The Density-Gradient Correction as a Disguised Pilot Wave of de Broglie

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Abstract

Recent papers on advanced semiconductor devices adopt a model called *density-gradient correction*, in which the standard electric potential acting on the carriers is modified by a non-linear term involving the carrier concentration and its second derivatives. When applied to cases where quantum effects are not negligible, the modified model improves the results with respect to the standard approach. The paper shows how, starting from a straightforward derivation of the density-gradient correction from the Schrödinger equation, its interpretation as an addition to the potential energy is questionable, and makes a few considerations for further investigation on the subject.

1 Introduction

In the modeling of nanoscale devices it is necessary to account for the quantum effects, that play a non-negligible role due to the device size and to the presence of sharp variations in the electric potential. To this purpose, in the frame of a semiclassical picture of carrier transport in semiconductors, a model call *density-gradient correction* is often used, in which the standard electric potential acting on the carriers is modified by a term proportional to $(\nabla^2\sqrt{n})/\sqrt{n}$, with n the carrier concentration. The adoption of this model provides better results than the standard approach when applied to cases where quantum effects are important. The model was proposed in [1], basing on thermodynamical considerations, for the case of an infinite system with no current flow. A following paper [2] refined the model by determining the numerical coefficient of the correction, basing on the asymptotic solution of the Wigner equation obtained by perturbation. Different forms of the correction are discussed in [3] and references therein. The inclusion of the density-gradient correction is made by simply adding it to the potential energy of the standard model, to obtain an “equivalent” field acting on the carriers. It will be shown in the following sections that the density-gradient correction possesses some properties that make such procedure questionable. A subtler point is that the adoption of the correction as such violates the applicability limits of the Ehrenfest approximation, upon which the semiclassical equations for the modeling of semiconductor devices are based. Further investigations on the subject are then of importance, both from the conceptual viewpoint and to provide a sound basis for the models to be adopted in practical applications.

2 Theory

The starting point is the Schrödinger equation $j\hbar\,\partial\psi/\partial t = \mathcal{H}\psi$ which, in this form, holds for a system of particles and for a non-conservative case as well. Considering a system of identical particles of mass m and neglecting the magnetic part of the force, the single-particle Hamiltonian reads $\mathcal{H} = \hat{\boldsymbol{p}}\bullet\hat{\boldsymbol{p}}/(2m) + V_w$, where $\hat{\boldsymbol{p}} = -j\hbar\,\nabla$ and V_w accounts for the effect of the other particles and possible external forces. Here, the wave function ψ is defined over a domain Ω, which may be infinite, and is assumed normalized. The Schrödinger equation is easily split into two real equations by considering the real and imaginary part of ψ. However, it is more sensible to use the expression $\psi = \alpha\,\exp(j\beta)$, $\alpha \geq 0$, which reminds one of that used to derive the eikonal equation of geometrical optics. In this case the two real equations read

$$\frac{\partial\alpha}{\partial t} = -\frac{\hbar}{2m}\left(\alpha\,\nabla^2\beta + 2\nabla\alpha\bullet\nabla\beta\right)\,, \tag{1}$$

$$\frac{\partial(\hbar\beta)}{\partial t} + \frac{1}{2m}|\nabla(\hbar\beta)|^2 + V_w - \frac{\hbar^2}{2m}\,\frac{\nabla^2\alpha}{\alpha} = 0\,. \tag{2}$$

The dimensions of α^2 and $\nabla\hbar\beta$ are the inverse of a volume and a momentum, respectively. Letting $P = \alpha^2$, $S = \hbar\beta$, $\boldsymbol{v}_e = \nabla S/m$, $Q = -\hbar^2/(2m)\,(\nabla^2\alpha/\alpha)$, $H_Q = mv_e^2/2 + Q + V_w$, and multiplying (1) by 2α, the set of two equations (1,2) become

$$\frac{\partial P}{\partial t} + \mathrm{div}(P\boldsymbol{v}_e) = 0\,, \qquad \frac{\partial S}{\partial t} + H_Q = 0\,, \tag{3}$$

with

$$\int_\Omega P\,\mathrm{d}^3r = \int_\Omega |\psi|^2\,\mathrm{d}^3r = 1\,, \tag{4}$$

namely, two differential equations in the unknowns α, β, the first of which is the standard continuity equation for the probability density. As for the second of (3), its limit for $\hbar \to 0 \implies Q \to 0$ is the Hamilton-Jacobi equation of classical mechanics and, as a consequence, the classical limit of S is the Hamilton principal function [4, Ch. VI-4]. It should also be noted that, in the limit $Q \to 0$, equations (3) become decoupled from each other. Without the limit, the term Q may be manipulated by considering an ensemble of N replicas of the particle, to find

$$Q = -\frac{\hbar^2}{2m}\,\frac{\nabla^2\alpha}{\alpha} = -\frac{\hbar^2}{2m}\,\frac{\nabla^2\sqrt{P}}{\sqrt{P}} = -\frac{\hbar^2}{2m}\,\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\,, \tag{5}$$

where $n = NP$ is dimensionally a concentration. Clearly, as n is a quantity proportional to the squared wave function of a single particle, its meaning is not that of concentration in a system of interacting particles. On the other hand, it is interesting to note that the last form of Q in (5) reproduces that of the density-gradient correction. The derivation above shows that such a term is inherent in the Schrödinger equation and is derived from it without approximations. In the time-independent case (3) reduce to

$$\mathrm{div}(P\boldsymbol{v}_e) = 0\,, \qquad \frac{1}{2}mv_e^2 + Q + V_w = E\,, \tag{6}$$

coherently with the fact that in this case Hamilton's principal function becomes $S = W - Et$, with W the time-independent Hamilton characteristic function. Although $\boldsymbol{v}_e$ plays the role of an average velocity in the continuity equation of (3) or (6), determining the expectation value needs a further averaging: in fact, taking the usual definition of expectation value and observing that the normalization makes the integral of $\nabla\alpha^2$ to vanish, yields

$$m\,\langle \boldsymbol{v}_e \rangle = \int_\Omega \psi^*\,\hat{\boldsymbol{p}}\psi\,\mathrm{d}^3 r = \int_\Omega \alpha^2\,\nabla(\hbar\beta)\,\mathrm{d}^3 r = m\int_\Omega \alpha^2\,\boldsymbol{v}_e\,\mathrm{d}^3 r\,. \tag{7}$$

3 Is the density-gradient correction a potential energy?

The second of (6) suggests that Q is a potential energy to be added to V_w. This is not necessarily true, as shown by the calculation of the expectation value of the kinetic energy T:

$$\langle T \rangle = \frac{1}{2m}\int_\Omega \psi^* \hat{\boldsymbol{p}}^2 \psi\,\mathrm{d}\Omega = -\frac{\hbar^2}{2m}\int_\Omega \alpha\exp(-j\beta)\,\nabla^2\left[\alpha\exp(j\beta)\right]\,\mathrm{d}\Omega =$$

$$= \int_\Omega \psi^*\left(\frac{1}{2}m v_e^2 + Q\right)\psi\,\mathrm{d}\Omega\,, \tag{8}$$

showing that the presence of Q is essential for correctly determining the expectation value of T. To better investigate the meaning of Q it is useful to consider alternative expressions of $\langle Q \rangle$, like

$$\langle Q \rangle = \frac{\hbar^2}{2m}\int_\Omega |\nabla\alpha|^2\,\mathrm{d}\Omega = \frac{1}{2m}\left(\langle \hat{\boldsymbol{p}}^2 \rangle - \langle p_e^2 \rangle\right)\,, \qquad \boldsymbol{p}_e = m\boldsymbol{v}_e\,, \tag{9}$$

whose derivation is straightforward and follows the same pattern as that of (8). The first form shows that $\langle Q \rangle$ is positive definite irrespective of the shape of α. The second one is the analogue of the definition of dispersion around the average found in classical statistics. By analogy with the classical case one may think that the term $p_e^2/(2m)$ provides the analogue of the convective part of the kinetic energy, while Q provides the analogue of the thermal part of it. By way of example, assume that at a given instant of time the wave function be the minimum-uncertainty packet of the one-dimensional case,

$$\alpha = \frac{1}{\sqrt[4]{2\pi}\,\sqrt{\sigma}}\,\exp\left[-\frac{(x-x_0)^2}{4\sigma^2}\right]\,, \qquad \beta = k_0 x\,, \tag{10}$$

which is normalized for any σ. One finds $\langle x \rangle = x_0$, $\mathrm{d}\hbar\beta/\mathrm{d}x = \hbar k_0$, $\langle p_e \rangle = \hbar k_0$,

$$\left\langle \frac{p_e^2}{2m} \right\rangle = \frac{\hbar^2 k_0^2}{2m}\,, \qquad \langle Q \rangle = \frac{\hbar^2}{8m\sigma^2}\,, \qquad \langle T \rangle = \frac{\hbar^2}{2m}\left(k_0^2 + \frac{1}{4\sigma^2}\right)\,. \tag{11}$$

As a consequence, for a fixed $\langle T \rangle$ all non-negative values of the "convective" and "thermal" parts that add up to $\langle T \rangle$ are allowed. In the particular case of a free particle, where $\langle T \rangle = \langle E \rangle$, the above shows that different values of the average momentum and dispersion may combine to yield the same total energy.

In view of the meaning of $\langle Q \rangle$ that stems from the above observations, the assumption that $-\nabla Q$ provides an additional contribution to the field acting on the particles, in an otherwise unchanged transport equation, becomes questionable.

4 Conclusion and historical remark

The transport equation commonly used for the description of semiconductor devices is derived by combining the Hamilton equations for the expectation values of position and momentum, supplemented with the Ehrenfest approximation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \boldsymbol{r}\rangle = \langle \boldsymbol{v}_e\rangle \,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle \boldsymbol{p}_e\rangle = -\int_\Omega \alpha^2 \nabla V_w \,\mathrm{d}\Omega \simeq -\nabla V_w \,, \tag{12}$$

with the continuity equation in the phase space $\boldsymbol{r}, \boldsymbol{p}_e$. The adoption of the density-gradient correction is equivalent to replacing the last term in (12) with $-\nabla(V_w + Q)$. This, on the other hand, yields Hamiltonian relations that can not be derived by the standard procedure of quantum mechanichs and, moreover, violates the applicability limits of the Ehrenfest approximation. Another difficulty is that the expression of Q written in terms of the carrier concentration introduces a dependence on the device temperature, which is obviously missing in the equivalent expression of Q in terms of α: consensus is still lacking as for the extension of the theory from a pure state to the statistical ensemble. Despite these aspects, the results obtained by introducing the density-gradient correction are encouraging in several practical applications. Quoting a recent paper, "DG *theory is a macroscopic approximation to quantum mechanics ... The theory built on this simple foundation, though obviously incomplete, has been found to be surprisingly accurate ... in practical situations*" [5]. The considerations of sections 3 and 4 provide a clue for a sound formalization of the density-gradient correction, namely, that of seeking for a more general form of the Hamiltonian relations (12).

It is interesting to note that the analogy between the Schrödinger equation and a set of a continuity and a Hamilton-Jacobi-like equations had been noted by de Broglie, who introduced the concept of *pilot wave* in [6]. This cost him severe criticism by Pauli at the Fifth Solvay Conference. He resumed the idea more than twenty years later, stimulated by the papers by Bohm introducing the concept of *quantum potential*, see e.g., [7]. The most recent paper by de Broglie on the subject is [8], published when the author was seventy-nine years old. The density-gradient correction for a pure state is nothing more than the quantum potential of Bohm, and is correctly identified as such, e.g., in [3].

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