A solution to the density matrix equation

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The authors derive a solution for the density matrix of an electron moving in a spatially periodic field. The solution corresponds to a mixed state of the system.

Consider the motion of a one-dimensional electron in a periodic field described by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U\sin kx,$$

where U and k are arbitrary real constants.

The corresponding equation for the density matrix can be written as follows:[1]

$$i\hbar\frac{\partial}{\partial t}\rho(x, x', t) = (\hat{H} - \hat{H}'^{*})\rho(x, x', t); \qquad (1)$$

where H' is the same operator acting on x'. It is easy to verify by direct substitution that equation (1) has an exact, steady-state solution:

$$\rho(x, x') = C\exp\left\{-\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\cos\left[\frac{k}{2}(x - x')\right] - \alpha U\sin\left[\frac{k}{2}(x + x')\right]\right\}; \qquad (2)$$

where C is a normalization constant and α is an arbitrary constant.

Let the one-dimensional motion occur in a segment $x\in[0,L]$. We impose the periodic boundary conditions

$$\rho(x+L, x') = \rho(x, x'), \quad \rho(x, x'+L) = \rho(x, x'). \qquad (3)$$

Substituting (2) into (3) one finds that the boundary conditions are satisfied only if

$$k = \frac{4\pi}{L}\nu, \quad \nu = 1, 2, 3, \ldots \qquad (4)$$

The normalization constant C is determined by the condition

$$\int_0^L \rho(x, x)\,dx = 1$$

whence

$$C = \exp\left[\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\right]\left[\int_0^L \exp(-\alpha U\sin kx)\,dx\right]^{-1} = \tilde{C}\exp\left[\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\right],$$

where

$$\tilde{C} = \left[\int_0^L \exp(-\alpha U\sin kx)\,dx\right]^{-1}. \qquad (5)$$

For $\rho(x, x')$ we find, ultimately,

$$\rho(x, x') = \tilde{C}\exp\left[-\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\left\{\cos\left[\frac{k}{2}(x - x')\right] - 1\right\} - \alpha U\sin\left[\frac{k}{2}(x + x')\right]\right]. \qquad (6)$$

Let us now derive the Wigner function corresponding to solution (6). We proceed from the general formula[2]

$$f(p, x) = \int_0^\infty \rho\left(x + \frac{t}{2},\ x - \frac{t}{2}\right)\exp\left(-\frac{ipt}{\hbar}\right)\frac{dt}{2\pi\hbar}. \qquad (7)$$

Substituting (6) into (7) we obtain

$$f(p, x) = \tilde{C}\exp(-\alpha U\sin kx)\cdot \times\exp\left[-\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\right]\sum_{n=-\infty}^{\infty} I_n\left(\frac{m}{\alpha}\left(\frac{2}{\hbar k}\right)^2\right)\delta\left(p - \frac{n\hbar k}{2}\right), \qquad (8)$$

where $I_n(z)$ is the modified Bessel function of order n; $\delta(z)$ is the delta function; $n = 0, \pm 1, \pm 2, \ldots$. One can verify by direct substitution that the normalization condition is satisfied:[2]

$$\int f(p, x)\,dp\,dx = 1.$$

From expression (8) we can solve for the mean value of the electron momentum

$$\langle p\rangle = 0.$$

Analogously, we find using (8) that

$$\left\langle\frac{p^2}{2m}\right\rangle = \frac{1}{2\alpha}.$$

The classical limit of $f(p, x)$ can be easily obtained by taking the $\hbar\to 0$ limit of (8):

$$f(p, x) = \tilde{C}\left(\frac{\alpha}{2\pi m}\right)^{1/2}\exp\left(-\frac{\alpha p^2}{2m} - \alpha U\sin kx\right). \qquad (9)$$

Note that if parameter α^{-1} is interpreted as a temperature T (in energy units), then solution (9) transforms into the classical Gibbs distribution for a particle in a field $U\sin kx$:

$$f(p, x) = \frac{\tilde{C}}{(2\pi mT)^{1/2}}\exp\left(-\frac{H(p, x)}{T}\right).$$

Recall that the C of this formula is given by equation (5).

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[1] L. D. Landau and E. M. Lifshits, *Quantum Mechanics: Non-Relativistic Theory*, 2nd ed., Pergamon Press, Oxford, 1962 [Russ. original, Nauka, M., 1963].

[2] R. Feynmann, *Statistical Mechanics*, Benjamin, N. Y., 1972 [Russ. transl., Mir, M., 1975].

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