

THE MOTION OF AN ELECTRON IN A CRYSTAL LOCATED IN AN EXTERNAL FIELD

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Various forms of the equations of motion of an electron with an arbitrary dispersion law in a uniform magnetic and arbitrary electric fields are considered. A transition from the exact equation to approximate ones involves neglected values which are estimate. Special attention is paid to the nondiagonal terms (due to neighboring energy bands).

In a previous paper¹ the equation of motion of an electron with an arbitrary dispersion law in a magnetic field was obtained and solved. In the present paper this solution is extended to the case in which in addition to the uniform magnetic field $H = H_z$ there is also an arbitrary electrical field V in the crystal and, consequently, the eigenfunction of the electron satisfies equation:

$$-\frac{\hbar^2}{2m_0} \Delta \Psi - i\mu_0 H y \frac{\partial \Psi}{\partial x} + \left(\frac{e^2 H^2 y^2}{2m_0 c^2} + V_p + V - E \right) \Psi = 0 \quad (1)$$

(V_p is the periodic field of the crystal). In the absence of external fields ($V = 0, H = 0$) Eq. (1) has a known solution (s is the number of the energy band):

$$\psi_{ks} = e^{ikr} u_s(\mathbf{k}, \mathbf{r}) = e^{ikr} \sum_{\mathbf{h}} b_{\mathbf{h}s}(\mathbf{k}) e^{2\pi i \mathbf{h} \cdot \mathbf{r}}; \quad (2)$$

$$E = E_s(\mathbf{k}) = \sum_{\mathbf{h}} A_{\mathbf{h}s} e^{i\mathbf{k} \cdot \mathbf{h}}. \quad (3)$$

For crystals with a center of symmetry the coefficients $b_{\mathbf{h}s}(\mathbf{k})$ in the expansion of the Bloch function (2) are real, even functions of arguments $\mathbf{k} + 2\pi\mathbf{h}$. They satisfy relation:

$$\sum_{\mathbf{h}} b_{\mathbf{h}s}(\mathbf{k}) b_{\mathbf{h}s'}(\mathbf{k}) = \delta_{ss'}. \quad (4)$$

Any sum over all \mathbf{h} of the form $\sum_{\mathbf{h}} f(\mathbf{k} + 2\pi\mathbf{h})$ is a periodic function of the wave vector \mathbf{k} and can be written in the form completely similar to (3). Taking advantage of this, let us introduce the notation

$$\sum_{\mathbf{g}} b_{\mathbf{g}s}(\mathbf{k}) \frac{\partial^{l_1+l_2+l_3} b_{\mathbf{h}+\mathbf{g}, s'}}{\partial k_1^{l_1} \partial k_2^{l_2} \partial k_3^{l_3}} = \sum_{\mathbf{m}} B_{\mathbf{m}, \mathbf{h}, s, s'}^{l_1 l_2 l_3} e^{i\mathbf{k} \cdot \mathbf{m}}; \quad B_{\mathbf{m}0ss'}^1 \equiv B_{\mathbf{m}ss'}^1; \quad (5)$$

$$\sum_{\mathbf{g}} b_{\mathbf{g}s}(\mathbf{k}) \frac{\partial^{l_1+l_2+l_3} b_{\mathbf{h}+\mathbf{g}, s'}}{\partial k_1^{l_1} \partial k_2^{l_2} \partial k_3^{l_3}} (k_2 + 2\pi g_2) = \sum_{\mathbf{m}} C_{\mathbf{m}, \mathbf{h}, s, s'}^{l_1 l_2 l_3} e^{i\mathbf{k} \cdot \mathbf{m}}. \quad (6)$$

Generally speaking, in order of magnitude,

$$B^{l_1 l_2 l_3} \sim a^{l_1+l_2+l_3}, \quad C^{l_1 l_2 l_3} \sim a^{l_1+l_2+l_3-1} \quad (7)$$

(a is the lattice constant), with the exception of the special cases examined below.

In the following discussion the properties of the $B_{\mathbf{m}}$ coefficients, expressed by formulas (8) through (10), are important:

$$B_{\mathbf{m}ss}^{100} = B_{\mathbf{m}ss}^{010} = B_{\mathbf{m}ss}^{001} = 0. \quad (8)$$

When $s \neq s'$ these coefficients are different from zero [therefore they are the principal representatives of the neighboring bands, i.e., of the nondiagonal terms of Eq. (1)] and have the property:

$$B_{\mathbf{m}ss'}^{100} = -B_{\mathbf{m}s's}^{100} \text{ etc.} \quad (9)$$

Notice also that

$$B_{\mathbf{m}ss'}^{000} = \delta_{ss'} \delta_{\mathbf{m}0}. \quad (10)$$

We seek the solution of (1) in the form of expansion:

$$\Psi = \sum_{\mathbf{s}} \int g_{\mathbf{s}}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} u_s(\mathbf{k} + i\mathbf{y}/\alpha_0^2, \mathbf{r}) d\mathbf{k}, \quad (11)$$

\mathbf{i} is the unit vector of the X axis, $\alpha_0 = \sqrt{\hbar c/eH}$ is a quantity having the meaning of the least "radius of rotation" of a free electron in a magnetic field.

For fields $H \ll 10^9$ oersteds, $\alpha_0 \gg a$ (a is the lattice constant). With a field $H = 10^4$ oersteds, $\epsilon = a/\alpha_0 \approx 10^{-2}$.

The equation of electron motion in \mathbf{k} space, i.e., the equation for $g_{\mathbf{s}}(\mathbf{k})$, will be obtained by substituting (11) in (1), multiplying by the integrand function $e^{i\mathbf{k}' \cdot \mathbf{r}} u_{s'}(\mathbf{k}' + i\mathbf{y}/\alpha_0^2, \mathbf{r})$, and integrating over the entire space.

In reference 1 we retained only the first two terms of the expansion with respect to parameter $\epsilon^2 = a^2/\alpha_0^2$ (ϵ^0 and ϵ^2); here we retain terms $\sim \epsilon^0, \epsilon^2$, and ϵ^4 , and neglect only terms $\sim \epsilon^6$ and exponentially small ones of the type $\exp(-1/\epsilon^2)$. For this reason the equation will be cumbersome;

however, simpler forms will be used below, and in each case we shall be able to assess the error resulting from ignoring the small terms. Terms of the order ϵ^6 or $\exp(-1/\epsilon^2)$ (recalling that usually $\epsilon \sim 10^{-2}$) will hardly be necessary, and thus the equation written below can be considered as accurate as equation (1):

$$\begin{aligned} & \sum_n A_{ns} \exp \left\{ i \mathbf{k} \mathbf{n} - i \frac{n_1 n_2}{2\alpha_0^2} \right\} g_s \left(k_2 - \frac{n_1}{\alpha_0^2} \right) \\ & - \frac{1}{\alpha_0^2} \sum_{\mathbf{m}, s' \neq s} e^{i \mathbf{k} \mathbf{m}} \left\{ B_{\mathbf{m} s s'}^{010} \sum_n A_{n s'} (m_1 + n_1) \right. \\ & \times \exp \left\{ i \mathbf{k} \mathbf{n} - i \frac{n_1 n_2}{\alpha_0^2} \right\} g_{s'} \left(k_2 - \frac{n_1 + m_1}{\alpha_0^2} \right) \\ & + \left(\frac{i \hbar^2}{m_0} C_{\mathbf{m} s s'}^{100} - m_1 E B_{\mathbf{m} s s'}^{010} \right) g_{s'} \left(k_2 - \frac{m_1}{\alpha_0^2} \right) \left. \right\} + \frac{1}{2\alpha_0^4} \sum_{s'} H_{s s'}^{(2)} g_{s'} \\ & + \sum_{\substack{\mathbf{m}, \mathbf{h}, s, s' \\ \mathbf{l}, \mathbf{h}}} B_{\mathbf{m} s s'}^{\mathbf{l}} \frac{e^{i \mathbf{k} \mathbf{m}}}{l_1! l_2! l_3!} \int g_{s'}(\mathbf{k}') V(\mathbf{k}' - \mathbf{k} + \mathbf{j} \frac{m_1}{\alpha_0^2} + 2\pi \mathbf{h}) \\ & \times (k'_1 - k_1)^{l_1} (k'_2 - k_2)^{l_2} (k'_3 - k_3)^{l_3} d\mathbf{k}' = E g_s(\mathbf{k}). \quad (I) \end{aligned}$$

We have introduced here the symbols

$$V(\mathbf{x}) = \int e^{i \mathbf{x} \mathbf{r}} V(\mathbf{r}) d\tau, \quad (12)$$

\mathbf{j} is the unit vector of the y axis, and $g(k_1, k_2 - k_2^0, k_3)$ is understood for $g(k_2 - k_2^0)$. An explicit expression for the term of the order α_0^{-4} is written out in the Appendix.

The "magnetic terms" of Eq. (I) contain no components with $\mathbf{h} \neq 0$, because they are exponentially small [$\sim \exp(-1/\epsilon^2)$]. Let us explain the cases in which we can drop these components in the last term connected with the electrical field $V(\mathbf{r})$, of the left part of (I).

This can be done, for example, in the particular case when $V(\mathbf{r})$ reduces to a polynomial (and, in addition, $H = 0$), since then (12) will be expressed in terms of $\delta(\mathbf{k}' - \mathbf{k} + 2\pi \mathbf{h})$ and its derivatives, while the point $\mathbf{k}^1 = \mathbf{k} - 2\pi \mathbf{h}$ lies outside the elementary \mathbf{k} -space cell over which the integration is performed. If $V(\mathbf{r})$ is an analytic function having no poles with $V(\infty) = 0$, and if the distance at which it essentially disappears is equal to A , then the integral (12) for $\mathbf{h} \neq 0$ will be of the order $e^{-A/a}$, or even $\exp\{- (A/a)^2\}$. Therefore when $A \gg a$ it is possible to drop from (I) terms with $\mathbf{h} \neq 0$ as exponentially small. If however $V(\mathbf{r})$ has a pole (for example, $V \sim 1/r$) or merely a discontinuity of the derivative at any point (for example, $e^{-\alpha r}$), the terms with $\mathbf{h} \neq 0$, generally speaking, cannot be dropped. In these cases an additional investigation of (I) is necessary.

Let us now examine the problem of the influence of neighboring bands. It is best to examine first

the nondiagonal "electrical" terms. Two obvious questions arise: 1) at which $V(\mathbf{r})$ are the non-diagonal terms most substantial, and 2) which features of the neighboring bands are capable of making their contribution to (I) more substantial.

The answer to the first question comes from the fact that, according to (9), $B_{\mathbf{S} \mathbf{S}'}^{000} = \delta_{\mathbf{S} \mathbf{S}'}$; i.e., when $s = s'$, there are no multipliers $(k'_1 - k_1)^{l_1}$ etc. in the integrand of (I). Therefore the contribution of neighboring bands will be small if $V(\mathbf{r})$ is a smooth function, varying little over the lattice constant. If $V(\mathbf{r})$ changes substantially over the distance A , and $A \gg a$, then the contribution of neighboring bands can be written as a series in powers of the small parameter, a/A (beginning, generally speaking, with the first power of this parameter, since $B_{\mathbf{S} \mathbf{S}'}^{100} \neq 0$). We assume, of course, that coefficients $B_{\mathbf{S} \mathbf{S}'}^{100}$ (meaning also $B_{\mathbf{S} \mathbf{S}'}^{010}$ and $B_{\mathbf{S} \mathbf{S}'}^{001}$) are of the order a [see Eq. (7)].

The answer to the second question is exactly connected with the possible deviations from the relation $B_{\mathbf{S} \mathbf{S}'}^{100} \sim a$. We recall that these values are determined by formula (5), which in the given case has the form

$$\sum_{\mathbf{m}} B_{\mathbf{m} s s'}^{100} e^{i \mathbf{k} \mathbf{m}} = \sum_{\mathbf{h}} b_{\mathbf{h} s} \partial b_{\mathbf{h} s'} / \partial k_1.$$

Thus the coefficients B^{100} can be very large if derivatives $\partial b_{\mathbf{h} s'} / \partial k_1$ are large. If we express $E_{\mathbf{S}}(\mathbf{k})$ by $b_{\mathbf{h} s}$ using formula $E_{\mathbf{S}} = \int \psi_{\mathbf{k} \mathbf{S}}^* H \psi_{\mathbf{k} \mathbf{S}} d\tau$ and expand $E_{\mathbf{S}}$ in powers of $(k_1 - k_1^0)^2$ near the point of effective mass, the derivatives $\partial b_{\mathbf{h} s} / \partial k_1$ and $\partial^2 b_{\mathbf{h} s} / \partial k_1^2$ will enter the coefficients of $(k_1 - k_1^0)^2$. Therefore, generally speaking, the larger these derivatives, the smaller will be the effective mass. Thus, we can expect anomalously large values of $B_{\mathbf{S} \mathbf{S}'}^{100}$ in cases in which effective mass m^* in the neighboring bands is anomalously small (as was pointed out in another way by Adams²), or in general the coefficients $b_{\mathbf{h} s}$, and consequently the energy, have an anomalously rapid variation with change in the wave vector. Thus, for example, in the approximation of weakly bound electrons, for values of \mathbf{k} close to the boundaries of the band, we have $\partial b_{\mathbf{h}} / \partial k_1 \sim a (\hbar^2 / m_0 a^2 V_g)$, which can also be written as $\partial b_{\mathbf{h} s} / \partial k_1 \sim a m_0 / m^*$. Here V_g is the Fourier coefficient of the potential, and in this approximation $V_g \ll \hbar^2 / m_0 a^2$, and therefore $\partial b / \partial k$ is not of the order a , but is significantly greater. The coefficients $B_{\mathbf{S} \mathbf{S}'}^{100}$ increase correspondingly, and along with them the contribution of the neighboring bands.

The diagonal coefficient $B_{\mathbf{S} \mathbf{S}}^{200}$ can also become anomalously large for the same reason, but the contribution of values $B^{\mathbf{l}}$ with large $|\mathbf{l}|$ is gen-

erally less, because of the factors $(k_1' - k_1)^l$ in the integrand.

The influence of the neighboring bands in the "magnetic terms" of Eq. (I) is usually weaker and is easier to evaluate, since there is always a small multiplier α_0^{-2} standing before each nondiagonal magnetic term. Therefore their contribution cannot be greater than $a\alpha_0^{-2}B^{010}$, while at the same time the contribution of the neighboring bands in the "electrical terms" is of the order B^{100}/A . Here A is the distance at which $V(\mathbf{r})$ changes significantly,* $\alpha_0/a \sim 10^2$ and $\alpha_0 \sim 2 \times 10^{-6}$ cm with fields $H \sim 10^4$ oersteds, so that $\alpha_0^2/a \sim 10^{-4}$ cm. If $A \ll \alpha_0^2/a$, the effect of neighboring bands in the "electrical" terms is more substantial than in the "magnetic" ones.

If the contribution of neighboring bands can be considered as a perturbation, it will be less than the foregoing estimates, because the product of rapidly oscillating (for levels not too low) and noncoincident functions g_s and $g_{s'}$ will enter into the perturbation matrix element. In the case in which the electrical field is absent,¹ this gives, in addition to multiplier α_0^{-2} , another multiplier $\epsilon = a/\alpha_0$, or even an exponentially small one.[†]

In the case when $V(\mathbf{r})$ changes so slowly that we can drop in Eq. (I) terms with $\mathbf{h} \neq 0$ and the nondiagonal terms describing the neighboring bands, Eq. (I) assumes the simple form

$$\sum_n A_{ns} \exp \{ikn - in_1 n_2 / 2\alpha_0^2\} g_s \left(k_1, k_2 - \frac{n_1}{\alpha_0^2}, k_3 \right) + \int g_s(k') V(k' - k) dk' = E g_s(k). \quad (\text{II})$$

If we set here $H = 0$, i.e., $\alpha_0^2 = \infty$, the first term on the left will simply take the form $E_s(\mathbf{k}) g_s(\mathbf{k})$, while Eq. (II) changes into the Slater equation³ written in the \mathbf{k} representation. A particular consequence is the effective-mass method. The Vannier function method used by Slater and several other authors makes it difficult to evaluate errors which occur in going from the accurate equation (I) to the "quasi-classical" equation (II).

Equation (II) is of the integro-difference type. In a number of cases it can be written also in a differential-difference form. This includes, in particular, the case when $V(\mathbf{r})$ is a polynomial. For each term of the polynomial $x^n y^m z^l$ there is a corresponding Fourier component

$$(x^n y^m z^l)_{k'-k} = i^{-(n+m+l)} \delta_{(k_1'-k_1)}^{(n)} \delta_{(k_2'-k_2)}^{(m)} \delta_{(k_3'-k_3)}^{(l)}$$

*The distance at which $V(A) \sim E_s(\mathbf{k}) - E_{s'}(\mathbf{k})$ (see the last of the examples given below).

†Depending on whether the \mathbf{k} trajectories are intersected in zones s and s' . "Trajectory" means the intersection between a surface $E(\mathbf{k}) = \text{const}$ and a plane perpendicular to the magnetic field.

[the δ -function is taken to mean everywhere $\int e^{i\mathbf{k}\mathbf{r}} d\tau$ without the multiplier $(2\pi)^{-3}$]. After integrating with $g(\mathbf{k})$ in (II) this term takes the form

$$i^{n+m+l} \partial^{n+m+l} g(\mathbf{k}) / \partial k_1^n \partial k_2^m \partial k_3^l.$$

Consequently the integral in (II) can be written in this case in the form of a differential operator $V(\hat{x}, \hat{y}, \hat{z})$, where $\hat{x} = i\partial/\partial k_1$, $\hat{y} = i\partial/\partial k_2$, $\hat{z} = i\partial/\partial k_3$. Equation (II) takes the form

$$\sum_n A_{ns} \exp \{ikn - in_1 n_2 / 2\alpha_0^2\} g_s(k_1, k_2 - n_1/\alpha_0^2, k_3) + V(i\partial/\partial k_1, i\partial/\partial k_2, i\partial/\partial k_3) g_s = E g_s(\mathbf{k}). \quad (\text{III})$$

Equation (II) can be written in the same form also in the general case in which integration with respect to \mathbf{k} in (II) can be extended over the entire \mathbf{k} space (which corresponds to replacing the quasi-momentum with the momentum).

The left part of (III) can be represented completely in operator form, if we account for the fact that, as shown in reference 4, the first sum in (III) (under the condition of using the operation of total symmetrization⁴) can be written as $E_s(\hat{k}_1, k_2, k_3)$, where $\hat{k}_1 = k_1 - (1/i\alpha_0^2) \partial/\partial k_2$:

$$E_s \left(k_1 - \frac{1}{i\alpha_0^2} \frac{\partial}{\partial k_2}, k_2, k_3 \right) g_s + V \left(i \frac{\partial}{\partial \mathbf{k}} \right) g_s = E g_s. \quad (\text{IV})$$

As an example, let us examine the motion of an electron in crossed electric ($V = Fy$) and magnetic fields. We first neglect the nondiagonal terms, thereby obtaining the equation

$$\sum_n A_{ns} \exp \left\{ ikn - i \frac{n_1 n_2}{2\alpha_0^2} \right\} g_s \left(k_2 - \frac{n_1}{\alpha_0^2} \right) + iF \frac{\partial g_s}{\partial k_2} = E g_s(\mathbf{k}). \quad (\text{13})$$

As shown in reference 5, the quasi-classical solution of equation (13) does not differ at all in principle from the solution of the equation when $F = 0$. The electron in this case moves in \mathbf{k} -space along a trajectory shifted in the direction perpendicular to both fields. It is easy to show that nondiagonal terms will give a correction of the order ϵ^3 or less (see footnote*) compared with the corresponding diagonal ones.

As another example, let us examine the motion of an electron in a field $V = Fy$ without a magnetic field. Neglecting nondiagonal terms, we obtain from (13):

$$E_s(\mathbf{k}) g_s(\mathbf{k}) + iF \partial g_s / \partial k_2 = E g_s(\mathbf{k}). \quad (\text{14})$$

A solution of this equation is

$$g_s(\mathbf{k}) = \exp \left\{ \frac{1}{iF} \int [E - E_s(\mathbf{k})] dk_2 \right\}. \quad (\text{15})$$

For a free particle, when $E(\mathbf{k}) = \hbar^2 k^2 / 2m$, we obtain the \mathbf{k} -representation Airy function.⁶ With an

arbitrary periodic $E_S(\mathbf{k})$ we obtain the \mathbf{k} -representation of a function which could be called the "Airy crystal function." We recall that the eigenfunction in ordinary space is expressed by formula (11), which in the given case has the form $\Psi_S = \int g_S(\mathbf{k}) \psi_{\mathbf{k}S} d\mathbf{k}$. If the field F is weak, this integral can be computed by the steepest-descent method. Since $\psi_{\mathbf{k}S}$ contains a multiplier $e^{i\mathbf{k}_2 y}$, then Ψ oscillates in the interval where the derivative with respect to k_2 of

$$k_2 y - \frac{1}{F} \int_0^{k_2} [E - E_s] dk_2$$

vanishes. From this we immediately get a number of known facts concerning the motion of an electron in a uniform electric field. The motion of a free electron is bounded on one side, and the motion of an electron in a band is bounded on two sides by the limits $y_{\max} = (E - E_{S \min})/F$, $y_{\min} = (E - E_{S \max})/F$. Outside this interval, Ψ diminishes exponentially.

Now let us examine the motion of an electron in a field $V = Fy$, with allowance for the nondiagonal terms (assuming them to anomalously large). It is sufficient to examine two bands, s and r . Equation (I) in this case will be written in the form of the system

$$\begin{aligned} iF \partial g_s / \partial k_2 + (E_s - E) g_s + iFB g_r &= 0, \\ iF \partial g_r / \partial k_2 + (E_r - E) g_r - iFB g_s &= 0. \end{aligned} \quad (16)$$

Here the property (9) is accounted for and the symbol $B = \sum B_{\mathbf{m}S\mathbf{r}}^{010} e^{i\mathbf{k}\mathbf{m}}$ is introduced. By substituting

$$\begin{aligned} g_s &= \exp \left\{ \frac{1}{iF} \int [E - \frac{1}{2}(E_s + E_r)] dk_2 \right\} \psi_s, \\ g_r &= \exp \left\{ \frac{1}{iF} \int [E - \frac{1}{2}(E_s + E_r)] dk_2 \right\} \psi_r \end{aligned}$$

we bring system (16) to a more symmetrical form

$$\begin{aligned} iF \psi'_s + (E_s - E_r) \psi_s + iFB \psi_r &= 0, \\ iF \psi'_r - (E_s - E_r) \psi_r - iFB \psi_s &= 0. \end{aligned} \quad (17)$$

Assuming the field F to be weak, we seek a quasi-classical solution. We find that if we write $\psi_S = \exp(i\Phi_1/F)$, the solution for the second band has the form $\psi_r = iF\Phi_2 \exp(i\Phi_1/F)$, where Φ_1 and Φ_2 can be expanded by powers of iF .

$$\begin{aligned} \Phi_1 &= \frac{1}{2} \int (E_s - E_r) dk_2 + F^2 \int \frac{B^2}{E_s - E_r} dk_2 + \dots, \\ \Phi_2 &= -\frac{B}{E_s - E_r} - iF \left(\frac{B}{E_s - E_r} \right)' \frac{1}{E_s - E_r} + \dots \end{aligned} \quad (18)$$

In this manner, the solution has the following final form:

$$\begin{aligned} g_s &= \exp \left\{ \frac{1}{iF} \int_0^{k_2} (E - E_s) dk_2 + iF \int_0^{k_2} \frac{B^2}{E_s - E_r} dk_2 + \dots \right\} \\ g_r &= -\frac{iFB}{E_s - E_r} \\ &\times \exp \left\{ \frac{1}{iF} \int_0^{k_2} (E - E_s) dk_2 + iF \int_0^{k_2} \frac{B^2}{E_s - E_r} dk_2 + \dots \right\} \end{aligned} \quad (19)$$

In these formulas we can interchange s and r and thereby obtain a second solution.

As expected, the weaker the field F , the less the significance of the second band. Its contribution is the more significant the larger B is and the stronger the bands overlap, i.e., the smaller the difference $E_s - E_r$ (for a given \mathbf{k}). If the difference $E_S(\mathbf{k}) - E_R(\mathbf{k})$ is very small in any region of \mathbf{k} values, while the value of B is large, the contribution of both bands may become commensurate.

APPENDIX

Terms of the order $1/\alpha_0^4$ in Eq. (I) have the following explicit form:

$$\begin{aligned} \frac{1}{2\alpha_0^4} \sum_{s'} H_{ss'} g_{s'} &= \frac{1}{2\alpha_0^4} \left\{ \sum_{\mathbf{m}, s'} B_{\mathbf{m}ss'}^{020} e^{i\mathbf{k}\mathbf{m}} \sum_{\mathbf{n}} A_{\mathbf{n}s'} e^{i\mathbf{k}\mathbf{n}} (m_1 + n_1)^2 g_s \right. \\ &\times \left(k_2 - \frac{m_1 + n_1}{\alpha_0^2} \right) - E \sum_{\mathbf{m}, s'} B_{\mathbf{m}ss'}^{020} e^{i\mathbf{k}\mathbf{m}} g_{s'} \left(k_2 - \frac{m_1}{\alpha_0^2} \right) \\ &+ \frac{2i\hbar^2}{m_0} \sum_{\mathbf{m}, s'} (B_{\mathbf{m}ss'}^{100} + C_{\mathbf{m}ss'}^{110}) e^{i\mathbf{k}\mathbf{m}} g_{s'} \left(k_2 - \frac{m_1}{\alpha_0^2} \right) \\ &+ \frac{1}{4} \sum_{\mathbf{n}} A_{\mathbf{n}s} e^{i\mathbf{k}\mathbf{n}} n_1^2 n_2^2 g_s \left(k_2 - \frac{n_1}{\alpha_0^2} \right) \\ &\left. - \frac{\hbar^2}{m_0} \sum_{\mathbf{m}, s'} B_{\mathbf{m}ss'}^{200} e^{i\mathbf{k}\mathbf{m}} g_{s'} \left(k_2 - \frac{m_1}{\alpha_0^2} \right) \right\}. \end{aligned}$$

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