^{(\Delta)}(r,r'\mid\epsilon) \\ ie^{i\phi}\mathcal{C}_m^{(\Delta)}(r,r'\mid\epsilon) & ie^{i(\phi-\phi')}\mathcal{D}_m^{(\Delta)}(r,r'\mid\epsilon) \end{pmatrix}. \quad (10)$$

We substitute this representation in Eq. (2), take into account the following representation for the δ function

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{\delta(r-r')}{2\pi\sqrt{rr'}}\sum_{m=-\infty}^{\infty}e^{im(\phi-\phi')}, \quad (11)$$

and obtain:

$$(\epsilon - V(r) - \Delta)\mathcal{A}_m^{(\Delta)} - \frac{\partial\mathcal{C}_m^{(\Delta)}}{\partial r} - \frac{m+1}{r}\mathcal{C}_m^{(\Delta)} = \frac{\delta(r-r')}{\sqrt{rr'}},$$
$$(\epsilon - V(r) + \Delta)\mathcal{C}_m^{(\Delta)} + \frac{\partial\mathcal{A}_m^{(\Delta)}}{\partial r} - \frac{m}{r}\mathcal{A}_m^{(\Delta)} = 0. \quad (12)$$

Functions $\mathcal{D}_m^{(\Delta)}$ and $\mathcal{B}_m^{(\Delta)}$ can be expressed through $\mathcal{A}_m^{(\Delta)}$ and $\mathcal{C}_m^{(\Delta)}$ as follows:

$$\mathcal{D}_m^{(\Delta)} = \mathcal{A}_{-m-1}^{(-\Delta)}, \quad \mathcal{B}_m^{(\Delta)} = -\mathcal{C}_{-m-1}^{(-\Delta)}. \quad (13)$$

Therefore, to calculate Green's function, it is necessary to solve two equations (12).

4. ELECTRON WAVE FUNCTION IN THE POTENTIAL WELL

To calculate the induced charge density, it is necessary to find the wave function for the electron $\psi_n(\mathbf{r})$ in the potential well (see (3)). The equation for the wave function has the form [18]

$$[\epsilon - V(r) - \boldsymbol{\sigma}\cdot\mathbf{p} - \Delta\sigma_z]\psi(\mathbf{r}) = 0. \quad (14)$$

The wave function and the spectrum depend on the specific shape of the potential. Let us consider in detail the solutions in the case of a potential well:

$$V(r) = -U\theta(R - r), \quad (15)$$

where $\theta(x)$ is the Heaviside step function; R and U are the radius and depth of the potential well. The wave functions for the potential are known; see e.g., [22]. The substitution of the wave function in the form

$$\psi_n(\mathbf{r}) = \begin{pmatrix} u_n(r) \\ id_n(r)e^{i\phi} \end{pmatrix}e^{im\phi} \quad (16)$$

to (14) leads to the solution [22]

$$u_n(r) = h\begin{cases} J_{|m|}(\mu_n r), & r < R \\ gK_{|m|}(\tilde{\mu}_n r), & r > R, \end{cases} \quad (17)$$

$$d_n(r) = h\begin{cases} \dfrac{\sigma\mu_n}{\epsilon_n + U + \Delta}J_{|m|+\sigma}(\mu_n r), & r < R \\ \dfrac{g\tilde{\mu}_n}{\epsilon_n + \Delta}K_{|m|+\sigma}(\tilde{\mu}_n r), & r > R, \end{cases} \quad (18)$$

where $\sigma = 1$ for $m \geq 0$ and $\sigma = -1$ for $m < 0$, ϵ_n is the bound state energy, and $\mu_n = \sqrt{(\epsilon_n + U)^2 - \Delta^2}$ is the Bessel function of the first kind. The bound state energy $\tilde{\mu}_n = \sqrt{\Delta^2 - \epsilon_n^2}$, $J_a(b)$ is the Bessel function. Energy ϵ_n depends on m. Coefficients g and h can be found from the wave function normalization condition and from the continuity conditions for the functions $u_n(r)$ and $d_n(r)$ at $r = R$ [22]:

$$g = \frac{J_{|m|}(\mu_n R)}{K_{|m|}(\tilde{\mu}_n R)}, \quad (19)$$

$$h^2 = \frac{\epsilon_n + U + \Delta}{2\pi UR^2}\left(\frac{\Delta J_m^2(\mu_n R)}{\Delta + \epsilon_n} + \frac{\Delta J_{m+1}^2(\mu_n R)}{\Delta - \epsilon_n}\right.$$
$$+ \frac{\Delta(U + 2\epsilon_n) - (2m+1)(\Delta^2 + \epsilon_n(1 + \epsilon_n))}{R\mu_n\tilde{\mu}_n^2}$$
$$\left.\times J_m(\mu_n R)J_{n+1}(\mu_n R)\right)^{-1}. \quad (20)$$

The continuity conditions lead to the equation for the bound state energies ϵ_n:

$$\frac{\sigma\mu_n(\epsilon_n + \Delta)}{\tilde{\mu}_n(\epsilon_n + U + \Delta)}\frac{J_{|m|+\sigma}(\mu_n R)}{J_{|m|}(\mu_n R)} = \frac{K_{|m|+\sigma}(\tilde{\mu}_n R)}{K_{|m|}(\tilde{\mu}_n R)}. \quad (21)$$

One can check that each energy level ϵ_n smoothly decreases from Δ to $-\Delta$ as U increases from zero to some critical value of the potential depth U_c, at which the energy level reaches the value $-\Delta$ and disappears from the discrete spectrum. At this potential depth value, the processes of electron–hole pair creation arise [22, 23] (the analogue of the of electron–positron pair creation in quantum electrodynamics). As an example, in Fig. 2 we show the dependence of the energy of the lowest bound state on the potential depth for $R\Delta = 1$. The value of the critical depth of the potential U_c is different for different energy levels. The min-
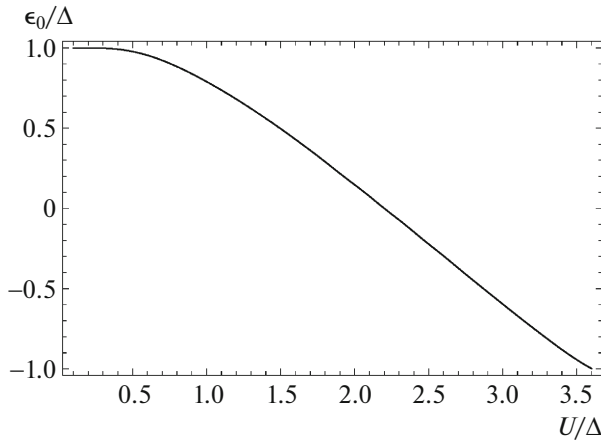
Fig. 2. Dependence of ratio ϵ_0/Δ on U/Δ for $R\Delta = 1$.

imum value of U_c corresponds to the disappearance of the lowest bound state. At the critical value of the potential depth, the peculiarities of the induced charge density arise (see, e.g., [17]).

To obtain the induced charge density, it is necessary to calculate the potential depths U_0 at which the energies of the bound states become equal to zero (see (3)). Also, to study the behavior of the induced charge near the critical value of the potential depth, it is necessary to calculate the value U_c. The values U_0 and U_c can be found numerically for arbitrary values of Δ and R. For this, Eq. (21) is solved numerically for $\epsilon_n = 0$ and $\epsilon_n = -\Delta$, respectively. However, when the parameters R and Δ satisfy the relations $R\Delta \ll 1$ or $R\Delta \gg 1$, the values U_0 and U_c can be found analytically. So, we set ϵ_0 in Eq. (21) and find solutions in the leading and next-to-leading order over smallness parameters. In the case $R\Delta \ll 1$, we have

$$U_0 \approx \frac{g_c}{R} - \Delta \ln \frac{1}{R\Delta}. \tag{22}$$

For $R\Delta \gg 1$, we obtain

$$U_0 \approx \Delta + \frac{g_c^2}{2R^2\Delta}, \tag{23}$$

where g_c is the smallest positive solution of the equation $J_0(g_c) = 0$ ($g_s \approx 2.4$). To find U_c, we set $\epsilon_0 = -\Delta$ in (21), for U_c solve the equation, and obtain

$$\frac{U_c}{\Delta} = 1 + \sqrt{1 + \frac{g_c^2}{R^2\Delta^2}}, \tag{24}$$

In the case $R\Delta$, the solution has the form

$$U_c \approx \frac{g_c}{R} + \Delta. \tag{25}$$

When $R\Delta \ll 1$, we have

$$U_c \approx 2\Delta + \frac{g_c^2}{2R^2\Delta}. \tag{26}$$

Note that, in the case of $R\Delta \gg 1$, the values of U_0 and U_c coincide in the leading order in $R\Delta \ll 1$; i.e.,

$$U_0 \approx U_c. \tag{27}$$

5. ASYMPTOTIC BEHAVIOR OF THE INDUCED CHARGE DENSITY

The asymptotic behavior of the induced charge density depends on the relation between the distance r, the characteristic width R of the potential well $V(r)$, and the Compton wavelength of electron in the material $1/\Delta$. We will consider two cases. In the first case, $R \ll r \ll \Delta^{-1}$. The second case corresponds to the relations $r \gg R$ and $r \gg \Delta^{-1}$, but the relation between R and Δ is arbitrary. In the first case ($R \ll r \ll \Delta^{-1}$), when calculating the asymptotics of the induced charge density, the main contribution to integral over energy ϵ comes from the region $\epsilon \sim 1/r$. At such energies, the band gap can be neglected, since $r\Delta \ll 1$. Therefore, the result for the asymptotics of the induced charge density $r_{\text{ind}}(\mathbf{r})$ coincides with the result of [17], where the induced charge density in graphene was considered. We consider the second case in detail below.

To calculate $\tilde{\rho}^{(1)}(\mathbf{r})$ at $r \gg R$, we substitute Green's function (9) to Eq. (7) and obtain

$$\tilde{\rho}^{(1)}(\mathbf{r})$$
$$= -\frac{eN}{2\pi^3} \int_0^\infty d\epsilon \int d\mathbf{r}' V(r')\{(\epsilon^2 - \Delta^2)K_0^2(\kappa\rho) - \kappa^2 K_1^2(\kappa\rho)\}, \tag{28}$$

where $\rho = |\mathbf{r} - \mathbf{r}'|$. The main contribution to the integral over the variable r' comes from the region R. Since $r \gg R$ and $r \gg \Delta^{-1}$, the argument of the Macdonald function obeys the condition $\kappa\rho \gg 1$. Substituting the asymptotics of the Macdonald function for large arguments [24],

$$K_m(x) \approx \sqrt{\frac{\pi}{2x}} e^{-x}, \tag{29}$$

in Eq. (28), using the Laplace method, we calculate the integral over ϵ and obtain

$$\tilde{\rho}^{(1)}(\mathbf{r}) = \frac{eN}{2\sqrt{\pi}}\left(\frac{\Delta}{r}\right)^{3/2} \int \frac{d\mathbf{r}'}{2\pi} V(r')e^{-2\rho\Delta}. \tag{30}$$

Below we also assume that the following relation is fulfilled:

$$\frac{R^2\Delta}{r} \ll 1. \tag{31}$$

In this case we integrate over directions of the vector $\mathbf{r}'$ and obtain

$$\tilde{\rho}^{(1)}(\mathbf{r}) = F(r)\mathcal{L}_V^{(1)}, \tag{32}$$

where

$$F(r) = -\frac{eN\sqrt{\Delta}e^{-2r\Delta}}{2\sqrt{\pi}r^{3/2}}, \tag{33}$$

$$\mathcal{L}_V^{(1)} = -\Delta\int\limits_0^\infty dr'r'V(r')I_0(2r'\Delta), \tag{34}$$

and $I_m(x)$ is the modified Bessel function of the first kind. One can see that the linear in the potential contribution to the induced charge density decreases exponentially at large distances.

To calculate the asymptotics of $\tilde{\rho}^{(2)}(\mathbf{r})$, we substitute Green's functions (9) and (10) in Eq. (8); then we set $r_1 = 0$ and $r_2 = 0$ in the arguments of the functions $G^{(0)}$, use the asymptotics of the Macdonald function (29), integrate over the directions of the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, take into account the condition (31), use relations (13), and get

$$\tilde{\rho}^{(2)}(\mathbf{r}) = \frac{eN\Delta}{2r}\int\limits_{-\infty}^\infty \frac{d\epsilon}{2\pi}e^{-2\kappa r}\int\limits_0^\infty\int\limits_0^\infty dr_1dr_2r_1r_2V(r_1)V(r_2)$$
$$\times\sum_{s=-1,1}\sum_{m=-\infty}^\infty I_m(\kappa r_2)\{I_m(\kappa r_1)\mathcal{A}_m^{(s\Delta)}(r_1,r_2\mid i\epsilon) \tag{35}$$
$$- sI_{m+1}(\kappa r_1)\mathcal{C}_m^{(s\Delta)}(r_1,r_2\mid i\epsilon)\}.$$

Here, $\mathcal{A}_m^{(\pm\Delta)}(r_1,r_2|i\epsilon)$ and $\mathcal{C}_m^{(\pm\Delta)}(r_1,r_2|i\epsilon)$ are the solutions of Eqs. (12).

Following the results of [17], we introduce the functions

$$a_m^{(\pm\Delta)}(r,i\epsilon) = \int\limits_0^\infty dr'r'V(r')I_m(\kappa r')\mathcal{A}_m^{(\pm\Delta)}(r,r'\mid i\epsilon), \tag{36}$$

$$c_m^{(\pm\Delta)}(r,i\epsilon) = \int\limits_0^\infty dr'r'V(r')I_m(\kappa r')\mathcal{C}_m^{(\pm\Delta)}(r,r'\mid i\epsilon), \tag{37}$$

that satisfy the equations

$$\left(\frac{\partial}{\partial r} - \frac{m}{r}\right)a_m^{(\pm\Delta)}(r,i\epsilon)$$
$$+ (i\epsilon - V(r) \pm \Delta)c_m^{(\pm\Delta)}(r,i\epsilon) = 0,$$
$$(i\epsilon - V(r) \mp \Delta)a_m^{(\pm\Delta)}(r,i\epsilon) \tag{38}$$
$$+ \left(\frac{\partial}{\partial r} + \frac{m+1}{r}\right)c_m^{(\pm\Delta)}(r,i\epsilon) = V(r)I_m(\kappa r).$$

To obtain these equations, we multiply both sides of Eqs. (12) by $r'V(r')I_m(\kappa r')$ and integrate over r'. The boundary conditions for functions have the form

$$a_m^{(\pm\Delta)}(0,i\epsilon) < \infty, \quad c_m^{(\pm\Delta)}(0,i\epsilon) < \infty,$$
$$\lim_{r\to\infty} a_m^{(\pm\Delta)}(r,i\epsilon) = \lim_{r\to\infty} c_m^{(\pm\Delta)}(r,i\epsilon) = 0. \tag{39}$$

We express $\tilde{\rho}^{(2)}(\mathbf{r})$ through $a_m^{(\pm\Delta)}(r,\ i\epsilon)$ and $c_m^{(\pm\Delta)}(r,\ i\epsilon)$ and obtain

$$\tilde{\rho}^{(2)}(\mathbf{r}) = \frac{eN\Delta}{2r}\int\limits_{-\infty}^\infty \frac{d\epsilon}{2\pi}e^{-2\kappa r}\int\limits_0^\infty dr_1r_1V(r_1)$$
$$\times\sum_{s=-1,1}\sum_{m=-\infty}^\infty \{I_m(\kappa r_1)a_m^{(s\Delta)}(r_1,i\epsilon) \tag{40}$$
$$- sI_{m+1}(\kappa r_1)c_m^{(s\Delta)}(r_1,i\epsilon)\}.$$

Thus, to calculate function $\rho_{ind}^{(2)}(\mathbf{r})$, it is necessary to find the functions $a_m^{(\Delta)}(r,i\epsilon)$ and $c_m^{(\Delta)}(r,i\epsilon)$.

Let us assume that functions $a_m^{(\Delta)}(r,\ i\epsilon)$ and $c_m^{(\Delta)}(r,\ i\epsilon)$ do not contain singularities at small ϵ; then the integral over energy can be calculated analytically using the Laplace method:

$$\tilde{\rho}^{(2)}(\mathbf{r}) = F(r)\mathcal{L}_V^{(2)}, \tag{41}$$

where

$$\mathcal{L}_V^{(2)} = -\frac{\Delta}{2}\sum_{s=-1,1}\sum_{m=-\infty}^\infty \int\limits_0^\infty dr_1r_1V(r_1)\{I_m(\kappa r_1)$$
$$\times a_m^{(d\Delta)}(r_1,0) - sI_{m+1}(\kappa r_1)c_m^{(s\Delta)}(r_1,0)\}. \tag{42}$$

One can see that the dependence of the induced charge density on the distances and parameters of the potential are factorized. Below, using potential (15) as the example, we show that the dependence of the functions $a_m^{(\Delta)}(r,\ i\epsilon)$ and $c_m^{(\Delta)}(r,\ i\epsilon)$ can be omitted for the wide range of the parameters of the potential. However, expression (41) is not correct for values of the potential depth U close to U_0, i.e., such that the pole of Green's function corresponding to the bound state is located close to the integration contour. In this case, the calculation of the integral over ϵ must be performed more carefully, since the functions $a_m^{(\Delta)}(r,\ i\epsilon)$ and $c_m^{(\Delta)}(r,\ i\epsilon)$ contains the singularities (see below).

Functions $a_m^{(\Delta)}(r,\ i\epsilon)$ and $c_m^{(\Delta)}(r,\ i\epsilon)$ depend on the shape of the potential well $V(r)$; therefore, below we investigate the charge density induced by the potential

(15). The solutions of Eqs. (38) for the potential (15) have the form

$$
\begin{aligned}
&a_m^{(\pm\Delta)}(r,i\epsilon) \\
&= \begin{cases} H_m^{(\pm)} J_{|m|}(\varkappa r) - \dfrac{U \pm \Delta + i\epsilon}{U + 2i\epsilon} I_m(\kappa r), & r < R \\ G_m^{(\pm)} K_m(\kappa r), & r > R, \end{cases}
\end{aligned} \quad (43)
$$

$$
\begin{aligned}
&c_m^{(\pm\Delta)}(r,i\epsilon) \\
&= \begin{cases} -\dfrac{\varkappa\sigma H_m^{(\pm)} J_{|m|+\sigma}(\varkappa r)}{U \pm \Delta + i\epsilon} - \dfrac{\kappa I_{|m|+\sigma}(\kappa r)}{U + 2i\epsilon} I_m(\kappa r), & r < R \\ \dfrac{\varkappa}{i\epsilon \pm \Delta} G_m^{(\pm)} K_{|m|+\sigma}(\kappa r), & r > R, \end{cases}
\end{aligned} \quad (44)
$$

where $\varkappa = \sqrt{(U - i\epsilon)^2 - \Delta^2}$. Coefficients $H_m^{(\pm)}$ and $G_m^{(\pm)}$ can be found from the continuity conditions for the functions $a_m^{(\pm\Delta)}(r, i\epsilon)$ and $c_m^{(\pm\Delta)}(r, i\epsilon)$ at $r = R$. We do not demonstrate the explicit form of the coefficients due to their cumbersomeness.

We substitute (43) and (44) to (40), perform simple transformations, integrate over r_1, and obtain the following expression:

$$
\begin{aligned}
\tilde{\rho}^{(2)}(\mathbf{r}) = {}& \frac{eNUR\Delta}{2r} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{U + i\epsilon}{(U + 2i\epsilon)\kappa} e^{-2\kappa r} I_1(2\kappa R) \\
& - \frac{eN\Delta}{r} \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{e^{-2\kappa r}(M_m\gamma_m + P_m\gamma_{m+1})}{\kappa R(U + 2i\epsilon)^2 D_m},
\end{aligned} \quad (45)
$$

where

$$
\gamma_m = y I_{m+1}(y) J_m(x) + x I_m(y) J_{m+1}(x), \quad (46)
$$

$$
\begin{aligned}
M_m = {}& \tilde{B}_m(\kappa[(U + i\epsilon)\kappa - U\Delta] \\
& + Uy[(\kappa^2 - i\epsilon U)A_m + \kappa\Delta\tilde{A}_m]) \\
& + \varkappa(i\epsilon\kappa + Uy[\kappa A_m + \Delta\tilde{A}_m])B_m m
\end{aligned} \quad (47)
$$

$$
\begin{aligned}
P_m = {}& B_m(\kappa([(U + i\epsilon)\kappa - U\Delta] \\
& + Uy[(\kappa^2 - i\epsilon U)\tilde{A}_m + \kappa\Delta A_m]) \\
& - \varkappa(i\epsilon\kappa + Uy[\kappa\tilde{A}_m + \Delta A_m])\tilde{B}_m,
\end{aligned} \quad (48)
$$

$$
D_m = \kappa\varkappa(B_m^2 - \tilde{B}_m^2) + 2B_m\tilde{B}_m(\kappa^2 - i\epsilon U), \quad (49)
$$

$$
A_m = I_m(y)K_{m+1}(y), \quad \tilde{A}_m = I_{m+1}(y)K_m(y), \quad (50)
$$

$$
B_m = J_m(x)K_{m+1}(y), \quad \tilde{B}_m = J_{m+1}(x)K_m(y), \quad (51)
$$

$x = \varkappa R$, $y = \kappa R$. On the right-hand side of Eq. (45) we calculate the integral in the first term using the Laplace method, since $r \gg R$ and $r \gg 1/\Delta$. Then we sum the result for $\tilde{\rho}^{(2)}(\mathbf{r})$ with the function $\tilde{\rho}^{(1)}(\mathbf{r})$ calculated for the potential well (15) (see (32)) and obtain

$$
\begin{aligned}
\tilde{\rho}(\mathbf{r}) = {}& -\frac{eN\Delta}{Rr} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{e^{-2\kappa r}}{\kappa(U + 2i\epsilon)^2} \\
& \times \sum_{m=0}^{\infty} \frac{M_m\gamma_m + P_m\gamma_{m+1}}{D_m}.
\end{aligned} \quad (52)
$$

Let us consider the dependence of the function $\tilde{\rho}(\mathbf{r})$ on the depth of the potential well.

For $r \gg 1/\Delta$, the function $e^{-2\kappa r}$ changes sufficiently at $\epsilon \sim \Delta/\sqrt{r\Delta}$, i.e., at $\epsilon \ll \Delta$. Assuming that the denominator D_m does not have singularities at small ϵ, we calculate the integral and get

$$
\tilde{\rho}(\mathbf{r}) = F(r)\mathscr{L}_V, \quad (53)
$$

where

$$
\mathscr{L}_V = \frac{U}{\Delta} \sum_{m=0}^{\infty} \frac{J_m(x)J_{m+1}(x)}{(B_m^2 + \tilde{B}_m^2) + 2yB_m\tilde{B}_m}\bigg|_{\epsilon=0}. \quad (54)
$$

Thus, the function $\tilde{\rho}(\mathbf{r})$ is the product of the function depending on r and the coefficient $\mathscr{L}_V$, which depends on the parameters of the potential and does not depend on r.

In the case $U \ll \Delta$, we obtain

$$
\mathscr{L}_V = \frac{URI_1(2R\Delta)}{2}. \quad (55)
$$

This result is consistent with the contribution $\tilde{\rho}^{(1)}$ for the potential (15). The denominator in the expression (54) equals to zero at potential values $U = U_0$ that satisfy Eq. (21) at $\epsilon_n = 0$. Therefore, for $U = U_0$, the function $\mathscr{L}_V$ has the singularity. In order to calculate correctly the function $\tilde{\rho}(\mathbf{r})$ (52) for U close to U_0, we extract the dependence of the denominator D_m on ϵ at small ϵ. To do this, we expand the denominator D_m over ϵ, keep the linear in ϵ terms, and obtain the following expression:

$$
\tilde{\rho}(\mathbf{r}) = -\frac{eNU}{Rr} \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{J_m(x_0)J_{m+1}(x_0)e^{-2\kappa r}}{\beta_m + i\epsilon\alpha_m}, \quad (56)
$$

where $x_0 = R\sqrt{U^2 - \Delta^2}$, $\beta_m = D_m|_{\epsilon=0}$,

$$
\begin{aligned}
\alpha_m = {}& -\frac{2U^2 R\Delta}{\sqrt{U^2 - \Delta^2}} K_m(R\Delta)K_{m+1}(R\Delta) \\
& \times \left(J_m^2(x_0) + J_{m+1}^2(x_0) + \frac{U - (2m+1)\Delta}{x_0\Delta} J_m(x_0)J_{m+1}(x_0) \right).
\end{aligned} \quad (57)
$$

Let us investigate the behavior of one of the terms of the sum in (56) when U changes. As an example, we consider the term with $m = 0$. For convenience, we denote it as $\tilde{\rho}_0(\mathbf{r})$. The integral over energy contains the large parameter $r\Delta$ in the exponent and the param-

eter β_0 in the denominator, which becomes small when U close to U_0. Using U and U_0, we build the dimensionless parameter $\lambda = r|\beta_0/\alpha_0|$. If $\lambda \ll 1$, then we put $\epsilon = 0$ in the denominator, because the convergence of the integral is determined by the exponential function and the integral converges on the scales $\epsilon \sim \Delta/\sqrt{r\Delta}$. In this case, the result for this term coincides with that obtained earlier. If the parameter $\lambda \ll 1$, then the convergence of the integral is determined by the denominator, so we can neglect the energy dependence in the exponential function. Calculating the integral, we find

$$\tilde{\rho}_0(\mathbf{r}) = -\frac{eN}{Rr} e^{-2r\Delta} \frac{\text{sign}(U_0 - U)J_0(x_0)J_1(x_0)}{2|\alpha_0|}. \quad (58)$$

Note that for $\lambda \ll 1$, the dependence of the function $\tilde{\rho}_0(\mathbf{r})$ on r differs from its behavior for the case $\lambda \gg 1$. However, for a fixed U different from U_0, i.e., for a fixed ratio β_0/α_0, one can find a sufficiently large r such that the asymptotics (52) is correct.

Despite the fact that the function $\tilde{\rho}_0(\mathbf{r})$ has discontinuity at $U = U_0$,

$$\tilde{\rho}_0(\mathbf{r})|_{U=U_0-0} = -\tilde{\rho}_0(\mathbf{r})|_{U=U_0+0},$$

the induced charge density has no such behavior at $U = U_0$. Because when the pole of Green's function appears in the left half-plane, we must add the contribution of this pole to the function $\tilde{\rho}(\mathbf{r})$ (see (3)). Substituting (17)−(20) in (16) and setting $m = 0$, $\epsilon_0 = 0$, we obtain the contribution of the pole at $U = U_0 + 0$:

$$-eN|\psi_0(\mathbf{r})|^2|_{\epsilon=0} = 2\tilde{\rho}(\mathbf{r})\text{sign}(U_0 - U). \quad (59)$$

Thus, the induced charge density is continuous at $U = U_0$.

For the values of the potential depth close to U_c, i.e., when the ground state energy is close to $-\Delta$, the function $\tilde{\rho}(\mathbf{r})$ decreases as $e^{-2r\Delta}/r^{3/2}$ (see (53)), while the square of the wave function decreases as $h^2g^2K_1^2(r\sqrt{\Delta^2 - \epsilon^2})$, (see (17), (18)). This means that, at large distances $r\sqrt{\delta\epsilon\Delta} \gg 1$, the main contribution to the induced charge density gives the wave function corresponding to the state with energy $\epsilon = -\Delta + \delta\epsilon$. Here, $\delta\epsilon \ll \Delta$. However, the coefficient h^2g^2 tends to zero as the energy level approaches the valence band ($\delta\epsilon \to 0$). Therefore, there is the region of the distances at which $|\tilde{\rho}(\mathbf{r})| \gg |e||\psi_0(r)^2|$. Assuming $\delta\epsilon$ to be sufficiently small, we obtain a condition for this region:

$$\max(\Delta^{-1}, R) \ll r \ll r_\star, \quad (60)$$

$$r_\star = \frac{1}{\Delta} \ln \left| \frac{R^3\Delta^3}{\sqrt{r\delta\epsilon}} \ln^2(R\sqrt{\delta\epsilon\Delta}) \right|. \quad (61)$$

At such distances, the induced charge density coincides with the function $\tilde{\rho}(\mathbf{r})$; i.e., $\rho_{\text{ind}}(\mathbf{r}) = \tilde{\rho}(\mathbf{r})$. At $r \gtrsim r_\star$, the behavior of the induced charge density is determined by the behavior of the wave function, so $\rho_{\text{ind}}(\mathbf{r})$ decreases as $\exp\{-2r\sqrt{2\delta\epsilon\Delta}\}$. For $U = U_c$, the bound state disappears from the discrete spectrum. It leads to a steplike change in the induced charge density when U reaches U_c:

$$\rho_{\text{ind}}(\mathbf{r})|_{U=U_c+0} - \rho_{\text{ind}}(\mathbf{r})|_{U=U_c-0} = eN|\psi_0(\mathbf{r})|^2. \quad (62)$$

At $U = U_c + 0$, the process of electron−hole pair creation occurs. The electrons are localized on scales much smaller than r, while holes go to infinity. Therefore, at $U > U_c$ the total induced charge differs from zero and equals eN (see [17], [23]).

Let us consider the behavior of the induced charge density in the case of $R\Delta \ll 1$. For $U < \Delta$, we substitute the asymptotics of the Macdonald function for small arguments

$$K_m(y) \approx -\ln(y)\delta_{m,0} + (1 - \delta_{m,0})\frac{2^{m-1}\Gamma(m)}{y^m}, \quad (63)$$

to Eq. (54); use the analytic continuation of the Bessel function; and get

$$\mathcal{L}_V \approx UR^2\Delta/2, \quad (64)$$

where $\Gamma(x)$ is the Euler gamma function. The main contribution to $\mathcal{L}_V$ comes from the term with $m = 0$; the other terms are suppressed by powers of the parameter $R\Delta$. The substitution of Eqs. (64), (33) to (53) gives

$$\tilde{\rho}_{\text{ind}}(\mathbf{r}) = -\frac{eNUR^2e^{-2r\Delta}}{4\sqrt{\pi}}\left(\frac{\Delta}{r}\right)^{3/2}. \quad (65)$$

This result coincides with $\tilde{\rho}^{(1)}(\mathbf{r})$ calculated for the potential (15) in the case of $R\Delta \ll 1$ (see (32)). The corrections in the parameter U can be found easily. To calculate the corrections, it is necessary to expand the Bessel functions in Eq. (54).

In the case of $U > \Delta$, we extract the leading contribution in parameter $R\Delta$ and get

$$\mathcal{L}_V \approx \frac{UR\Delta}{\sqrt{U^2 - \Delta^2}} \frac{J_1(R\sqrt{U^2 - \Delta^2})}{J_0(R\sqrt{U^2 - \Delta^2})}. \quad (66)$$

The function $\mathcal{L}_V$ is regular at $U = \Delta$ and equals (64). In the case $U \ll \Delta$, we have

$$\mathcal{L}_V \approx R\Delta \frac{J_1(UR)}{J_0(UR)}. \quad (67)$$

One can see that function $\mathcal{L}_V$ has a singularity at $U = g_c/R$. This value of the potential is obtained in the leading order in $R\Delta$. As was mentioned earlier, the singularity occurs at $U = U_0$, but with our accuracy $U = U_c$

(see (27)). Because the two values coincided and for $U > U_c$ the bound state with the minimum energy disappears from the spectrum, the induced charge density coincides with the function $\tilde{\rho}$. Thus, for $R\Delta \ll 1$ we get

$$\rho_{\text{ind}}(\mathbf{r}) = \tilde{\rho}(\mathbf{r}).$$

We emphasize that this expression is not valid for the value of the potential depth close to U_c. Note also that the sign of the induced charge density changes abruptly at $U = U_c$.

Let us study the behavior of the induced charge located at large distances in the case $R\Delta \ll 1$:

$$Q_>(r) = 2\pi \int_r^\infty dr' r' \rho_{\text{ind}}(r'). \tag{68}$$

To calculate $Q_>(r)$ in the leading order in $R\Delta$, we substitute $\tilde{\rho}(r')$ (see (56)) instead of $\rho_{\text{ind}}(r')$ to (68), keep the term with $m = 0$, calculate β_0 and α_0 in the leading order in the parameter $R\Delta$, integrate over r', change the variable $\epsilon \to \epsilon/\Delta$, and obtain

$$Q_>(r) = -eNR\Delta J_0(UR)J_1(UR)$$

$$\times \int_0^\infty d\epsilon \frac{e^{-2r\Delta\sqrt{1+\epsilon^2}}}{J_0^2(UR) + 4\epsilon^2(R\Delta)^2 \ln^2(R\Delta)J_1^2(UR)}. \tag{69}$$

If

$$|J_0(UR)| \gg \frac{R\sqrt{\Delta}|\ln(R\Delta)|}{\sqrt{r}},$$

then

$$Q_>(r) = -\frac{eN\sqrt{\pi\Delta}RJ_1(UR)}{2\sqrt{r}J_0(UR)}e^{-2r\Delta}. \tag{70}$$

If

$$|UR - g_c| \ll \frac{R\sqrt{\Delta}|\ln(R\Delta)|}{\sqrt{r}},$$

then

$$Q_>(r) = -\frac{eN\pi\operatorname{sgn}(g_c - UR)}{4|\ln(R\Delta)|}e^{-2r\Delta}. \tag{71}$$

Thus, the charge outside the circle of radius r changes abruptly when the critical depth of the potential is exceeded.

Let us consider the behavior of the induced charge $Q_<(r)$ inside the circle of the radius r. For $UR < g_c$, the total induced charge $Q_{\text{tot}} = Q_<(r) + Q_>(r) = 0$ equals zero; therefore, $Q_<(r) = -Q_>(r)$. When UR is greater than the minimum g_c, the total induced charge is $Q_{\text{tot}} = eNM$, where M is the number of critical values g_c less than UR; i.e., the number of levels that disappeared from the discrete spectrum. This is due to processes similar to those of the electron–positron pair creation [23]. Therefore, in the case of $R\Delta \ll 1$ and

when the parameter UR is greater than the minimum value g_c, we get $Q_<(r) = eNM + Q_>(r)$. Since the induced charge $Q_>(r)$ is exponentially small, we have $Q_<(r) \approx eNM$.

Note that the solutions for the induced charge and the induced charge density are correct when the potential depth less than g_c/R, because for g_c we obtain a many-body problem. For U greater than the minimum critical value, the field creates four electron–hole pairs. The holes go to infinity, and the electrons are localized either on R or on the scale of the Compton wavelength of an electron in the material $1/\Delta$; see [23, 25]. Therefore, when calculating the induced charge for $U > U_c$, it is also necessary to take into account the potential induced by the created electrons.

6. CONCLUSIONS

In this paper, we consider the behavior of the charge density induced by the potential well. We have shown that, in the wide range of the parameters of the potential well, the induced charge density can be represented as a product of the function depending on the distance r and the function depending on the parameters of the potential well; i.e., the dependences on distance and the parameters of the potential are factorized. As the potential depth approaches the critical value, there is the range of the distances (60) at which the induced charge density is represented in the factorized form. When the potential well depth exceeds the critical value, the induced charge density changes abruptly by a value proportional to the square of the wave function that disappeared from the discrete spectrum state (62). For the potential (15) in the case of $R\Delta \ll 1$, we found the analytical expression for the induced charge density (53), (33), (66). Also, we considered the behavior of the induced charge inside and outside the circle of large radius.

CONFLICT OF INTEREST

The author declares that he has no conflicts of interest.

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