ELECTRON IN A RANDOM FIELD

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An expression is obtained for the averaged Green's function of a nonrelativistic electron in a statistically homogeneous and isotropic random field; the expression does not depend on the time, and is valid under rather broad assumptions concerning the characteristics of the field.

THE question of the behavior of an electron in a random field is encountered in various problems, for example, in the analysis of the effect of random inhomogeneities on electrons in a solid. Mathematically, a similar formulation is used for the problem of the propagation of acoustic, thermal, and in some cases also electromagnetic waves in a medium with random properties, as well as many other problems[1].

A random field will henceforth be characterized by a pair correlation function of the potentials, $\langle V(\mathbf{x})\, V(\mathbf{y})\rangle$, where the angle brackets denote averaging over the ensemble. The main numerical characteristics of the field are in this case the magnitude of the fluctuations $\langle (V-\langle V\rangle)^2\rangle$ and the characteristic correlation length l. Our main problem is to calculate the averaged Green's function of the electron. We first find, for the case of large-scale inhomogeneities, a solution valid for any magnitude of the potential fluctuations (an expression of the quasiclassical type). The solution is then generalized to include inhomogeneities of arbitrary size; for small-scale inhomogeneities, limitations are imposed in this case on the magnitude of the potential.

To find the average value of the Green's function $\langle G\rangle$ it is necessary first to solve the Schrödinger equation in an arbitrary external field, and then average over all possible potentials.

We consider the equation for G:

$$\left[\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 + E - V(\mathbf{x})\right] G(E, \mathbf{x}, \mathbf{x}'\,|\,V) = -\delta(\mathbf{x}-\mathbf{x}'). \quad (1)$$

Taking the Fourier transform with respect to the difference in the coordinates

$$G(E,\mathbf{x},\mathbf{x}'\,|\,V) = \frac{1}{(2\pi)^3}\int d\mathbf{p}\, e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} G(E, \mathbf{p}, \mathbf{x}|\, V), \quad (2)$$

we obtain for the function $G(E, \mathbf{p}, \mathbf{x}\,|\,V)$ the equation

$$\left[\frac{\hbar^2}{2m}(\nabla_{\mathbf{x}}^2 - 2i\mathbf{p}\nabla_{\mathbf{x}} - p^2) + E - V(\mathbf{x})\right] G(E, \mathbf{p}, \mathbf{x}\,|\,V) = -1. \quad (3)$$

Its symbolic solution can be written directly (we choose a retarded Green's function):

$$G(E, \mathbf{p}, \mathbf{x}|V) = i\int_0^\infty dt \exp\left[-it\left(\frac{\hbar^2 p^2}{2m} - E - i\delta\right)\right] \times \exp\left[it\left(\frac{\hbar^2\nabla^2}{2m} - \frac{i\hbar^2}{m}\mathbf{p}\nabla - V\right)\right]. \quad (4)$$

The problem consists of expressing the last exponential in explicit form with maximum accuracy.

As will be shown later, each differentiation ∇ adds to $\langle G\rangle$ a quantity l^{-1}. In the case of large scale inhomogeneities (large l) the first step is to discard all the terms containing ∇. This actually corresponds to the classical approach; the corresponding Green's function was used by Bonch-Bruevich[2]. We shall take exact account here of the term $i\hbar^2\mathbf{p}\cdot\nabla/m$ and expand in powers of $\hbar^2\nabla^2/2m$. Criteria for the applicability of the resultant expressions will be given below.

We write the last exponential in (4) in the following form (to abbreviate the notation we omit $\hbar^2/2m$ for the time being):

$$\exp[it(\nabla^2 - 2i\mathbf{p}\nabla - V)] = \exp[-it(2i\mathbf{p}\nabla + V)]L(t). \quad (5)$$

Differentiating both halves of (5) with respect to t (the procedure is analogous to that given in[3]) we obtain an equation for L(t):

$$\frac{d}{dt}L(t) = \exp[it(2i\mathbf{p}\nabla + V)] \times \nabla^2 \exp[-it(2i\mathbf{p}\nabla + V)]L(t). \quad (6)$$

We confine ourselves to the first two terms of the expansion of L(t) in a series in ∇^2: $L = 1 + L_1(t)$. Recognizing that

$$\exp[-it(2i\mathbf{p}\nabla + V(\mathbf{x}))] = \exp(2t\mathbf{p}\nabla)\exp\left[i\int_0^{-t} dt'\, V(\mathbf{x}+2\mathbf{p}t')\right] \quad (7)$$

(this relation can be obtained with the aid of the same procedure of differentiating with respect to t), we obtain

$$\frac{dL_1}{dt} = i\exp\Big\{i\int_0^t dt'\,V(\mathbf{x}-2\mathbf{p}t')\Big\} \times \nabla^2\exp\Big\{-i\int_0^t dt'\,V(\mathbf{x}-2\mathbf{p}t')\Big\} \tag{8}$$

and, bearing in mind that L(t) acts on unity,

$$L_1(t) = \int_0^t dt'\int_0^{t'} dt''\nabla^2 V(\mathbf{x}-2\mathbf{p}t'') - i\int_0^t dt'\Big[\int_0^{t'} dt''\,\nabla V(\mathbf{x}-2\mathbf{p}t'')\Big]^2. \tag{9}$$

In this approximation the Green's function (4) is equal to

$$G(E,\mathbf{p},\mathbf{x}|V) = i\int_0^\infty dt\exp\Big\{-it(p^2-E-i\delta)-i\int_0^t dt'\,V(\mathbf{x}+2\mathbf{p}t')\Big\} \times\Big[1+\int_0^t dt'\int_0^t dt''\,\nabla^2 V(\mathbf{x}+2\mathbf{p}t-2\mathbf{p}t'') - i\int_0^t dt'\Big(\int_0^{t'} dt''\,\nabla V(\mathbf{x}+2\mathbf{p}t-2\mathbf{p}t'')\Big)^2+\ldots\Big]. \tag{10}$$

We now average this expression. In the averaging we assume that all the correlation functions of the potential $\langle V(\mathbf{x}_1)\ldots V(\mathbf{x}_n)\rangle$ are expressed in terms of the pair correlation function $\rho(\mathbf{x}_1-\mathbf{x}_2) = \langle V(\mathbf{x}_1)\,V(\mathbf{x}_2)\rangle$. The operation of averaging over the ensemble is reduced thereby to all possible pairings of the potentials in the sense used in quantum field theory. Such an assumption is equivalent to introducing a normal distribution[4] for the random function V(x). The perturbation-theory series for the average Green's function is then represented in the form of a sum of diagrams, and the average of Eq. (10) is itself expressed in terms of a continual integral, in complete analogy with the Green's function of the quantized field. (The propagation functions of the Bose field are replaced here by correlation functions; there are no diagrams containing the polarization of vacuum.)

Instead of calculating the continual integral, it will be more expedient for us to take functional derivatives of a suitably chosen expression, as is sometimes done in quantum field theory. Namely, using the properties of a normal distribution and following the procedure used by Fradkin[5], we can easily show that the averaging is equivalent to the operation of differentiation with respect to fictitious external sources:

$$\langle G(E,\mathbf{p},\mathbf{x}|V(\mathbf{x}))\rangle = G\Big(E,\mathbf{p},\mathbf{x}\Big|\frac{\delta}{\delta J(\mathbf{x})}\Big) \times\exp\Big\{\frac{1}{2}\int\int d\mathbf{x}_1\,d\mathbf{x}_2\,J(\mathbf{x}_1)\rho(\mathbf{x}_1-\mathbf{x}_2)J(\mathbf{x}_2)\Big\}\Big|_{J=0}. \tag{11}$$

We shall assume further that the average value of the potential is equal to zero [otherwise it is necessary to add to the Green's function a factor $\exp(-i\langle V\rangle t)$]. Averaging (10) with the aid of (11), we obtain

$$\langle G(E,\mathbf{p},\mathbf{x}|V)\rangle = G(E,p) = i\int_0^\infty dt\exp\Big\{-it(p^2-E) -\frac{1}{2}\int_0^t dt'\int_0^t dt''\,\rho(2\mathbf{p}t'-2\mathbf{p}t'')\Big\} \times\Big[1-\int_0^t dt'\int_0^{t'} dt_1\int_{t'}^t dt_2\,\nabla^2\rho(2\mathbf{p}t_1-2\mathbf{p}t_2) +i\int_0^t dt'\Big(\int_0^t dt_1\int_0^{t'} dt_2\,\nabla\rho(2\mathbf{p}t_1-2\mathbf{p}t_2)\Big)^2+\ldots\Big]. \tag{12}$$

We perform all possible integrations in (12), restore the correct dimensionalities, and introduce the following symbols: l—correlation length, defined by the relation

$$\int_0^\infty dx\,\rho(x) = l\rho(0) = l\langle V^2\rangle;\quad \rho = \langle V^2\rangle F(\xi),\quad \xi = x/l;$$

t_l—characteristic time, defined by

$$t_l = lm/p\hbar;\quad E_p = p^2\hbar^2/2m.$$

Carrying out a Fourier transformation with respect to energy, we obtain ultimately for a time $t > 0$ (when $t < 0$ we have $G(p,t) = 0$):

$$G(p,t) = i\exp\Big\{-iE_pt/\hbar - \frac{\langle V^2\rangle t_l^2}{\hbar^2}\int_0^{t/t_l} d\xi\,(t/t_l-\xi)F(\xi)\Big\} \times\Big[1+\frac{i\langle V^2\rangle t_l t}{2\hbar^2 pl}\Big(1-F\Big(\frac{t}{t_l}\Big)\Big) +\frac{i\langle V^2\rangle^2 t_l^4}{\hbar^4 pl}\int_0^{t/t_l} d\xi_1\int_{\xi_1}^{t/t_l-\xi_1} d\xi_2\Big(\frac{t}{t_l}-2\xi_2\Big)F(\xi_1)F(\xi_2)+\ldots\Big]. \tag{13}$$

This is the amplitude of the probability that an electron with momentum $\mathbf{p}\hbar$ at $t = 0$ will be in the same state at the instant t.

Scattering by the inhomogeneities causes the amplitude to decrease with time. From (13) we see that, regardless of the form of $F(\xi)$, at sufficiently short times the decrease has a Gaussian character

$$G(p,t) \sim \exp\{-\langle V^2\rangle t^2/2\hbar^2\},\quad t \ll t_l, \tag{14}$$

and at large times an exponential character

$$G(p, t) \sim \exp\{-\langle V^2\rangle plt/2E_p\hbar\}, \quad t \gg t_l. \tag{15}$$

Which of the two types of fall-off predominates depends on whether $\langle V^2\rangle (pl)^2/E_p^2$ is very much larger than or very much smaller than unity. By substituting in (13) sufficiently simple concrete expressions for $F(\xi)$ we can easily obtain for $G(p, t)$ a final formula containing no integrations.

To clarify the character of the neglected quantities, we expand the exponential in (12)

$$\exp\left\{-\frac{1}{2}\int_0^t dt'\int_0^t dt''\rho(2\mathbf{p}t'-2\mathbf{p}t'')\right\} = \exp\left\{-\frac{1}{2(2\pi)^3}\right.$$
$$\left.\times\int d\mathbf{q}\tilde{\rho}(\mathbf{q})\int_0^t dt'\int_0^t dt''\exp[2i\mathbf{pq}(t'-t'')]\right\} \tag{16}$$

in a series and integrate term by term with respect to t ($\tilde{f}$ denotes henceforth the three dimensional Fourier transform of the function f). We obtain

$$G(E,p)=\frac{1}{E_p-E}+\frac{\langle V^2\rangle(pl)^2}{(2\pi)^3E_p}\frac{1}{(E_p-E)^2}$$
$$\times\int\frac{d\mathbf{q}\tilde{F}(\mathbf{q})}{p^2l^2-2mEl^2/\hbar^2+2l\mathbf{pq}} \tag{17}$$
$$\times\left(1-\frac{q^2}{p^2l^2-2mEl^2/\hbar^2+2l\mathbf{pq}}\right)+\ldots.$$

Comparing (17) with the perturbation-theory series, where the typical denominator corresponding to the free fermion propagator can be written in the form

$$l^2(p^2-2mE/\hbar^2)+2l\mathbf{p}\sum_i\mathbf{q}_i+\sum_i q_i^2+\sum_{i\neq j}\mathbf{q}_i\mathbf{q}_j, \tag{18}$$

we verify that the principal term in (12) or (13) corresponds to the sum of all the diagrams of perturbation theory, from each of which we discard the propagator terms that are quadratic in q_1. The correction in the square brackets accounts for all these terms in first order, the first of the terms corresponding to inclusion of terms of the type $\Sigma_i q_i^2$, and the second to inclusion of $\Sigma_{i\neq j}\mathbf{q}_i\mathbf{q}_j$.

We see from (17) and (18) that we actually deal with expansions in inverse powers of pl. An analysis of (13) shows indeed that in order for the expansion in the square brackets to be meaningful and for the corrections to $G(p, t)$ in the principal region of its variation (that is, before $G(p, t)$ becomes much smaller than unity in absolute value) to be small, it is necessary and sufficient to satisfy the condition

$$pl \gg 1. \tag{19}$$

If for some reason we are also interested in the value of $G(p, t)$ at a time when they are already much smaller than unity, then the regions of applicability can be found by simply requiring that the correction terms in the square brackets of (13) be small compared with unity. Since the corrections increase with time, we obtain by the same token a limitation on the permissible values of t.

We note that the method of discarding the terms that are quadratic in the virtual momentum was used to study the infrared asymptotic values of the Green's functions in quantum field theory, where a formula corresponding to the principal term in (12) was obtained[6,7].

To illustrate the possibility of applying the obtained results to questions of physical interest, let us find the change in the density of the energy states of the electron in a solid, due to its interaction with inhomogeneities described by an effective potential V (we have in mind, for example, deviations of the crystal lattice from ideal; l is the characteristic length over which the change in structure takes its place, and $\mathbf{p}\hbar$ is the quasimomentum). Confining ourselves to a limiting case requiring no complicated computations, we take for $G(p, t)$ the form (14), which is valid if the following conditions are satisfied

$$pl \gg 1, \quad \langle V^2\rangle(pl)^2/E_p^2 \gg 1. \tag{20}$$

The energy-state density $\rho(E)$ is determined by the following formula[8]

$$\rho(E)=\frac{1}{4\pi^4}\int d\mathbf{p}\,\mathrm{Im}\,G(E,\mathbf{p}). \tag{21}$$

From (14) and (21) we get

$$\mathrm{Im}\,G(E,p)=\left(\frac{\pi}{2\langle V^2\rangle}\right)^{1/2}\exp\left\{-\frac{(E_p-E)^2}{2\langle V^2\rangle}\right\},$$
$$\rho(E)=\frac{1}{4\sqrt{2}\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\langle V^2\rangle^{1/4}\exp\left(\frac{-E^2}{4\langle V^2\rangle}\right)D_{-3/2}\left(\frac{-E}{\langle V^2\rangle^{1/2}}\right) \tag{22}$$

($D_\alpha(x)$ is the parabolic-cylinder function). Relations (22), the most remarkable property of which is that they give a nonzero density of states in a hitherto forbidden band ($E < 0$), were obtained in a different fashion by L. V. Keldysh (unpublished), and also by Almazov[9].

We can now show that Eqs. (22) are applicable under the following conditions

$$\langle V^2\rangle^{1/2}ml^2/\hbar^2 \gg 1, \quad \langle V^2\rangle ml^2/\hbar^2 \gg |E|. \tag{23}$$

The first inequality in (23) is a consequence of (20), while the second is obtained from the requirement that an appreciable contribution be made to the integral (21) only by values of p satisfying (20). In addition, of course, it is necessary

to satisfy the conditions for the applicability of the single-band approximation. If the characteristics of the field are not satisfied by inequalities (23), then to obtain $\rho(E)$ it is necessary to use the more complete formula (13), or the later formula (25). We shall not stop here to discuss this question in greater detail, and proceed to generalize the expression for the Green's function.

We wish now to get rid of the limitation (19), taking into account some of the discarded terms. To this end we set up a Green's function which takes into account in each of the denominators of (18) not only the terms that are linear in q_i, but also terms of the type Σq_i^2 (but not $\Sigma_{i\neq j} q_i \cdot q_j$). For this end it is sufficient to modify somewhat the exponential in (12), replacing (16) by [1)]

$$\exp\left\{\frac{-1}{(2\pi)^3}\int d\mathbf{q}\tilde{\rho}(\mathbf{q})\int_0^t dt'\int_0^{t'} dt''\exp\left[i(2\mathbf{pq}-q^2)(t'-t'')\right]\right\}. \tag{24}$$

It is easy to check the correctness of this statement by again expanding the exponential (24) in a series and integrating the expression for $G(E, p)$ term by term with respect to t. We made such a check up to fourth order of perturbation theory, and the character of the resultant expressions has demonstrated the correctness of the chosen form (24) in any order.

Calculation of the integrals in (24) now leads to the following expression for the Green's function when $t > 0$:

$$G(p,t)=i\exp\left\{-\frac{iE_pt}{\hbar}-\frac{e^{-3i\pi/4}\langle V^2\rangle}{2\sqrt{2}\pi E_p^2}(pl)^{5/2}\int_0^\infty d\xi\,\xi F(\xi)\right.$$
$$\left.\times\sin pl\xi\int_0^{t/t_l} ds\frac{t/t_l-s}{s^{3/2}}\exp\left[\frac{ipl}{2}\left(s+\frac{\xi^2}{s}\right)\right]\right\}. \tag{25}$$

Of course, when $pl \gg 1$ this expression goes over into the principal term of (13), inasmuch as the expansion in the $(pl)^{-1}$ has not been disturbed. We note nevertheless that even when $pl \gg 1$ it is preferable to use (25) and not (13), since a comparison carried out for several trial functions $F(\xi)$, of the first and second correction terms in (13), which give the corrections in the quantities $\Sigma_i q_i^2$ and $\Sigma_{i\neq j} q_i \cdot q_j$ respectively, shows that the second of the corrections does not exceed several per cent of the first. This is due to the fact that $\Sigma_i q_i^2$ is always positive, whereas $\Sigma_{i\neq j} q_i \cdot q_j$ reverses sign when integrated with respect to angle, and has a zero mean value.

The main advantage of taking into account the terms of the type $\Sigma_i q_i^2$ lies in the fact that this yields correctly the lower order with respect to $\langle V^2\rangle$ in $G(p, t)$ since terms of the type $\Sigma_{i\neq j} q_i \cdot q_j$ appear only for $\langle V^2\rangle^2$. More accurately speaking, in this case complete account is taken of all the diagrams corresponding to the lower order with respect to $\langle V^2\rangle$ in the mass operator. This circumstance enables us to state, as we shall show below, that (25) is suitable also for a description of the case $pl \ll 1$.

At sufficiently small correlation lengths (the required criteria will be indicated below), the Green's function (25) has in the main region of its variation the form

$$G(p,t)=i\exp\left\{-\frac{iE_pt}{\hbar}-\frac{\langle V^2\rangle tpl}{E_p\hbar}\int_0^\infty d\xi F(\xi)\left(1-e^{2ipl\xi}\right)\right\},\quad t>0, \tag{26}$$

corresponding to

$$G(E,p)=\left[E_p-E-\frac{i}{2}\frac{\langle V^2\rangle pl}{E_p}\int_0^\infty d\xi F(\xi)\left(1-e^{2ipl\xi}\right)\right]^{-1} \tag{27}$$

(an additional factor arises on going over from (25) to (26) and (27), but the difference between this factor and unity can be neglected when the conditions written out below are satisfied).

Expression (27) can be obtained independently by calculating the mass operator in the lower approximation in $\langle V^2\rangle$:

$$M_2(E,p)=\frac{\langle V^2\rangle}{E_p}(pl)^2 l^{-3}\int d\mathbf{x}G_0(E,\mathbf{x})F(\mathbf{x})e^{i\mathbf{px}}, \tag{28}$$

provided we improve somewhat the free Green's function of the electron

$$G_0(E,x)=(4\pi x)^{-1}\exp\left(i\sqrt{2m}Ex/\hbar\right),$$

by replacing in it the free-motion momentum $\sqrt{2mE}$ by $p\hbar$ (when $\langle V^2\rangle (pl)^2/E_p^2 \ll 1$ the motion is close to free and such a replacement is inessential).

We see therefore that at sufficiently small pl the use of (25) leads to the same result as an account of the lower order in the mass operator. This is usually perfectly sufficient, since the interaction of the electron with the small-scale inhomogeneities is on the average weak and is well described by perturbation theory, as can be seen from the criterion given below for the applicability of (31). It is essential here that the perturbation-theory variant, in which the expansion is carried out in the mass operator [and by the same token in the argument of the exponential in (26)] does not require that the variation of the Green's func-

[1)] A formula of the same type was obtained previously by Fradkin in quantum electrodynamics[10].

tion be small compared with the free one; it is merely required that the contribution from the next order be small. We are therefore justified in using (26) for G(p, t) even at those values of the time when its absolute value differs appreciably from unity.

Let us explain finally the conditions for the applicability of expression (26) when $pl \ll 1$. Formula (25) goes over into (26) when $t \gg t_1/pl$. In order for the region $t \lesssim t_1/pl$ to be inessential it is necessary that the characteristic damping time of the exponential in (26) be appreciably larger than t_1/pl; this leads to the condition

$$\langle V^2\rangle (pl)^3 / E_p^2 \ll 1. \tag{29}$$

The same condition ensures smallness of the damping over one wave length.

To estimate the correction terms it is necessary to find the mass operator in the next higher order in $\langle V^2\rangle$. Fourth-order calculations lead to the expression

$$M_4 = \frac{i}{2}\frac{\langle V^2\rangle^2}{E_p^3} p^6 \left(\frac{\hbar^2}{2mE}\right)^{1/2} l^5 \int_0^\infty d\xi \cdot \xi F(\xi) \int_0^\infty d\xi \cdot \xi^2 F(\xi)$$

$$pl \ll 1. \tag{30}$$

Comparing with the damping in M_2 (that is, $\mathrm{Im}M_2$), we find that in order to obtain a small correction at a time when G(p, t) is still not much smaller in absolute value than unity, it is necessary to satisfy the condition

$$\langle V^2\rangle (pl)^2 / E_p^2 \ll 1. \tag{31}$$

We note that (31) is a more stringent requirement on the value of $\langle V^2\rangle$ than (29). Nonetheless, it enables us to consider strong fields, which can be larger than the kinetic energy. This indeed is the cause of the good applicability of perturbation theory when $pl \ll 1$. We note that estimates of a similar kind were made by Tatarskiĭ and Gertsenshteĭn[11,12] for the scattering of electromagnetic waves in a turbulent medium. In an estimate of a quantity similar to M_4, Tatarskiĭ[12] obtained an expression which is literally equivalent to (30), but the final estimate corresponds there to (29), and not to (31) as in our case. The reason for it is that Tatarskiĭ[12] required that M_4 be small compared with $\mathrm{Re}M_2$, without paying attention to the fact that M_4 is imaginary.

When $pl \sim 1$, estimates in the fourth order of the mass operator lead to the rather stringent requirement:

$$\langle V^2\rangle / E_p^2 \ll 1, \tag{32}$$

which replaces both (29) and (31). We cannot state, however, that this condition is necessary, for when $\langle V^2\rangle \sim E_p^2$ the function G(p, t) no longer has the form (26), and the use of perturbation theory in the mass operator is not justified. In this case (25) can be regarded as an interpolation formula between large and small values of pl, which describes qualitatively the intermediate region. It is hardly possible to obtain directly a solution in this region, for when $pl \sim 1$ and $\langle V^2\rangle \sim E_p^2$ there are no small parameters left in the problem.

As already stated, the employed method has great generality and can be used in various problems involving wave equations in a medium with random properties. We plan in the future to apply the obtained results to the question of the propagation of electromagnetic waves in a medium with a fluctuating dielectric constant, especially to find the region of applicability of various types of solutions.

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Note added in proof (24 March 1965). A direct calculation of $\rho(E)$ in accordance with formulas (21) and (13), in which simpler concrete functions were taken in lieu of $F(\xi)$, has led to a more precise definition of the conditions of applicability of (22). Namely, it turned out that the second inequality in (23) should be replaced by the following stronger inequality:

$$\langle V^2\rangle^2 m l^2 / \hbar^2 \gg |E|^3.$$

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