C Numerical Calculation of Carrier Trajectories

> Mutationem motus proportionalem esse vi motrici impressae, et fieri secundum lineam rectam qua vis illa imprimitur.
>
> *(Sir Isaac Newton, Pricipia Mathematica)*

Electron trajectories in an arbitrary electrostatic potential $V(\mathbf{r})$ can be simulated by numerically integrating the semiclassical equations of motion [1]

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k}) \qquad \text{and} \tag{C.1}$$

$$\hbar\dot{\mathbf{k}} = -e\big[\mathbf{E}(\mathbf{r}) + \dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r})\big], \tag{C.2}$$

where $\mathbf{r}$ and $\mathbf{k}$ denote position and crystal momentum, $E(\mathbf{k})$ is the energy dispersion, q the charge, $\mathbf{E}(\mathbf{r}) = -\nabla_{\mathbf{r}} V(\mathbf{r})$ the electric field, and $\mathbf{B}(\mathbf{r})$ the magnetic field. The equations of motion for electron holes with energy $E_{\mathrm{h}}(\mathbf{k})$ are obtained by replacing $E(\mathbf{k})$ by $-E_{\mathrm{h}}(\mathbf{k})$ in Eq. (C.1) and $-e$ by e in Eq. (C.2) [2].

Integrating the equations of motion of one or more particles is an ubiquitous problem, and a number of general algorithms have been developed for this purpose, particularly in the context of molecular dynamics simulations. For the present work I have chosen an approach based on Beeman's algorithm [3], which gives both position and momentum up to third order in the time step and provides for improved energy conservation compared to the

unmodified Verlet algorithm. In this scheme, the position and momentum at the next time step are

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + \dot{\mathbf{r}}(t)\delta t + \frac{2}{3}\ddot{\mathbf{r}}\delta t^2 - \frac{1}{6}\ddot{\mathbf{r}}(t-\delta t)\delta t^2 \qquad \text{and} \tag{C.3}$$

$$\mathbf{k}(t+\delta t) = \mathbf{k}(t) + \frac{5}{12}\dot{\mathbf{k}}(t+\delta t)\delta t + \frac{3}{2}\dot{\mathbf{k}}(t)\delta t - \frac{1}{12}\dot{\mathbf{k}}(t-\delta t)\delta t. \tag{C.4}$$

If $\mathbf{B}(\mathbf{r}) \neq \mathbf{0}$, according to Eq. (C.2) the force and hence the momentum change $\dot{\mathbf{k}}$ depends on the velocity $\dot{\mathbf{r}}$. As $\dot{\mathbf{r}}(t+\delta t)$ is not known yet, one cannot determine $\dot{\mathbf{k}}(t+\delta t)$ in Eq. (C.4) directly. Instead, a predictor–corrector method is used, in which Eq. (C.4) is replaced by

$$\mathbf{k}_0(t+\delta t) = \mathbf{k}(t) + \frac{3}{2}\dot{\mathbf{k}}(t)\delta t - \frac{1}{2}\dot{\mathbf{k}}(t-\delta t)\delta t \qquad \text{and} \tag{C.5}$$

$$\mathbf{k}_{n+1}(t+\delta t) = \mathbf{k}(t) + \frac{1}{3}\dot{\mathbf{k}}(t+\delta t)\delta t + \frac{5}{6}\dot{\mathbf{k}}(t)\delta t - \frac{1}{6}\dot{\mathbf{k}}(t-\delta t)\delta t \tag{C.6}$$

and Eq. (C.6) is iterated until the correction $\mathbf{k}_{n+1}(t+\delta t) - \mathbf{k}_n(t+\delta t)$ falls below a predetermined threshold.

If $\mathbf{B}(\mathbf{r}) = (0, 0, B_z)$ independent of $\mathbf{r}$ and $\partial V(\mathbf{r})/\partial z = 0$, corresponding to a laterally modulated two-dimensional electron gas (2DEG) in a perpendicular magnetic field, Eqs. (C.1) and (C.2) can be written in terms of x, y, k_x, and k_y as

$$\dot{x} = \frac{1}{\hbar}\frac{\partial E(k_x, k_y)}{\partial k_x}, \qquad \dot{y} = \frac{1}{\hbar}\frac{\partial E(k_x, k_y)}{\partial k_y}, \tag{C.7}$$

$$\hbar\dot{k}_x = e\frac{\partial V(x,y)}{\partial x} - e\dot{y}B_z, \qquad \text{and} \qquad \hbar\dot{k}_y = e\frac{\partial V(x,y)}{\partial y} + e\dot{x}B_z. \tag{C.8}$$

A square lattice of antidots with period a can be represented by a phenomenological potential of the form [4]

$$V(x,y) = V_0\left[\cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{a}\right)\right]^{2\alpha} \qquad \text{with} \quad \alpha \in \mathbb{Z}^+, \tag{C.9}$$

where $V_0 < 0$ and α is a parameter controlling the steepness. A weak potential modulation corresponds to $-eV_0 \ll E_\mathrm{F}$, where E_F is the Fermi energy, while $-eV_0 > E_\mathrm{F}$ implies the local depletion of the carrier sheet. If $-eV_0 \gg E_\mathrm{F}$, the intersection contours $-eV(x,y) = E_\mathrm{F}$

are approximately circular and one can identify the diameter of the antidots as $d \approx a\big[\frac{1}{2} - \sqrt[2\alpha]{E_\mathrm{F}/(-eV_0)}/\pi\big]$.

It is convenient to express Eqs. (C.7), (C.8) and (C.9) using dimensionless variables. The lattice constant gives the natural scale for the position, leading to $\tilde{x} \stackrel{\text{def}}{=} x/a$ and $\tilde{y} \stackrel{\text{def}}{=} y/a$, while the energy scale is set by E_F so that one can define $\tilde{U} \stackrel{\text{def}}{=} -eV/E_\mathrm{F}$. With these definitions Eq. (C.9) simplifies to

$$\tilde{U}(x,y) = \tilde{U}_0\big[\cos(\pi\tilde{x})\cos(\pi\tilde{y})\big]^{2\alpha}, \tag{C.10}$$

where $\tilde{U}_0 = -eV_0/E_\mathrm{F} \approx [\cos(\pi d/2a)]^{-2\alpha}$. The energy dispersion should be scaled accordingly as $\tilde{E} \stackrel{\text{def}}{=} E/E_\mathrm{F}$, while the momentum coordinates will be $\tilde{k}_x \stackrel{\text{def}}{=} k_x/k_0$ and $\tilde{k}_y \stackrel{\text{def}}{=} k_y/k_0$. If $k_0 = \sqrt{2m_\mathrm{c}E_\mathrm{F}/\hbar^2}$, where m_c is the cyclotron effective mass at E_F, and one further defines $\tilde{t} = t/t_0$ and $\tilde{B} = B_z/B_0$ with $t_0 = \sqrt{2m_\mathrm{c}a^2/E_\mathrm{F}}$ and $B_0 = 2\sqrt{2m_\mathrm{c}E_\mathrm{F}}/ea$, Eqs. (C.7) and (C.8) become

$$\frac{d\tilde{x}}{d\tilde{t}} = \frac{\partial\tilde{E}(\tilde{k}_x,\tilde{k}_y)}{\partial\tilde{k}_x}, \qquad \frac{d\tilde{y}}{d\tilde{t}} = \frac{\partial\tilde{E}(\tilde{k}_x,\tilde{k}_y)}{\partial\tilde{k}_y}, \tag{C.11}$$

$$\frac{d\tilde{k}_x}{d\tilde{t}} = -\frac{\partial\tilde{U}(\tilde{x},\tilde{y})}{\partial\tilde{x}} - 2\frac{d\tilde{y}}{d\tilde{t}}\tilde{B}, \qquad \text{and} \qquad \frac{d\tilde{k}_y}{d\tilde{t}} = -\frac{\partial\tilde{U}(\tilde{x},\tilde{y})}{\partial\tilde{y}} + 2\frac{d\tilde{x}}{d\tilde{t}}\tilde{B}. \tag{C.12}$$

For nearly free electrons, $E(k_x,k_y) = \hbar^2(k_x^2+k_y^2)/2m^*$, so that $m_\mathrm{c} = m^*$ and a well-defined Fermi wave number k_F and Fermi velocity v_F exist. The above definitions then imply $k_0 = k_\mathrm{F}$ and $t_0 = 2a/v_\mathrm{F}$, while $B_0 = 2m^*v_\mathrm{F}/ea$ is the field for which the cyclotron radius $R_\mathrm{c} = m^*v_\mathrm{F}/eB_z$ equals $a/2$.

For electron holes, Eqs. (C.11) and (C.12) need to be modified as described above, so that one now has

$$\frac{d\tilde{x}}{d\tilde{t}} = -\frac{\partial\tilde{E}(\tilde{k}_x,\tilde{k}_y)}{\partial\tilde{k}_x}, \qquad \frac{d\tilde{y}}{d\tilde{t}} = -\frac{\partial\tilde{E}(\tilde{k}_x,\tilde{k}_y)}{\partial\tilde{k}_y}, \tag{C.13}$$

$$\frac{d\tilde{k}_x}{d\tilde{t}} = -\frac{\partial\tilde{U}(\tilde{x},\tilde{y})}{\partial\tilde{x}} + 2\frac{d\tilde{y}}{d\tilde{t}}\tilde{B}, \qquad \text{and} \qquad \frac{d\tilde{k}_y}{d\tilde{t}} = -\frac{\partial\tilde{U}(\tilde{x},\tilde{y})}{\partial\tilde{y}} - 2\frac{d\tilde{x}}{d\tilde{t}}\tilde{B}\cdot \tag{C.14}$$

If the hole band $E_\mathrm{h}(\mathbf{k})$ is given by Eq. (5.8), the reduced energy $\tilde{E}(\tilde{k}_x,\tilde{k}_y)$ becomes

$$\tilde{E}(\tilde{k}_x,\tilde{k}_y) = \frac{E_\mathrm{g}}{E_\mathrm{F}} - 2\frac{m_\mathrm{c}}{m_\mathrm{e}}\left[|A|\big(\tilde{k}_x^2+\tilde{k}_y^2\big) - \sqrt{B^2\big(\tilde{k}_x^2+\tilde{k}_y^2\big)^2 + C^2k_x^2k_y^2}\right], \tag{C.15}$$

where—as before—I take the anisotropy parameters to be $A = -14{\cdot}3$, $B = -10{\cdot}4$, and $C = 13{\cdot}5$ [5]. With this dispersion relation, one finds $m_c \approx 0{\cdot}185 m_e$ independent of energy. The scale B_0 then identifies the magnetic field for which the unperturbed cyclotron orbit has the same area as a circle of radius $a/2$.

Bibliography

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