Motion of a quasiparticle with position-dependent effective mass

I. M. Sokolov

P. N. Lebedev Physics Institute, Academy of Sciences of the USSR

(Submitted 9 January 1985)
Zh. Eksp. Teor. Fiz. **89**, 556–561 (August 1985)

The problem of the motion of a quasiparticle in an inhomogeneous crystal is considered. The form of the quasiparticle kinetic energy operator in the effective-mass approximation and the conditions for admissible spatial dependence of the effective mass are obtained from the general requirements of hermiticity of the Hamiltonian, probabilistic interpretation of the wave function, and Galilean invariance.

The effective mass approximation is often employed in the investigation of the effects connected with the quantization of the motion of quasiparticles in thin films and heterostructures. It is then necessary to find the conditions for the matching of the wave functions in the various regions. Also of interest is the problem in which the effective mass is a continuous function of the coordinates, as in, say, a semiconductor with variable doping. Similar problems are considered in, for example, Refs. 1–5. The main difficulty here consists in the choice of the right form of the kinetic-energy term in the Hamiltonian. Various Hermitian operators that go over into the usual operator $-(\hbar^2/2m)\Delta$ in the case of a homogenous sample have been postulated for this term. The various operators lead, naturally, to different results.[4] The assertion is made in Ref. 3 that this operator is, in principle, not unique, and, consequently, the effective mass approximation is not suitable for the description of the motion of a particle in an inhomogeneous medium. As a matter of fact, the kinetic energy operator is uniquely defined. An additional condition that makes a unique choice possible is that the solution to the corresponding Schrödinger equation should be a wave function, i.e., it should admit of a probabilistic interpretation.

Let us first consider as an example the following one-dimensional case. Let the coordinate of the boundary between two regions be $x = 0$, and let the effective masses in the regions to the left and right of the boundary be respectively equal to m_- and m_+. We shall assume here that the motion in each region is exactly described by the effective-mass equation, i.e., that the kinetic energy operator in the ith region has the form

$$T_i = -(\hbar^2/2m_i)\Delta. \tag{1}$$

Assuming that the model does not contain any parameters having the dimensions of length, and describing the boundary, we are forced to require that

$$\psi(+0)=\delta\psi(-0), \quad \psi'(+0)=\gamma\psi'(-0),$$

where δ and γ are dimensionless quantities. Then the hermiticity condition for the Hamiltonian:

$$\int \psi_1^* H\psi_2 dx = \int \psi_2^* H\psi_1 dx, \tag{2}$$

where $\psi_{1,2}$ are arbitrary square-integrable functions satisfying the matching conditions, leads us (after integration by parts in the $x < 0$ and $x > 0$ regions) to the requirement that $\gamma = \mu/\delta^*$, where $\mu = m_+/m_-$, i.e., that

$$\psi(+0)=\delta\psi(-0), \quad \psi'(+0)=(\mu/\delta^*)\psi'(-0). \tag{3}$$

For $\mu = 1$, the continuity condition for ψ'/ψ, which follows from the momentum-conservation requirement, should be fulfilled at the boundary. Accordingly, $\delta = 1$ when $\mu = 1$. When $\mu \neq 1$, this requirement is not legitimate, on account of the inhomogeneity of the space, and δ becomes a free parameter. Let us find out what this parameter depends on, and what the form of the dependence is.

Let us consider a crystal with smoothly varying properties, in which the mass will be a continuous function of the coordinates. The probability of finding the particle in the vicinity of the point x is proportional to the square of the modulus of the true wave function:

$$w(\mathbf{x}) = |\Psi(\mathbf{x})|^2 \approx |u_0(\mathbf{x})|^2 |\varphi(\mathbf{x})|^2, \tag{4}$$

where $u_0(\mathbf{x})$ is the Bloch function corresponding to the bottom (top) of the band in question in the spatial region under investigation, a region which is large compared to the interatomic distance, while $\varphi(\mathbf{x})$ is a slowly-varying envelope function, for which the effective mass approximation is valid in this region. The latter implies that the quasimomentum operator acts on the function φ, and is equal to $p_i = -i\hbar\partial/\partial x_i$, while the kinetic energy in the "classical limit" (i.e., in the limit of a homogeneous sample or a sufficiently rapidly varying φ) has the form

$$T = \sum_{i,k} \frac{1}{2} \gamma_{ik} p_i p_k,$$

where γ_{ik} is an element of the reciprocal effective mass tensor.

Averaging (4) over a scale large compared to the interatomic distance, we obtain

$$\overline{w(\mathbf{x})} = g(\mathbf{x}) |\varphi(\mathbf{x})|^2, \tag{5}$$

where $g(\mathbf{x})$ is the average value of $|u_0(\mathbf{x})|^2$ in a unit volume, i.e., is a quantity that is inversely proportional to the volume of the unit cell. Thus, the scalar product of the envelope

0038-5646/85/080317-04$04.00

functions should be defined as

$$(\varphi_1, \varphi_2) = \int g(\mathbf{x}) \varphi_1(\mathbf{x}) \varphi_2(\mathbf{x}) \, d\mathbf{x}. \tag{6}$$

In complete analogy with the problem of quantization in Riemannian space,[6] it is not difficult to show that in this case the kinetic energy operator acting in the space of the functions φ has the form

$$T = -\frac{\hbar^2}{2} \sum_{i,k} g^{-1}(\mathbf{x}) \frac{\partial}{\partial x_i} g(\mathbf{x}) \gamma_{ik}(\mathbf{x}) \frac{\partial}{\partial x_k}. \tag{7}$$

Let us note in parentheses that, for the case of Riemannian space the correctness and uniqueness of precisely this form of the operator T can be verified through a direct change of variables.[7]

The analysis of the problem in the space of the functions φ is not convenient, in view of the fact that φ is not a wave function, since $|\varphi|^2$ does not have the meaning of a probability density, and

$$\frac{i\hbar}{2} \gamma_{ik} \left(\varphi \frac{\partial \varphi^*}{\partial x_k} - \varphi^* \frac{\partial \varphi}{\partial x_k} \right)$$

does not have the meaning of a probability-flux density. Therefore, let us introduce in place of the envelope functions effective-mass approximation wave functions, for which these combinations have the meaning of averages over a small, but macroscopic range of values of the corresponding quantities. Clearly, these functions are connected with the functions φ by the relation

$$\psi(\mathbf{x}) = g^{1/2}(\mathbf{x}) \varphi(\mathbf{x}). \tag{8}$$

The Schrödinger equation for the function ψ in the case when all the parameters are continuous has the form

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2} \frac{1}{g^{1/2}} \frac{\partial}{\partial x_i} g \gamma_{ik} \frac{\partial}{\partial x_k} \frac{1}{g^{1/2}} \psi + U\psi, \tag{9}$$

with the kinetic energy operator having the form of a symmetric monomial—in complete agreement with the results obtained in Ref. 4. But let us note that here the quasimomentum operator acting in the space of the ψ functions is equal to

$$p = -i\hbar \frac{1}{g^{1/2}(\mathbf{x})} \nabla + \frac{i\hbar}{2} \frac{\nabla g(\mathbf{x})}{g^{3/2}(\mathbf{x})},$$

where $g(\mathbf{x})$ is a real function. Thus, we have to pay for the introduction of the wave functions by having the commutation relations violated, and the requirement that these relations be valid leads to the necessity of defining the scalar product in the form (6), i.e., of working in space with curvature.

The assertion is made in Ref. 3 that the Schrödinger equation with the Hamiltonian in which the mass depends on the coordinates leads to results that are not invariant under the Galilean transformations

$$x' = x + vt, \quad t' = t. \tag{10}$$

This assertion is valid not for all such Hamiltonians, but only for the spherically symmetric model considered in that paper.

The Galilean transformations change the equation

$$ih\dot{\psi} = (T + U)\psi \tag{11}$$

into the equation

$$i\hbar\psi_1 + i\hbar \, v \nabla \psi_1 = (T + U)\psi_1. \tag{12}$$

The solution to (12) should be related with the solution to (11) by a unitary transformation:

$$\psi_1(x) = \psi(x) \exp[i\theta(\mathbf{x})]. \tag{13}$$

Substituting (13) into (12), and equating to zero the coefficients of those space derivatives of ψ which are not contained in (11), we see that such a transformation exists only if the system of equations

$$\frac{\partial \theta}{\partial x_i} = \frac{1}{\hbar} \sum_j m_{ij} v_j, \tag{14}$$

where the m_{ij} are the elements of the effective mass tensor, i.e., the inverse of the tensor γ_{ij}, possesses a solution. The equality of the mixed derivatives, i.e., the relation

$$\partial^2\theta / \partial x_i \partial x_j = \partial^2 \theta / \partial x_j \partial x_i \tag{15}$$

leads to the conditions

$$\partial m_{jk} / \partial x_i = \partial m_{ik} / \partial x_j, \tag{16}$$

which, together with the requirement that the tensor m_{ij} be symmetric, lead to the result that this tensor is always a tensor composed of the second derivatives of some scalar field:

$$m_{ij} = \frac{\partial^2}{\partial x_i \, \partial x_j} M(\mathbf{x}). \tag{17}$$

The only case in which the tensor m_{ij} satisfies (17) and realizes the spherical symmetry of the operator T is the case corresponding to $m = \text{const}$, as demonstrated in Ref. 3. Thus, the conclusion, drawn in Ref. 3, that a Hamiltonian with a variable mass is not Galilean invariant is not correct. The invariance of the physical processes under the Galilean transformations leads to the requirement (17). The corresponding tensor may not only not have identical diagonal elements, it may, in the general case, not even be simultaneously reducible to the principal axes at all points in the crystal.

Returning to the case with a sharp boundary, we shall not easily understand the origin of the parameter δ. In order for the kinetic energy operator to have the form (1) everywhere, except in the boundary region, we shall have to set $g(x) = g_- = \text{const}$ for $x < 0$ and $g(x) = g_+ = \text{const}$ for $x > 0$. Then from Eq. (9) we immediately obtain the matching conditions

$$\psi(+0) = \left(\frac{g_+}{g_-} \right)^{1/2} \psi(-0), \qquad \psi'(+0) = \mu \left(\frac{g_-}{g_+} \right)^{1/2} \psi'(-0), \tag{18}$$

which correspond to (3) with $\delta = (g_+/g_-)^{1/2}$. For the boundary between crystals with the same symmetry and lattice constant $\delta = 1$, and the matching conditions coincide with those obtained in Refs. 5 and 8. Let us point out that the condition (3), which does not require the validity of the effective-mass approximation inside the boundary region, is more general that (18). This should be understood in the sense that, if the boundary is sharp on the microscopic scale, the condition (3) is fulfilled, but the relation $\delta = (g_+/g_-)^{1/2}$ does not hold. We shall verify this with the example given at the end of the paper.

The quantity δ is, in the effective-mass approximation, an important parameter, which describes the boundary. Knowing it, we can easily determine, for example, the coefficient of reflection from the boundary between the materials:

$$R=\left|\frac{|\delta|^2-[\mu(1-U/E)]^{1/2}}{|\delta|^2+[\mu(1-U/E)]^{1/2}}\right|^2, \qquad (19)$$

where U is the potential jump at the boundary. When $U=0$ and $\mu>0$, the quantity R is equal to zero at $|\delta|=\mu^{1/4}$ and to unity when $\delta=0$, ∞.

Now let us consider as an example how the equations (7) and (9) and the condition (3) can be obtained within the framework of the simplest microscopic approach: the tight-binding approximation. Let our one-dimensional model be described by the Hamiltonian

$$H=\sum_n e_n|n\rangle\langle n|+\sum_{n\neq m} V_{nm}|n\rangle\langle m|, \qquad (20)$$

whose matrix elements e_n and V_{nm} depend on the site number, with $V_{nm}\neq 0$ only for sites that are nearest neighbors. For the amplitude φ_n of the excitation at the nth site we have the difference equation

$$(E-e_n)\varphi_n=V_{n,\,n-1}\varphi_{n-1}+V_{n,\,n+1}\varphi_{n+1}. \qquad (21)$$

When $e_n=e$ and $V_{nm}=-V$ the dispersion law is given by the relation

$$E(k)=e-2V\cos ka, \qquad (22)$$

where a is the interatomic distance. For $V>0$ the bottom of the band corresponds to $k=0$, and the effective mass

$$m=\frac{\hbar^2}{2}\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}_{k=0}=\frac{\hbar^2}{2}\frac{1}{Va^2} \qquad (23)$$

is determined by the parameters V and a.

Introducing in place of the discrete variable n a continuous variable y that assumes the value n at the nth site, and setting

$$V_{n,\,n-1}=V(y-{}^1\!/_2), \qquad V_{n,\,n+1}=V(y+{}^1\!/_2),$$

we obtain, on going over to the continuous case, the differential equation

$$\frac{\partial}{\partial y}V\frac{\partial}{\partial y}\varphi=(E-U(y))\varphi,$$
$$U(y)=e(y)+2V(y)+\frac{1}{4}\frac{d^2V(y)}{dy^2} \qquad (24)$$

which is valid provided $E-U(y)\ll 1$. Let us now go over from the dimensionless variable y to the variable x according to the rule $y=x/a(x)$, where $a(x)$ is the interatomic distance in the vicinity of the point x. This corresponds to the substitution

$$(\partial/\partial y)V(\partial/\partial y)\to a(x)(\partial/\partial x)m^{-1}(x)a^{-1}(x)(\partial/\partial x).$$

The last expression has the form of (7), with the function $g(x)=1/a(x)$.

It is also not difficult to consider within the framework of this model the case of a microscopically sharp boundary. Let $e_n=e_1$, $V_{n-1,\,n}=-V_1$ for $n\leqslant 0$ and $e_n=e_2$, $V_{n,\,n+1}=-V_2$ for $n\geqslant 1$, and let a_1 and a_2 be respectively the interatomic distances in the regions to the left and right of the point 0. In order to investigate the matching conditions in the pure form, and avoid a jump and a singularity in the effective potential at the boundary, we shall have to set

$$e_1-2V_1=e_2-2V_2, \qquad V_{01}=(V_1V_2)^{1/2}.$$

Thus, our model with $U=0$ contains two dimensionless parameters: the ratios $\nu=V_1/V_2$ and $\alpha=a_1/a_2$, with $\mu=\nu\alpha^2$.

If $\nu=1$, then

$$\varphi_n=Ae^{ikn}+Be^{-ikn}.$$

The quantity $\psi(x_n)$, where x_n is the coordinate of the nth site, differs from φ_n only by a constant factor, which has different values in the regions to the right and left of the boundary because of the different modes of normalization adopted for φ and ψ. Thus, when $\nu=1$ the function ψ undergoes a jump:

$$\psi(+0)=\alpha^{1/2}\psi(-0)=\mu^{1/4}\psi(-0).$$

Since the presence of the boundary in this case is not in any way manifested in the Hamiltonian (20), there is no reflection from it, so that $\delta=\mu^{1/4}$, in complete agreement with (19). For arbitrary ν and α

$$\psi(+0)=(\nu\alpha)^{1/2}\psi(-0),$$
$$\psi'(+0)=\nu^{1/2}\alpha^{3/2}\psi(-0)=\mu(\nu\alpha)^{-1/2}\psi'(-0), \qquad (25)$$

so that $\delta=(\nu\alpha)^{1/2}$. If by chance $V_{01}\neq(V_1V_2)^{1/2}$, but the effective-mass approximation is valid for both $x<0$ and $x>0$, then the matching condition has, in first order in $\omega=V_{01}-(V_1V_2)^{1/2}$, the form

$$\psi_+=\delta\psi_-, \qquad \psi_+'=\frac{\mu}{\delta}\psi_-'+\frac{\omega}{(V_1V_2a_1a_2)^{1/2}}\psi_+. \qquad (26)$$

The correction, proportional to ω, to the derivative can be interpreted as the contribution of a δ-function potential located to the right of the boundary:

$$U_+^{imp}=\hbar^2\omega\delta(x+0)/2m_+(V_1V_2a_1a_2)^{1/2}.$$

This "impurity" potential can also be considered to be located to the left of the boundary; the second equation in (26) can then be written in the form

$$\psi_+'=\frac{\mu}{\delta}\psi_-'+\frac{\omega}{V_2a_2}\psi_-.$$

The expression obtained from (25) for δ does not coincide with the expression obtained from (18), since (25) corresponds to the limiting case of a microscopically sharp boundary, whereas (18) was obtained under the assumption that all the quantities vary smoothly on the microscopic scale. The general relation (3) is naturally valid for both cases.

The author is grateful to P. V. Elyutin for indicating to him the connection between the above-considered problem and the problem of quantization in Riemannian space, as well as L. V. Keldysh and A. P. Silin for extremely useful discussions.

[1] T. Gora and F. Williams, Phys. Rev. **177**, 1179 (1969).
[2] Q.-C. Zhu and H. Kroemer, Phys. Rev. B **27**, 3519 (1983).
[3] O. Ross, Phys. Rev. B **27**, 7547 (1983).
[4] R. A. Morrow and K. R. Borwnstein, Phys. Rev. B **30**, 678 (1984).
[5] V. Milanovic and D. Tjapkin, Phys. Status Solidi B **110**, 687 (1982).
[6] P. V. Elyutin and V. D. Krivchenkov, Teor. Mat. Fiz. **16**, 419 (1973).
[7] B. Podolsky, Phys. Rev. **32**, 812 (1928).
[8] G. Bastard, Phys. Rev. B **24**, 5693 (1981).

Translated by A. K. Agyei