QUASIBOUND STATES IN A MAGNETIC FIELD AND IMPURITY FIELD. I. WEAK MAGNETIC FIELDS AND BORN POTENTIALS

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Approximate equations for finding the energy levels of quasibound states are formulated for an arbitrary short-range Born impurity potential in a weak magnetic field. The solutions of these equations are obtained in the quasiclassical case for a model with an isotropic quadratic dispersion and a Yukawa potential.

BOUND and quasibound states of an electron in a weak magnetic field at an impurity were investigated in[1-3]. However, in[1,2] the potential was assumed to be δ-like, which is incorrect in the case of a normal metal, and in[3] potentials of a special type were investigated. In this article we formulate a sufficiently simple algorithm for finding the spectrum and the damping of quasibound states on an arbitrary short-range Born potential in a crystal, and demonstrate its applicability to an isotropic model and a Yukawa potential in the quasiclassical case. It can be stated that the general character of the spectrum of the quasibound state remains in force for any short-range potential (particularly $1/r$ as $r \to 0$) and for any dispersion law that admits of closed extremal sections in the quasiclassical case.

1. GENERAL FORMULAS

We shall consider the problem of the energy levels of an electron in a magnetic field and an impurity field with a short-range potential $V(\mathbf{r})$. The effective radius of the potential will be denoted by r_0, and we introduce immediately the quantity[1)] $E_0 = 1/mr_0^2$, where m is a quantity on the order of the characteristic effective mass. If V is the mean value of the potential over a region with a dimension on the order of its effective radius (i.e., $V \sim r_0^{-3}\int V(\mathbf{r})d\mathbf{r}$), then $V/E_0 \ll 1$ is the condition under which the given potential is of the Born type and consequently the probability of appearance of a bound level in it in the absence of a magnetic field is small. These are precisely the potentials which we shall consider here. Thus, if $\hat{H}$ is the Hamiltonian of an electron in a magnetic field without an impurity, then we must investigate the "bound" level of the equation

$$(\hat{H} + V)\Psi = \omega\Psi$$

or, equivalently,

$$\Psi = GV\Psi, \tag{1}$$

where G is the Green's function of the problem without the impurity:

$$G = (\omega - \hat{H})^{-1} = \sum_{\mu} G_\mu(\omega)\Phi_\mu(\mathbf{r})\Phi_\mu^*(\mathbf{r}').$$

Here $\mu = (P_X, N, P_Z)$ is the aggregate of the corresponding quantum numbers, if the gauge of the vector potential is such that $A = \{-Hy, 0, 0\}$,

$$\hat{H}\Phi_\mu = \varepsilon_\mu\Phi_\mu,\ \varepsilon_\mu \equiv \varepsilon_{NP_z},\ \int \Phi_\mu^*\Phi_{\mu'}\,d\mathbf{r} = \delta_{\mu\mu'},\ G_\mu(\omega) = 1/(\omega - \varepsilon_\mu)$$

For concreteness we assume, unless otherwise stipulated, that $\mathrm{Im}\ \omega > 0$).

It is convenient to consider in lieu of (1) another equation (with an integrated singularity in G (see below)):

$$\psi = VG\psi, \tag{2}$$

where $\psi = V\Psi$ (from which it follows that $\Psi = G\psi$). If we rewrite Eq. (2) in the μ representation and separate the summation with respect to N, we obtain

$$\psi_N = \sum_{N'} \hat{K}_{NN'}\psi_{N'}, \tag{3}$$

where $\hat{K}_{NN'}$ are integral operators with two-dimensional kernels:

$$\hat{K}_{NN'}(\mathbf{PP}') = V_{P_xNP_z,\,P_x'N'P_z'}\,G_{N'P_z'}$$

($\mathbf{P}$ is the two-dimensional vector $\{P_X 0 P_Z\}$).

Let now $\omega \to \epsilon_{M0}$ (for simplicity we assume that $P_Z = 0$ is the point at which $\partial\epsilon_{MP_Z}/\partial P_Z = 0$. As will be shown below, terms of the type $\hat{K}_{NM}\psi_M$ then become infinite, and we shall therefore separate them in (3):

$$\psi_M = \hat{K}_{MM}\psi_M + \sum{}' \hat{K}_{MN}\psi_N, \tag{4}$$

$$\psi_N = \hat{K}_{NM}\psi_M + \sum{}' \hat{K}_{NN'}\psi_{N'}. \tag{4a}$$

The prime at the summation sign denotes that it does not include the term with N = M (or N′ = M).

We now express ψ_N of (4a) in terms of ψ_M and substitute in (4):

$$\psi_N = \sum{}'(1 - \hat{K})^{-1}_{NN'}\hat{K}_{N'M}\psi_M = \hat{K}_{NM}\psi_M + \sum{}'\hat{K}_{NN'}\hat{K}_{N'M}\psi_M + \sum{}'\hat{K}_{NN'}\hat{K}_{N'N''}\hat{K}_{N''M}\psi_M + \cdots$$

It is important that none of the summation indices (N′, N″, ...) assumes the value M, and therefore the ratio of any succeeding term to the preceding one (in terms of the normalization of the operators) is a quantity of the order of V/E_0; consequently, we can confine ourselves in the Born approximation to the first terms, and write

$$\psi_N \approx \hat{K}_{NM}\psi_M. \tag{4b}$$

[1)] We put $\hbar = 1$.

From (4) we now obtain an equation for ψ_M:

$$\psi_M \approx \hat{K}_{MM}\psi_M + \sum{}' \hat{K}_{MN}\hat{K}_{NM}\psi_M, \tag{5}$$

where the second term is smaller than the first (in terms of the normalization of the operators) by a factor V/E_0, but it determines the damping of the bound level if it is located inside the spectrum G (it is easily understood that the terminated series in (5) corresponds to the total scattering amplitude in the absence of a magnetic field, but we need not calculate it completely in the Born approximation). It is important that the regions of the values of the operators $\hat{K}_{MM}$ and $\Sigma'\hat{K}_{MN}\hat{K}_{NM}$ can readily be shown to coincide (even in the case of degenerate potentials). We can therefore construct for the calculations a corresponding perturbation theory, by regarding $\hat{K}_{MM}$ as the "unperturbed" operator. To this end, however, it is necessary to determine the function X^* that is conjugate to ψ (and does not coincide with ψ^*, since VG is not a self-adjoint operator):

$$X^* = X^*VG, \quad (X^*\psi) = \int X^*\psi d\mathbf{r} = 1.$$

A procedure similar to that carried out for ψ leads to the equation

$$X_M^* \approx X_M^*\hat{K}_{MM} + \sum{}' X_M^*\hat{K}_{MN}\hat{K}_{NM}, \tag{5a}$$

where

$$X_M^* = \int X^*(\mathbf{r})\Phi_M(\mathbf{r})\,d\mathbf{r}.$$

Proceeding in the sense of perturbation theory, we should solve the unperturbed equations

$$\psi_M^0 = \hat{K}_{MM}\psi_M^0, \quad X_M^{0*} = X_M^{0*}\hat{K}_{MM},$$
$$(X_M^{0*}\psi_M^0) \equiv \sum_P X_{MP}^{0*}\psi_{MP}^0 = 1 \tag{6}$$

and then determine from these functions the shift and the damping of the bound state. To this end, let us consider Eq. (6) in greater detail. We introduce the quantity $\xi = \omega - \epsilon_{M0}$ and rewrite (6) in the form (L_X and L_Z are the corresponding crystal dimensions)

$$\psi_{MP}^0 = \frac{L_z}{2\pi}\sum_{P_x'}\int dP_z'[\xi - (\varepsilon_{MP_z'} - \varepsilon_{M0})]^{-1}V_{MP,MP'}\psi_{MP'}^0.$$

It is now clear that if $\psi^0_{P_XM_0} \neq 0$, then the right-hand side of this equation tends to infinity as $\xi \to 0$. It is easily understood that it is precisely these solutions which correspond to the quasilocal levels (this will also be seen from the subsequent analysis). Accurate to $(\xi/E_0)^{1/2} \ll 1$, we can write

$$\psi_{MP}^0 \approx \frac{L_z}{2\pi}\sum_{P_x'}V_{MP,P_x'M0}\psi^0_{P_x'M0}\int dP_z'[\xi - (\varepsilon_{MP_z'} - \varepsilon_{M0})]^{-1} \approx \frac{L_z}{2\pi}f(\xi)\sum_{P_x'}V_{MP,P_x'M0}\psi^0_{P_x'M0}.$$

Here $f(\xi) = -i\pi/\sqrt{\alpha\xi}$, where $\alpha = \frac{1}{2}d^2\epsilon_{NP_Z}/dP_Z^2|_{P_Z=0}$. In the quasiclassical case (when $M \gg 1$), we can also write

$$\alpha = -\frac{1}{2}\frac{\partial^2 S}{\partial P_z^2}\left(\frac{\partial S}{\partial \omega}\right)^{-1}\Big|_{P_z=0},$$

where $S(\omega, P_Z)$ is the area of the corresponding equal-energy surface. The quantity α is thus half the reciprocal local effective mass. The root in $f(\xi)$ is so defined that $\sqrt{\alpha\xi} > 0$ when $\alpha\xi > 0$, Im $\xi = +0$ with a cut in the $\alpha\xi$ plane from 0 to ∞.

Thus we see that the solutions of (6) are obtained from the one-dimensional integral equation (which is independent of the energy)

$$\psi^0_{P_xM0} = q\sum_{P_x'}V_{P_xM0,P_x'M0}\psi^0_{P_x'M0}, \tag{7}$$

and the energy levels ξ_n^0, in the zeroth approximation with respect to V/E_0, are calculated from the equation

$$\frac{L_z}{2\pi}f(\xi_n^0) = q_n, \quad \xi_n^0 = -\frac{1}{\alpha}\left(\frac{L_z}{2q_n}\right)^2. \tag{7a}$$

It is clear that the q_n are real (since $V_{P_XP_X'} = V^*_{P_X'P_X}$), and that

$$\operatorname{sign} q_n = \operatorname{sign}\xi_n^0 = -\operatorname{sign}\alpha,$$

i.e., the bound states in an attracting potential lie lower (in energy) than the Landau level and appear in the case of positive local mass; in a repulsive potential they appear at negative local masses (holes) and lie above the Landau level.

It is now necessary to consider the second equation in (6). Since the function X_M^{0*} has a singularity as $\xi \to 0$, we introduce the function

$$\chi_M^{0*} = X_M^{0*}V_{MM} \equiv \sum_{P'}X_{MP'}^{0*}V_{MP',MP}, \quad X_{MP}^{0*} = \chi_{MP}^{0*}G_{MP_z},$$

where χ_M^{0*} satisfies the equation

$$\chi^{0*}_{P_xM0} = q\sum_{P_z'}\chi^{0*}_{P_x'M0}V_{P_x'M0,P_xM0},$$

from which it is clear that $\chi_M^{0*} = C\psi_M^{0*}$.

We can now consider the equation (5):

$$1 = (X_M^{0*}\psi_M^0) = (X_M^{0*}\hat{K}_{MM}(\xi)\psi_M^0) + \sum{}'(X_M^{0*}\hat{K}_{MN}\hat{K}_{NM}\psi_M^0)$$
$$= \frac{f(\xi)}{f(\xi^0)} + \sum_N{}'(\chi_M^{0*}G_MV_{MN}G_NV_{NM}G_M\psi_M^0) = \frac{f(\xi)}{f(\xi^0)}$$
$$+\left[\frac{L_z}{2\pi}f(\xi^0)\right]^2(\chi^{0*}_{P_xM0}T_{P_xM0,P_x'M0}\psi^0_{P_x'M0}) = \frac{f(\xi)}{f(\xi^0)} + \left[\frac{L_z}{2\pi}f(\xi^0)\right]^2 T.$$

In the second term we have written $f(\xi^0)$, since it constitutes a small increment. We use here the notation

$$T_{MP,MP'} = \sum_{N\neq M,Q}V_{MP,NQ}G_{NQ}V_{NQ,MP'}$$
$$= \int\Phi_{MP}^*(\mathbf{r})V(\mathbf{r})\tilde{G}(\mathbf{r}\mathbf{r}'\omega)V(\mathbf{r}')\Phi_{MP'}(\mathbf{r}')\,d\mathbf{r}d\mathbf{r}', \tag{8}$$

where $\tilde{G}$ is the Green's function of the crystal in the absence of a magnetic field (see Appendix B). Putting $\xi = \xi^0 + \delta\xi$ and recognizing that

$$f(\xi^0 + \delta\xi) = f(\xi^0) - \tfrac{1}{2}(f(\xi^0)/\xi^0)\delta\xi,$$

we obtain

$$\frac{\delta\xi_n}{\xi_n^0} = 2\left[\frac{L_z}{2\pi}f(\xi_n^0)\right]^2 T_{n,n} = 2q_n^2T_{n,n}, \tag{9}$$

where $T_{n,n}$ is the average of the operator (8) over the functions χ_n^{0*} and ψ_n^0 corresponding to the eigenvalue n of q_n of Eq. (7).

It is also useful to write out the normalization of the functions χ^* and ψ. It is obtained directly from (6):

$$1=(X^{0*}_{nM}\psi_{nM}{}^0)=(\chi^{0*}_{nM}G_M\psi_{nM}{}^0)=\frac{L_z}{2\pi}f(\xi_n{}^0)\sum_{P_x}\chi^{0*}_{nP_xM0}\psi^0_{nP_xM0}$$
$$=q_n(\chi^{0*}_{nM}\psi^0_{nM})^0. \tag{6b}$$

The upper index zero denotes here that the sum over P_X is taken at the extremal point of ϵ_{MP} (in our case, at $P_Z = 0$).

We shall investigate the resultant expressions (7)–(9) in further detail later, and present now certain general estimates. Since $\Phi_N \sim (L_XL_ZR_N)^{-1/2}$, where $R_N \sim (\epsilon_{N0}/m)^{1/2}/\Omega$ is the Larmor radius and Ω is the frequency of revolution of the electron in its orbit, then for $\omega \lesssim E_0$, in the entire interval ΔP_X of the summation in (7) ($\Delta P_X \sim \sigma R_M$, $\sigma = |e|H/c \sim m\Omega$), we have $V_{MM} \sim Vr_0^3/L_XL_ZR_M$, and therefore the smallest values are $q_0 \sim L_ZE_0\sqrt{mE_0}/V\Omega$ and $\xi_0^0 \sim (\Omega^2/E_0)(V/E_0)^2$. If $\omega \gtrsim E_0$, then the main contribution to (7) is made by the region $|P_X - P'_X| \lesssim 1/r_0$, where V_{MM} is, as before, of the order of $Vr_0^3/L_XL_ZR_M$, and $q_0 \sim L_ZE_0\sqrt{m\omega}/V\Omega$, $\xi_0^0 \sim (\Omega^2/\omega)(V/E_0)^2$. From (8) we can see that when $\omega \lesssim E_0$ we have $\mathrm{Re}\, q_0^2T_{00} \sim V/E_0$, $\mathrm{Im}\, q_0^2T_{00} \sim (V/E_0)(\omega/E_0)^{1/2}$, and when $\omega \gtrsim E_0$ we have $\mathrm{Re}\, q_0^2T_{00} \sim V/\omega$, $\mathrm{Im}\, q_0^2T_{00} \sim (V/E_0)(E_0/\omega)^{1/2}$, i.e., $\mathrm{Im}\, \delta\xi/\xi$ assumes a maximum value $\sim V/E_0$ when $\omega \sim E_0$.

Since Eq. (7) is obtained from (6) with accuracy $\sim\sqrt{\xi/E_0}$, we see from the foregoing estimates that it is suitable for $\omega \lesssim E_0$ if $\Omega \ll E_0$ or for $\omega \gtrsim E_0\sqrt{E_0/\omega}$ (the error in (7) should be much smaller than the subsequently calculated correction).

2. THE QUASICLASSICAL CASE

In normal metals, the case most frequently encountered is the quasiclassical one. Although the corresponding equations are perhaps easier to obtain in the coordinate representation, we shall adhere to the procedure described in Sec. 1. To this end we calculate the matrix element $V_{\mu\mu'}$, using formulas (A.13) and (A.14) of Appendix A:

$$V_{\mu\mu'}=2\pi\sigma\sum_{aa'}c_\mu{}^{a*}c_{\mu'}{}^{a'}\vartheta_a{}^*\vartheta_{a'}V_{Q_aQ_{a'}}\exp[i(\varphi_{a'}-\varphi_a)]. \tag{10}$$

Here

$$V_{QQ'}=\int\psi_{nQ}{}^*(\mathbf{r})\,V(\mathbf{r})\,\psi_{nQ'}(\mathbf{r})\,d\mathbf{r},\qquad Q_a=(P_xk_y{}^aP_z)$$

and the ϑ_a are taken outside the integral sign for reasons explained in Appendix A (following formula (A.14)). Eq. (7) is now written in the form

$$\psi_{P_x}=\sigma L_zf(\xi)\sum_{P_x'aa'}c_\mu{}^{a*}c_\mu{}^{a'}\vartheta_a{}^*\vartheta_{a'}V_{Q_aQ_{a'}}\psi_{P'_x}\exp[i(\varphi_{a'}-\varphi_a)]. \tag{11}$$

It is quite clear that it is convenient to seek a solution in the form

$$\psi_{P_x}=\sum_b c_\mu{}^{b*}\exp(-i\varphi_b)\vartheta_b{}^*\psi^b_{P_x}, \tag{12}$$

and it is obvious that on the right-hand side of (11) it is necessary to retain only the terms with $b = a'$ (if $b \neq a'$, strongly oscillating factors appear). We therefore obtain the following equation for ψ^a:

$$\psi^a_{P_x}=\sigma L_zf(\xi)|c_\mu|^2\sum_{P'_xa'}V_{Q_aQ_{a'}}\frac{\psi^{a'}_{P'_x}}{|v_y^{a'}|}.$$

We note now that the points Q_a and $Q_{a'}$ differ only in the value of k_γ^a, so that by introducing the two-dimensional vector $s = \{s_X, s_Y, 0\}$, we can write (substituting $|c_\mu|$ from (A.15)):

$$\psi_s=\Omega_\mu\frac{\Omega_0}{(2\pi)^3}f(\xi)\oint\frac{dl}{v_\perp}V_{ss'}\psi_{s'}. \tag{13}$$

Here $\Omega_\mu = \sigma/|m^*_\mu|$, and dl is the trajectory-arc element corresponding to the vector s'.

Equation (13) is convenient for numerical calculations and should be investigated separately for each concrete situation (the potential $V(r)$ and the dispersion law $\epsilon_n(k)$).

We now write out the normalization (6b) for ψ_s (it is clear that $\chi^*_s = -\psi^*_s$ for $\alpha > 0$ and $\chi^*_s = \psi^*_s$ for $\alpha < 0$:

$$1=-\frac{L_z}{2\pi}f(\xi)\,\mathrm{sign}\,\alpha\sum_{P_x{}^a}|c_\mu{}^a|^2|\vartheta_a|^2|\psi^a_{P_x}|^2=-\frac{\Omega_0}{(2\pi)^3}f(\xi)\cdot$$
$$\cdot\frac{\mathrm{sign}\,\alpha}{2\pi|m_\mu{}^*|}\oint\frac{dl}{v_\perp}|\psi_s|^2. \tag{14}$$

For the operator from (8) we obtain analogously

$$T_{\mu\mu'}=2\pi\sigma\sum c_\mu{}^{a*}c_{\mu'}{}^{a'}\vartheta_a{}^*\vartheta_{a'}T_{Q_aQ_{a'}}\exp[i(\varphi_{a'}-\varphi_a)],$$

where

$$T_{QQ'}=\int\psi_{nQ}{}^*(\mathbf{r})\,V(\mathbf{r})\,\bar G(\mathbf{r}\mathbf{r}'\omega)\,V(\mathbf{r}')\,\psi_{nQ'}(\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}',$$

after which it becomes clear that $T_{n,n}$ (see (9)) can be written in the form

$$T_{n,\,n}=-\,\mathrm{sign}\,\alpha\cdot2\pi\sigma|c_\mu|^4\sum_{P_x,\,P_x';\,a,\,a'}\frac{\psi^{a*}_{P_x}}{|v_y{}^a|}T_{Q_aQ_{a'}}\frac{\psi^{a'}_{P'_x}}{|v_y{}^{a'}|}=$$
$$=-2\pi\sigma\left[\frac{\Omega_0}{(2\pi)^3}\frac{2\pi}{L_z}\right]^2\frac{\mathrm{sign}\,\alpha}{(2\pi m_\mu{}^*)^2}\oint\frac{dl}{v_\perp}\frac{dl'}{v_\perp{}'}\psi_s{}^*T_{ss'}\psi_{s'}.$$

We therefore have in lieu of (9)

$$\frac{\delta\xi}{|\xi^0|}=4\pi\sigma\left[\frac{\Omega_0}{(2\pi)^3}f(\xi)\right]^2\frac{1}{(2\pi m_\mu{}^*)^2}\oint\frac{dl}{v_\perp}\frac{dl'}{v_\perp{}'}\psi_s{}^*T_{ss'}\psi_{s'}. \tag{15}$$

Thus, if we know the solutions of (13) with the normalization (14), we can determine the shift and damping of the quasilocal level from (15).

It should be noted, however, that in the derivation of (13) it is important to use the assumption that the functions are smooth (have a small number of oscillations compared with ϑ_a), so that the solutions obtained from (13) will correspond to reality only if the number of solutions n is such that $n \ll M$. As a rule, however, this is sufficient, since solutions with large n correspond to quasilocal levels that lie very close to the Landau level and are therefore strongly smeared out as a result of the fact that we are actually dealing with many impurity centers.

In the isotropic case we can proceed somewhat farther in the solution of (13). It is now necessary to assume that $\psi_{nQ} = \Omega_0^{-1/2}e^{iQr}$ (Ω_0 is perfectly arbitrary). We introduce polar coordinates s, φ (such that $s = s\{\cos\varphi, \sin\varphi, 0\}$); then $dl = sd\varphi$ and since

$$V_{ss'}=\Omega_0{}^{-1}V(|s-s'|)=\Omega_0{}^{-1}V(\varphi-\varphi'), \tag{16}$$

where

$$V(s)=V(|s|)=\int V(r)e^{-isr}\,dr_\perp$$

we can write (13) in the form

$$\psi(\varphi)=\frac{\Omega_\mu}{(2\pi)^3}f(\xi)\frac{s}{v}\int_0^{2\pi}d\varphi' V(\varphi-\varphi')\psi(\varphi') = \lambda\int_0^{2\pi}d\varphi' V(\varphi-\varphi')\psi(\varphi') \tag{13a}$$

(s = mv only in the case of a quadratic dispersion law). It is now obvious that it suffices to expand V in a Fourier series

$$V(\varphi-\varphi')=\sum V_n\exp[in(\varphi-\varphi')],\quad V_n=\frac{1}{2\pi}\int_0^{2\pi}d\varphi\, V(\varphi)\exp(-in\varphi), \tag{17}$$

since we obtain immediately

$$\psi_n(\varphi)=C_n e^{in\varphi},\quad \lambda_n=\frac{1}{2\pi V_n}\left(=\frac{\Omega_\mu}{(2\pi)^3}f(\xi_n^0)\frac{s}{v}\right). \tag{18}$$

From (14) we now obtain

$$1=-\operatorname{sign}\alpha\frac{\Omega_0}{\sigma}\frac{\lambda_n}{2\pi}\int_0^{2\pi}d\varphi|\psi_n|^2=\frac{\Omega_0}{\sigma}|\lambda_n||C_n|^2. \tag{14a}$$

It is obvious that

$$T_{ss'}=\Omega_0^{-1}\int d\mathbf{r}\,d\mathbf{r}' V(\mathbf{r})\bar{G}(\mathbf{r}\mathbf{r}'\omega)V(\mathbf{r}')\exp[i(\mathbf{s}'\mathbf{r}'-\mathbf{s}\mathbf{r})]$$

depends only on the angle between $\mathbf{s}$ and $\mathbf{s}'$, and therefore, denoting the latter integral by $T(\varphi-\varphi')=\Omega_0 T_{ss'}$ and expanding in a Fourier series

$$T(\varphi-\varphi')=\sum T_n\exp[in(\varphi-\varphi')],\quad T_n=\frac{1}{2\pi}\int_0^{2\pi}d\varphi\, T(\varphi)\exp(-in\varphi), \tag{19}$$

we obtain

$$\frac{\delta\xi_n}{|\xi_n^0|}=4\pi\sigma\left[\frac{f(\xi)}{(2\pi)^3 m_\mu^*}\frac{s}{v}\right]^2\Omega_0|C_n|^2T_n=\frac{4\pi}{\sigma}\Omega_0\lambda_n^2|C_n|^2T_n=4\pi|\lambda_n|T_n. \tag{15a}$$

Since $V(\varphi)=V(-\varphi)$, each ξ_n is doubly degenerate with wave functions $e^{in\varphi}$ and $e^{-in\varphi}$.

In the next section we shall demonstrate how to obtain the solutions in a model with an isotropic quadratic dispersion law and a Yukawa potential.

3. ISOTROPIC QUADRATIC DISPERSION LAW AND A YUKAWA POTENTIAL

Our potential now has the form $V(r)=\beta e^{-\kappa r}/r$, and

$$\bar{G}(\mathbf{r}\mathbf{r}'\omega)=-\frac{m}{2\pi}\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|},\quad k=\sqrt{2m\omega}, \tag{20}$$

with $k>0$ when $\omega>0$, $\operatorname{Im}\omega=+0$, and $\beta<0$,

$$V(s-s')=\frac{4\pi\beta}{(s-s')^2+\kappa^2}=\frac{4\pi\beta}{2k^2(1-\cos(\varphi-\varphi'))+\kappa^2}$$

(Since $|s|=|s'|=k$)

$$V_n=\frac{1}{2\pi}\int_0^{2\pi}\frac{4\pi\beta e^{-in\varphi}}{2k^2(1-\cos\varphi)+\kappa^2}d\varphi.$$

This integral is evaluated along the contour $|z|=1$ with the change of variables $z=e^{-i\varphi}$ for $n>0$ or $z=e^{i\varphi}$ for $n<0$ ($V_n=V_{-n}$):

$$V_n=2\pi\beta x^{2n}/\kappa k\nu, \tag{21}$$

where

$$x=\nu-\kappa/2k,\quad \nu^2=1+\kappa^2/4k^2.$$

Since $\lambda=f(\xi)\sigma/(2\pi)^3$ (see (13a)) and half the reciprocal local mass is $\alpha=(2m)^{-1}$, we obtain

$$\xi_n^0=-2m\left(\frac{\sigma V_n}{4\pi}\right)^2=-\frac{m\sigma^2\beta^2x^{4n}}{2\kappa^2k^2\nu^2}. \tag{22}$$

For $k\ll\kappa$ (if, of course, the quasiclassical approach is valid) we have $\nu\approx\kappa/2k+k/\kappa$ and $x\approx k/\kappa$, so that we obtain

$$\xi_n^0\approx-\frac{2m\sigma^2\beta^2}{\kappa^4}\left(\frac{k}{\kappa}\right)^{4n}, \tag{23}$$

i.e., some significance attaches to the quantity

$$\xi_0^0\approx-\frac{2m\sigma^2\beta^2}{\kappa^4}=-\frac{2m^3\Omega^2\beta^2}{\kappa^4}. \tag{23a}$$

This expression should be compared with the results obtained from the general formula (7) at low energies. Since the wave function changes little over distances on the order of r_0 when $kr_0\ll1$, it is clear that

$$V_{\mu\mu'}\approx\Phi_\mu^*(0)\Phi_{\mu'}(0)u,\quad u=\int V(r)\,dr. \tag{23b}$$

Therefore (7) can be solved immediately and yields

$$\psi_\mu=C\Phi_\mu^*(0),\quad qu\Lambda_{N0}(00)=1 \tag{23c}$$

(Λ is defined in Appendix B). In this case it is necessary to use formula (B.2) and, since $L_N(0)=1$, we obtain the well-known result[1,2]:

$$\xi_0^0=-m\frac{u^2\sigma^2}{8\pi^2}. \tag{23d}$$

For a Yukawa potential $u=4\pi\beta/\kappa^2$, from which (23a) follows directly.

When $k\gg\kappa$ we have $\nu\approx1$ and $x\approx1-\kappa/2k$, so that for the root with a given n we obtain $\xi_n^0\to\xi_0^0$ as $k\to\infty$.

We now turn to calculate T_n:

$$T(\varphi-\varphi')=\int V(s-q)\bar{G}(q\omega)V(q-s')\frac{dq}{(2\pi)^3}= =\frac{2\beta^2}{\pi}\int\left\{[(s-q)^2+\kappa^2][(s'-q)^2+\kappa^2]\left(\omega-\frac{q^2}{2m}\right)\right\}^{-1}dq.$$

Straightforward but cumbersome calculations yield for the second-order correction to the Born scattering amplitude the expression

$$T(\varphi)=-\frac{2\pi m\beta^2}{kt\gamma}\left(\frac{\pi}{2}-\operatorname{arctg}\frac{2k\gamma}{\kappa t}+\frac{i}{2}\ln\frac{\gamma+t}{\gamma-t}\right),$$

where $\gamma^2=\kappa^2\nu^2+t^2$, $t=k|\sin(\varphi/2)|$. Just as in the calculation of V_n, we write T_n in the form of an integral over the contour $|z|=1$, $z=e^{i\varphi}$ (it is clear that since $T(\varphi)$ is an even function of φ, the expansion is only in terms of the cosines, i.e., $T_n=T_{-n}$), but in this case there are no residues, and only branch points. If we make the substitution $t(z)=k(z-1)/2i\sqrt{z}$, $\gamma(z)=k\sqrt{(z_+-z)(z-z_-)}/2\sqrt{z}$ ($0\le\arg z<2\pi$), where

$$z_\pm=1+\frac{2\kappa^2\nu^2}{k^2}\pm\frac{2\kappa\nu}{k}\left(1+\frac{\kappa^2}{2k^2}\right), \tag{24}$$

then, as shown by a detailed analysis, the integral over the contour $|z|=1$, $0\le\arg z<2\pi$, for the quantity $\varphi_n=-T_nk^3/4\pi m\beta^2$ can be written in the form

$$\varphi_n=\int_C\frac{z^n\,dz}{(1-z)\sqrt{(z_+-z)(z-z_-)}}, \tag{25}$$

where the path C extends from the point 0 to the point z_1 and circles around the point z_- from below, with $\sqrt{(z_+-z)(z-z_-)}>0$ when $z>z_-$. The point z_1 is one of the branch points of $\tan^{-1}2k\gamma/\kappa t$:

$$z_1=1+\frac{2\kappa^2}{k^2}-\frac{2\kappa}{k}\sqrt{1+\frac{\kappa^2}{k^2}}=\left(\sqrt{1+\frac{\kappa^2}{k^2}}-\frac{\kappa}{k}\right)^2 \tag{26}$$

(It is easy to show that $z_- < z_1 < 1 < z_+$).

The integrals in (25) can be evaluated directly, but the resultant expressions are cumbersome and difficult to interpret, and contain triple sums with Chebyshev polynomials of the second kind U_n (see[4]), so that numerical results are more illustrative.

The calculations were performed by means of recurrence formulas expressing φ_{n+1} in terms of φ_n (see[4]). It follows from (18), (15a), and (21) that in this case $T_n = -4\pi m\beta^2\varphi_n/k^3$)

$$\frac{\delta\xi_n}{\xi_n^0} = \frac{2T_n}{V_n} = \frac{4m|\beta|}{\varkappa}\left(\frac{\varkappa}{k}\right)^2 \nu \frac{\varphi_n}{(\sqrt{z_-})^n} = \frac{4m|\beta|}{\varkappa}\tau_n\left(\frac{k}{\varkappa}\right) \tag{27}$$

(it is easily seen that x in (21) coincides with $z_-^{1/4}$ from (24)). The first ten functions τ_n, which depend on a single argument $k/\varkappa$, were calculated with the aid of a Ural-2 computer.

The results for the first three functions τ_0, τ_1, and τ_2 are shown in the figure, where the abscissas represent $k/\varkappa$ in a logarithmic scale. We note that the coefficient $4m|\beta|/\varkappa$ in (27) is of the order of V/E_0 (since, obviously, $V \sim \beta\varkappa$).

A simple investigation of the general formula (25) for φ_n shows that in limiting cases we can obtain the following expressions for τ_n:

$$\tau_n \approx \frac{1}{2^{2n+1}(2n+1)} + i\frac{2^n n!}{(2n+1)!!}\left(\frac{k}{\varkappa}\right)^{2n+1}, \quad k \ll \varkappa, \tag{28}$$

$$\tau_n \approx \frac{1}{4}\left(\frac{\varkappa}{k}\right)^2 + i\frac{\pi}{4}\frac{\varkappa}{k}, \quad k \gg \varkappa. \tag{28a}$$

When $k \ll \varkappa$ we obtain from (8) and (20) the following expression for $T_{\mu\mu'}$:

$$T_{\mu\mu'} \approx -\Phi_\mu^*(0)\Phi_{\mu'}(0)\frac{m}{2\pi}\int\frac{V(\mathbf{r})V(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}\,d\mathbf{r}' - i\frac{mk}{2\pi}u^2\Phi_\mu^*(0)\Phi_{\mu'}(0) \tag{29}$$

(For a definition of u see (23b). The wave functions of the "bound" approximation are known (see (23c)):

$$\psi_\mu = C\Phi_\mu^*(0), \quad \chi_\mu^* = -C^*\Phi_\mu(0),$$

and obviously (see (6c) and (B.1)),

$$-q|C|^2\Lambda_{N0}(00) = 1,$$

so that we obtain the well-known expression[2]

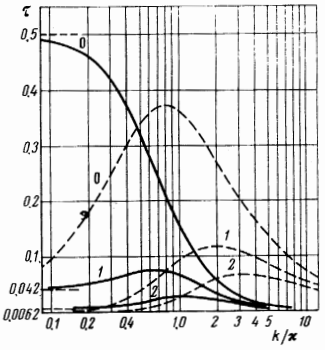
$$\mathrm{Im}\,\delta\xi_0/\xi_0^0 = -mku/\pi.$$

In our case $u = 4\pi\beta/\varkappa^2$ and

$$\mathrm{Im}\,\delta\xi_0/\xi_0^0 = 4mk|\beta|/\varkappa^2,$$

as follows also from (29) when n = 0.

The quasilocal levels are produced as a result of the fact that the problem in a magnetic field is in a certain sense one-dimensional: the energy depends only on one continuous parameter P_Z. Actually, however, besides the usual motion in the magnetic field, the particle is scattered by the impurity potential. This causes the scattering amplitude a (at zero magnetic fields) to appear as the potential in the corresponding one-dimensional equation ((4) or (5)) (for example, the decay of the "bound" state with $|P_Z| < \sqrt{m\Omega}$ is due to scattering into states with large P_Z). In the one-dimensional problem we have $\xi \sim U^2/E_0$,



Results of calculations for the functions τ_0 (0), τ_1 (1) and τ_2 (2). Solid lines—Re τ_n, dashed—Im τ_n. The horizontal dashed lines show the values of Re τ_n calculated from (28) as $k \to 0$.

where U is the average value of the potential "sensed" by the particle (see[5]). When $\Omega \ll E_0$, the particle is, in the main, outside the field of the potential, and therefore, as can be readily understood, $U \sim a\Omega/E_0$ when $\omega \lesssim E_0$ and $U \sim a\Omega/\sqrt{\omega E_0}$ when $\omega \gtrsim E_0$; further, Im a/Re a decreases when $\omega \to 0$ and $\omega \to \infty$, thereby explaining the character of the estimates at the end of Sec. 1 and of the curves in the figure.

An infinite number of levels is produced as a result of lifting of the degeneracy with respect to P_X, but when $\omega \to 0$ the potential can be regarded as δ-like, and therefore there actually remains only one eigenvalue ξ_0 (see Eq. (23)).

In conclusion, the author thanks R. G. Arkhipov for useful discussions and for interest in the work.

APPENDIX A

WAVE FUNCTIONS OF THE ELECTRONS IN A CRYSTAL IN A MAGNETIC FIELD

We consider here the quasiclassical case. A study of the wave functions is particularly simple if the technique developed by Zak is used[6]. Namely, $\Phi_\mu(\mathbf{r})$ is expanded in the eigenfunctions of the so called (k, x) representation

$$\Phi_\mu(\mathbf{r}) = \int d\mathbf{k}\,d\mathbf{x}\Phi_\mu(\mathbf{k},\mathbf{x})\psi_{\mathbf{kx}}(\mathbf{r}),$$
$$\psi_{\mathbf{kx}}(\mathbf{r}) = \sqrt{\Omega_0/(2\pi)^3}\sum_{\mathbf{a}}\delta(\mathbf{r}-\mathbf{x}-\mathbf{a})e^{i\mathbf{ka}}. \tag{A.1}$$

Here Ω_0 denotes the volume of the unit cell of the crystal, the integration over k and x extends over the volumes of the reciprocal and direct cells. If we write

$$\Phi_\mu(\mathbf{k},\mathbf{x}) = U_\mu(\mathbf{k},\mathbf{x})e^{i\mathbf{kx}},$$
$$U_\mu(\mathbf{k},\mathbf{x}) = \sum_n A_n(\mathbf{k})u_{n0}(\mathbf{x}) \tag{A.2}$$

(u_{n0} is the periodic part of the Bloch function at k = 0) then, as shown in[6], there exist functions[2)] $\Phi_\mu(\mathbf{k}, n)$ for which the equation in the lowest order in H can be written in the form

$$[\varepsilon_n(\mathbf{k})]\Phi_\mu(\mathbf{k}, n) = \varepsilon\Phi_\mu(\mathbf{k}, n) \tag{A.3}$$

[2)]These functions coincide with the $B_n(\mathbf{k})$ from Eqs. (64) and (67) of the first reference in [6]; they must not be confused with the $B_n(\mathbf{k})$ of Eq. (50) of the same reference.

and which in the lowest order in H are connected with $A_n(\mathbf{k})$ by the equation

$$A_n(\mathbf{k}) = \sum_m [S_{nm}(\mathbf{k})]\Phi_\mu(\mathbf{k}, m). \quad (A.4)$$

Here $[\epsilon_n(\mathbf{k})]$ is obtained from the dispersion law $\epsilon_n(\mathbf{k})$ in the absence of a magnetic field by symmetrizing all the components of the vector $\mathbf{k}$ and by replacing them with the operator $\kappa = \mathbf{k} - ec^{-1}\mathbf{A}(i\nabla_{\mathbf{k}})$. A similar operation is carried out on the matrix elements of the unitary transformation

$$u_{n\mathbf{k}}(\mathbf{x}) = \sum_m S_{mn}(\mathbf{k})u_{m0}(\mathbf{x}) \quad (A.5)$$

to obtain the operators $[S_{mn}(\mathbf{k})]$.

The solution of (A.3) is known (see, for example,[7]):

$$\Phi_\mu(\mathbf{k}, n) = \Delta(k_x - P_x)\delta(k_z - P_z)\tilde{\Phi}_\mu(k_y, n)\exp(P_x k_y / i\sigma), \quad (A.6)$$

if the gauge is $\mathbf{A} = \{-Hy, 0, 0\}$, with

$$\tilde{\Phi}_\mu(k_y, n) = \sum \tilde{c}_\mu^\alpha \Phi_\mu^\alpha(k_y, n),$$
$$\Phi_\mu^\alpha(k_y, n) = |v_x^\alpha(\pi_x, k_y, P_z)|^{-1/2}\exp(-S^\alpha(k_y)/i\sigma), \quad (A.7)$$
$$S^\alpha(k_y) = \int^{k_y} \pi_x^\alpha(k_y)\,dk_y, \quad \sigma = \frac{|e|H}{c}, \quad \mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}}\varepsilon_n(\mathbf{k}),$$

and the index α numbers the possible solutions of the equation

$$\varepsilon_n(\pi_x, k_y, P_z) = \varepsilon_\mu \quad (A.8)$$

and $\Delta(k_x)$ is a periodic δ function (with the period b_x of the reciprocal lattice).

From the quasiclassical-quantization condition we obtain immediately a formula for $\epsilon_\mu \equiv \epsilon_{NP}$:

$$S(\varepsilon_\mu P_z) = \oint \pi_x\,dk_y = 2\pi\sigma(N + 1/2), \quad (A.9)$$

where N is an integer suitable for cases when there is no self-intersection of the trajectories, magnetic breakdown, etc.

To calculate the wave function, we now employ, in the required order, all the numbered relations (A.1)–(A.6), and obtain

$$\Phi_\mu(\mathbf{r}) = \sqrt{\Omega_0/(2\pi)^3}\sum_{\mathbf{a}}\int d\mathbf{k}\,d\mathbf{x}\Phi_\mu(\mathbf{kx})\delta(\mathbf{r} - \mathbf{x} - \mathbf{a})e^{i\mathbf{ka}}$$
$$= \sqrt{\Omega_0/(2\pi)^3}\int d\mathbf{k}\Phi_\mu(\mathbf{k}\langle\mathbf{r}\rangle)e^{i\mathbf{ka}},$$

Here $\langle\mathbf{r}\rangle$ denotes $\mathbf{r}$ per unit cell and $\mathbf{a} = \mathbf{r} - \langle\mathbf{r}\rangle$.

We obtain further from (A.2), (A.4), and (A.5)[3]

$$\Phi_\mu(\mathbf{r}) = \sqrt{\Omega_0/(2\pi)^3}\int d\mathbf{k}\,e^{i\mathbf{kr}}U_\mu(\mathbf{k}, \langle\mathbf{r}\rangle)$$
$$= \sqrt{\Omega_0/(2\pi)^3}\sum_{n,m}\int d\mathbf{k}\,e^{i\mathbf{kr}}u_{n0}(\mathbf{r})[S_{nm}(\mathbf{k})]\Phi_\mu(\mathbf{k}, m)$$
$$= \sqrt{\Omega_0/(2\pi)^3}\sum_{n,m}\int d\mathbf{k}\,e^{i\mathbf{kr}}u_{n0}(\mathbf{r})S_{nm}(\pi_x + k_x - P_x, k_y, k_z)\Phi_\mu(\mathbf{k}, m)$$
$$= \sqrt{\Omega_0/(2\pi)^3}\sum_n\int dk e^{ik\mathbf{r}}u_{n\pi_x k_y k_z}(\mathbf{r})\Phi_\mu(\mathbf{k}, n)\exp[i(P_x - k_x)x],$$

after which (A.6) and (A.7) yield

$$\Phi_\mu(\mathbf{r}) = e^{i\mathbf{Pr}}\sum_{\alpha,n} c_\mu^\alpha \int dk_y u_{n\pi_x k_y P_z}(\mathbf{r})\Phi_\mu^\alpha(k_y, n)\exp\left(\frac{P_x - \sigma y}{i\sigma}k_y\right) \quad (A.10)$$

[3] The action of symmetrized operators on a quasiclassical wave function is described in [7].

By c_μ^α we denote here the quantities $[\Omega_0/(2\pi)^3]^{1/2}\tilde{c}_\mu^\alpha$ and $\mathbf{P}$ is a two-dimensional vector $(P_x, 0, P_z)$. We note that actually the summation over n need not be carried out here, since the quasiclassical wave function differs from zero only for one value of n having a bearing on our situation (i.e., entering in the equations (A.3) and (A.8)), if there are no close-lying bands (for other n′ the wave function is of the order $\exp(-|\epsilon_{n'}(\mathbf{k}) - \epsilon_n(\mathbf{k})|/\Omega)$.

For not too small v_y (see below) we can carry out the integration in (A.10) by the saddle-point method, if we recognize that $u_{n\mathbf{k}}$ changes appreciably over distances $\mathbf{k}$ on the order of the reciprocal-lattice vector $\mathbf{b}$ (this is connected with the fact that $\mathbf{k}$ numbers the number of nodes of the Bloch function $\psi_{n\mathbf{k}}$ in the entire crystal, whereas the variation of k over the reciprocal-lattice vector corresponds in a certain sense to a transition to the next band and thus changes the number of nodes in the unit cell by unity).

The integral in (A.10) can be written in the form

$$\int dk_y u_{n\pi_x k_y P_z}(\mathbf{r})|v_x^\alpha(\pi_x, k_y, P_z)|^{-1/2}\exp(\Sigma^\alpha(k_y)/i\sigma),$$

where $\Sigma^\alpha(k_y) = (P_x - \sigma y)k_y - S^\alpha(k_y)$. The stationary point Σ, $\partial\Sigma/\partial k_y = 0$, corresponds to the equation

$$P_x - \sigma y - \pi_x^\alpha = 0 \quad (A.11)$$

and further

$$\frac{\partial^2\Sigma}{\partial k_y^2} = -\frac{\partial\pi_x}{\partial k_y} = \frac{v_y}{v_x}$$

(π_x' is obtained from (A.8)). Integrating, we obtain

$$\Phi_\mu(\mathbf{r}) = e^{iPr}\sqrt{2\pi\sigma}\sum_a c_\mu^a e^{i\varphi_a}|v_y^a|^{-1/2}n_{nQ_a}(\mathbf{r})\exp\frac{(P_x - \sigma y)k_y^a - S^a}{i\sigma} \quad (A.12)$$

The letter a numbers here the possible solutions of (A.11),

$$Q_a = \{\pi_x^a, k_y^a, P_z\} \equiv \{P_x - \sigma y, k_y^a, P_z\}, \quad \mathbf{v}^a = \mathbf{v}(\mathbf{Q}_a),$$
$$S^a = S(k_y^a), \quad \varphi_a = -\frac{\pi}{4}\operatorname{sign}\Sigma_a'' = -\frac{\pi}{4}\operatorname{sign}\frac{v_y^a}{v_x^a}.$$

Since the stationary interval is Σ, $\delta k_y \sim \sqrt{\sigma/|\Sigma''|} \sim \sqrt{\sigma|v_x|/|v_y|}$, it is clear that (A.12) is suitable only for v_y such that $\sqrt{\sigma|v_x|/|v_y|} \ll b$ (we recall that the quasiclassical analysis is in general suitable only for fields such that $\sqrt{\sigma} \ll b$). If we introduce the notation

$$\vartheta_a = |v_y^a|^{-1/2}\exp\frac{P_x k_y^a - S^a}{i\sigma}, \quad (A.13)$$

then, as can be readily seen, (A.12) can be written in the convenient form

$$\Phi_\mu(\mathbf{r}) = e^{i\sigma xy}\sqrt{2\pi\sigma}\sum_a c_\mu^a e^{i\varphi_a}\vartheta_a\psi_{nQ_a}(\mathbf{r}). \quad (A.14)$$

In our problem $\Phi_\mu(\mathbf{r})$ is integrated with a potential $V(\mathbf{r})$ that differs from zero in the region $|\mathbf{r}| \sim r_0$, so that actually $\sigma xy \lesssim \sigma r_0^2 \sim \Omega/E_0 \ll 1$ and therefore the phase factor $e^{i\sigma xy}$ can be discarded. In addition, $\sigma_y \lesssim \sigma r_0 \ll b$, and we can therefore assume that $\mathbf{Q_a} \approx \{P_x, k_y^a, P_z\}$.

It is now necessary to calculate the normalization factor $|c_\mu^a|$. We use the expression (A.12) although, naturally, this can also be done more rigorously by using (A.1)–(A.7). We have

$$1 = \int|\Phi_\mu(\mathbf{r})|^2\,d\mathbf{r} = 2\pi\sigma\sum_a\int d\mathbf{r}|c_\mu^a|^2|u_{nQ_a}(r)|^2/|v_y^a|.$$

We note now that since Q_a changes little when y varies within the limits of one cell, we can write (assuming that $\int u_{nk}u_{n'k}d\mathbf{r} = \delta_{nn'}$)

$$1 = 2\pi\sigma\frac{L_x}{a_x}\frac{L_z}{a_z}\sum_a\sum_{a_y}\frac{|c_\mu^a|^2}{|v_y^a|}$$

$$= 2\pi\sigma\frac{L_xL_z}{\Omega_0}\sum_a\int\frac{dy}{|v_y^a|}|c_\mu^a|^2 = 2\pi\frac{L_xL_z}{\Omega_0}|c_\mu|^2\sum_a\int\frac{d\pi_x^a}{|v_y^a|}$$

$$= 2\pi\frac{L_xL_z}{\Omega_0}|c_\mu|^2\oint\frac{dl}{v_\perp} = (2\pi)^2|m_\mu^*|\frac{L_xL_z}{\Omega_0}|c_\mu|^2.$$

We have introduced here the notation $2\pi|m_\mu^*| = \oint dl/v_\perp = |\partial S/\partial\epsilon|$ (see[8]) and recognized that $|c_\mu^a|$ does not depend on the index a. We thus have

$$|c_\mu| = \sqrt{\frac{\Omega_0}{(2\pi)^2|m_\mu^*|}}\frac{1}{\sqrt{L_xL_z}}. \tag{A.15}$$

APPENDIX B

GREEN'S FUNCTION IN THE QUASICLASSICAL CASE

The wave functions for the quasiclassical case are given in Appendix A. We now derive an expression for the Green's function in a magnetic field in the coordinate representation (which, incidentally, will make clearer some of the statements of Sec. 1:

$$G(\mathbf{r},\mathbf{r}',\omega) = \sum_{NP_z}G_{NP_z}\sum_{P_x}\Phi_\mu(\mathbf{r})\Phi_\mu^*(\mathbf{r}') = \sum_{NP_z}G_{NP_z}\Lambda_{NP_z}(\mathbf{r},\mathbf{r}'). \tag{B.1}$$

Here (as in the derivation of the expression for the wave function) we disregard the dependence of the energy in the crystal on P_x, because when $\sqrt{\sigma} \ll b$ (b is the period of the reciprocal lattice) the number of levels for which this dependence is important is small. by Λ_{NP_Z} we denote the projector on the states with given N and P_z. We must now calculate it.

We can first write an exact expression for Λ in the isotropic case, when the wave functions are known (see[5]). With the aid of formula (7.377) of[4] we can readily obtain

$$\Lambda_{NP_z}(\mathbf{r},\mathbf{r}')$$

$$= \frac{\sigma}{2\pi L_z}\exp\left[iP_z(z-z') + i\frac{\sigma}{2}(x-x')(y+y') - \frac{\sigma^2}{4}\rho^2\right]L_N\left(\frac{\sigma\rho^2}{2}\right), \tag{B.2}$$

where $\rho^2 = (x-x')^2 + (y-y')^2$, and L_n is the corresponding Laguerre polynomial. We now proceed to calculate Λ in a crystal. To this end, we use the expression for the wave function in the form (A.10):

$$\Lambda_{NP_z}(\mathbf{r},\mathbf{r}') = \frac{L_x}{2\pi}\int dP_x e^{iP(\mathbf{r}-\mathbf{r}')}\sum_{\alpha\alpha'}c_\mu^\alpha c_\mu^{\alpha'*}\int dk_y\,dk_y' u_{n\mathbf{Q}}(\mathbf{r})$$

$$\times u_{n\mathbf{Q}'}(\mathbf{r}')|v_x^\alpha v_x^{\alpha'}|^{-1/2}\exp\left[\frac{\sigma(y'-y)-S^{\alpha'}-S^\alpha}{i\sigma} + iP_x\frac{k_y'-k_y}{\sigma}\right].$$

Here $\mathbf{Q} = \{\pi_X k_Y P_Z\}$. The integration with respect to P_X can easily be carried out and yields

$$2\pi\delta(x-x'+(k_y'-k_y)/\sigma).$$

We introduce the notation $\xi = x - x'$, $\eta = y - y'$; then

$$\Lambda_{NP_z}(\mathbf{r},\mathbf{r}') = \sigma L_x\sum_{\alpha\alpha'}c_\mu^\alpha c_\mu^{\alpha'*}\int dk_y\,u_{n\mathbf{Q}}(\mathbf{r})u_{n\mathbf{Q}'}^*(r')$$

$$\times|v_x^\alpha v_x^{\alpha'}|^{-1/2}\exp\left[\frac{\Sigma^{\alpha\alpha'}(k_y)}{i\sigma} + iP_z(z-z')\right], \tag{B.3}$$

with

$$\Sigma^{\alpha\alpha'}(k_y) = S^{\alpha'}(k_y-\sigma\xi) - S^\alpha(k_y) - \sigma\eta k_y - \sigma^2y'\xi.$$

In the general case the integration is carried out here by the saddle-point method and entails no difficulty, but the expression for G at large ρ (such that $\sigma\rho \gtrsim b$, $\rho^2 = \xi^2 + \eta^2$) is needed only to determine the asymptotic form of the wave function Ψ, whereas to solve Eq. (2) with ψ it is necessary only to have $\rho \sim r_0$, when $\sigma\rho \ll b$. In this case we can expand $\Sigma^{\alpha\alpha'}$:

$$\Sigma^{\alpha\alpha'}(k_y) \approx S^{\alpha'}(k_y) - S^\alpha(k_y) - \sigma\eta k_y - \sigma\xi\pi_x^{\alpha'}(k_y) - \sigma^2y'\xi.$$

Since the terms with $\alpha' \neq \alpha$ give a rapidly oscillating phase, they should be discarded and, recognizing that $\mathbf{Q} \approx \mathbf{Q}'$, we obtain the following expression for Λ:

$$\Lambda_{NP_z}(\mathbf{r},\mathbf{r}') = \sigma L_x|c_\mu|^2\exp[i\sigma y'(x-x')]F_{nP_z}(\mathbf{r},\mathbf{r}'), \tag{B.4}$$

where

$$F_{nP_z}(\mathbf{r},\mathbf{r}') = \oint\frac{dl}{v_\perp}\psi_{n\mathbf{Q}}(\mathbf{r})\psi_{n\mathbf{Q}}^*(\mathbf{r}').$$

This expression must be substituted in (B.1). We then obtain

$$G(\mathbf{r},\mathbf{r}',\omega) = \sigma L_x\exp[i\sigma y'(x-x')]\frac{L_z}{2\pi}\sum_N\int dP_z\frac{|c_\mu|^2}{\omega-\varepsilon_{NP_z}}F_{nP_z}(\mathbf{r},\mathbf{r}')$$

and when ω is close to ϵ_{M_0} we arrive, after quite obvious transformations, at the expression ($\xi = \omega - \epsilon_{M_0}$)

$$G(\mathbf{r},\mathbf{r}',\omega) = \exp[i\sigma y'(x-x')]\left[\frac{\sigma}{|m_\mu^*|}\frac{\Omega_0}{(2\pi)^3}f(\xi)\oint\frac{dl}{v_\perp}\psi_{nk_xk_y0}(\mathbf{r})\right.$$

$$\left.\times\psi_{nk_xk_y0}^*(\mathbf{r}') + \bar{G}(\mathbf{r}\mathbf{r}'\omega)\right], \tag{B.5}$$

where

$$\bar{G}(\mathbf{r}\mathbf{r}'\omega) = \Omega_0\int d\tau_{\mathbf{k}}\frac{\psi_{n\mathbf{k}}(\mathbf{r})\psi_{n\mathbf{k}}^*(\mathbf{r}')}{\omega-\varepsilon_n(\mathbf{k})}.$$

Here $d\tau_{\mathbf{k}} = d\mathbf{k}/(2\pi)^3$ and the integration extends over the volume of the reciprocal cell. In the problem in question, the phase factor $\exp[i\sigma y'(x-x')]$ can for obvious reasons be discarded (see Appendix A).

In the case of an isotropic quadratic dispersion law we obtain from (B.4)

$$\Lambda_{NP_z}(\mathbf{r},\mathbf{r}') = \frac{\sigma}{2\pi L_z}\exp[iP_z(z-z') + i\sigma y'(x-x')]J_0(Q_\perp\rho),$$

and as is clear from (A.9),

$$\pi Q_\perp^2 = 2\pi\sigma(N+1/2),$$

and we can write in the phase factor $(y+y')/2$ in place of y'.

We can now use relation (8.978) (2) of[4]:

$$J_0(Q_\perp\rho) = J_0(2\sqrt{\sigma(N+1/2)\rho^2/2})$$

$$\approx L_N(\sigma(N+1/2)\rho^2/2N) \approx L_N(\sigma\rho^2/2),$$

which must be compared with the exact formula (B.2).

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