Zitterbewegung of charge carriers in semiconductors

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Schrödinger equation (non relativistic)

Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m_0}$

Velocity $\hat{\mathrm{v}}_i = \frac{\partial \hat{H}}{\partial \hat{p}_i} = \frac{\hat{p}_i}{m_0}$

$$\frac{d\,\hat{\mathrm{v}}_i}{\mathrm{dt}} = \frac{1}{i\hbar}\left[\hat{\mathrm{v}}_i, \hat{H}\right] = \frac{1}{i\hbar m_0}\left[\hat{\mathrm{p}}_i, \hat{H}\right] = 0$$

v_i = const. Newton’s First Law

Schrödinger 1930

Dirac Equation $\mathrm{H} = c\vec{\alpha}\cdot\vec{p} + m_0 c^2 \beta$ α, β 4x4 matrices

velocity $\mathrm{v_i} = \frac{\partial H}{\partial p_i} = \alpha_i$ α and β anticommute

$$-i\hbar \frac{d\vec{\alpha}}{dt} = [H, \vec{\alpha}] = -\vec{\alpha}H - H\vec{\alpha} + H\vec{\alpha} + H\vec{\alpha} = -\{H, \vec{\alpha}\} + 2H\vec{\alpha} = -2c\vec{p} + 2H\vec{\alpha}$$

Differential equation for α (or v)

Finding solution and integrating $\vec{r}(t) = \vec{a} + c^2 H^{-1}\vec{p}t + \frac{1}{2} ic\hbar\eta_0 H^{-1} e^{-2iHt/\hbar}$

Zitterbewegung !

Frequency $\hbar\omega_Z \approx 2E \approx 2m_0 c^2$

Amplitude $\frac{\hbar c}{E} \approx \frac{\hbar c}{m_0 c^2} = \frac{\hbar}{m_0 c} = \lambda_C \approx 4\times 10^{-3}\ \mathring{\mathrm{A}}$

Narrow gap semiconductors

k.p theory $$\mathrm{H} = u\vec{\alpha}\cdot\vec{p} + \frac{\varepsilon_g}{2}\beta$$

correspondence to vacuum $2m_0c^2 \rightarrow \varepsilon_g \qquad m_0 \rightarrow m_0^*$

$$c = \left(\frac{2m_0c^2}{2m_0}\right)^{1/2} \rightarrow \left(\frac{\varepsilon_g}{2m_0^*}\right)^{1/2} = u \approx 10^8\,\mathrm{cm/s}$$

$$\varepsilon_g = 2m_0^*u^2 \qquad m_0^* \approx 0.02m_0$$

Zitterbewegung

frequency $\hbar\omega_Z \approx \varepsilon_g$

amplitude $\lambda_C \rightarrow \lambda_Z = \dfrac{\hbar}{m_0^*u} \approx 4\times10^{-3} * 3\times10^2 * 5\times10 \approx 60\,\mathrm{\mathring{A}}$

MONOLAYER GRAPHENE

Hamiltonian
$$\hat{H}_M = u\begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

where u≈1x10^{8}cm/s $\quad E = \pm u\hbar k \quad$ no gap!

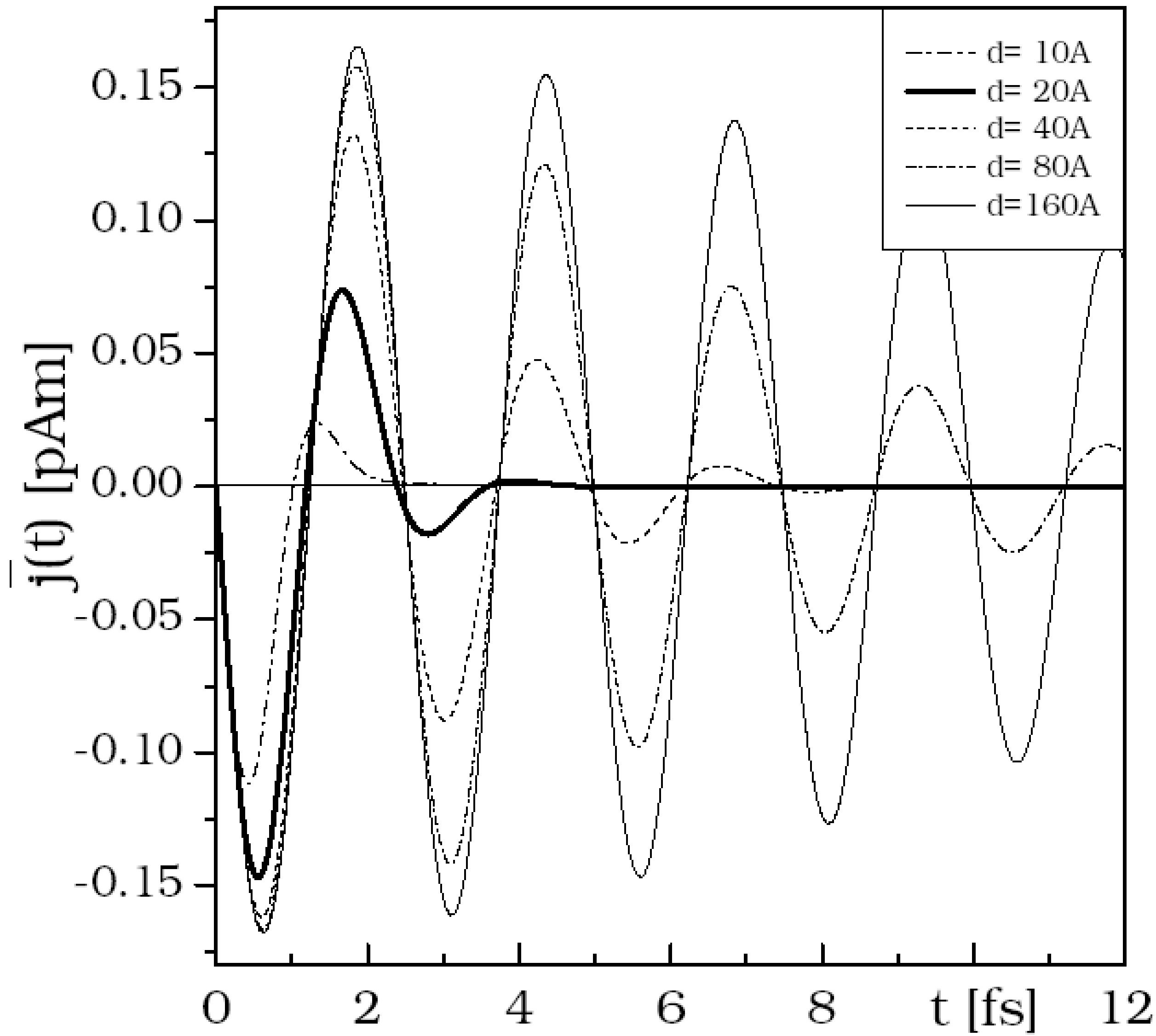
velocity
$$\hat{v}_i = \frac{\partial \hat{H}_M}{\partial \hat{p}_i} \qquad \hat{\mathbf{v}}(t) = e^{i\hat{H}_M t/\hbar}\,\hat{\mathbf{v}}\,e^{-i\hat{H}_M t/\hbar}$$

$$\hat{v}_x^{(11)}(t) = u\frac{k_y}{k}\sin(2ukt)$$

Frequency $\hbar\omega_Z = 2u\hbar k$

Current $\boldsymbol{j} = e\mathbf{v}$

2D Wave packet
$$\psi(\boldsymbol{r},t) = \frac{1}{2\pi}\frac{d}{\sqrt{\pi}}\int d^2\boldsymbol{k}e^{-\frac{1}{2}d^2k_x^2-\frac{1}{2}d^2(k_y-k_{0y})^2}e^{i\boldsymbol{kr}}\begin{pmatrix}1\\0\end{pmatrix}$$



Oscillatory electric current caused by the ZB in monolayer graphene *versus* time, calculated for a gaussian wave packet

ω_Z nearly constant, amplitude depends on the packet's width *d*

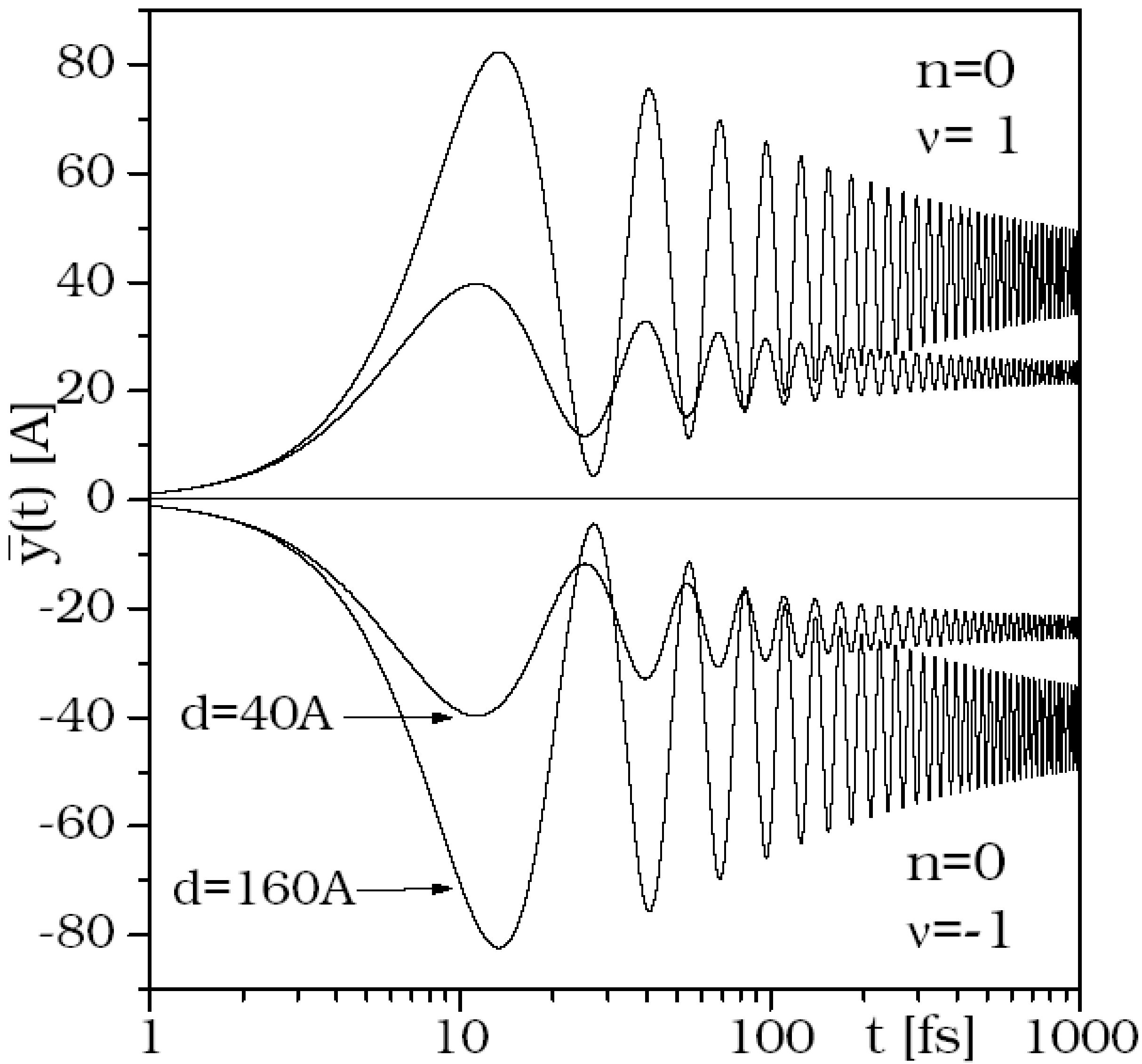
CARBON NANOTUBES

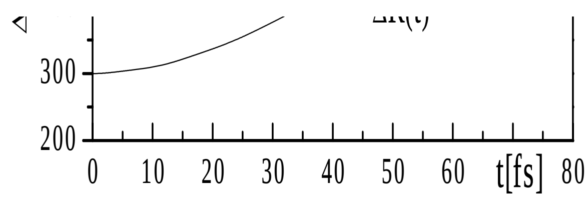
Hamiltonian

$$\hat{H}_{CNT} = u\begin{pmatrix} 0 & \hbar k_{n\nu} - ip_y \\ \hbar k_{n\nu} + ip_y & 0 \end{pmatrix}$$

Energy $$E = \pm\hbar u\sqrt{k_{n\nu}^2 + k_y^2}$$

IN GENERAL $$\hbar\omega_Z \approx \Delta E \qquad \lambda_Z \approx \frac{\hbar}{m^* u} \propto \frac{1}{\Delta E}$$





Zitterbewegung of two charge carriers in the ground subband of a single carbon nanotube of *L*=200A *versus* time

Time scale of damping: picoseconds

Spatial separation of ν=+1 and ν=-1 states

Here the SPREADING seems to be responsible for the transient character of ZB

Monolayer graphene + B

$$\hat{H} = u\begin{pmatrix} 0 & \hat{\pi}_x - i\hat{\pi}_y \\ \hat{\pi}_x + i\hat{\pi}_y & 0 \end{pmatrix}$$

π_i = p+|e|A

Exact solutions in harmonic oscillators

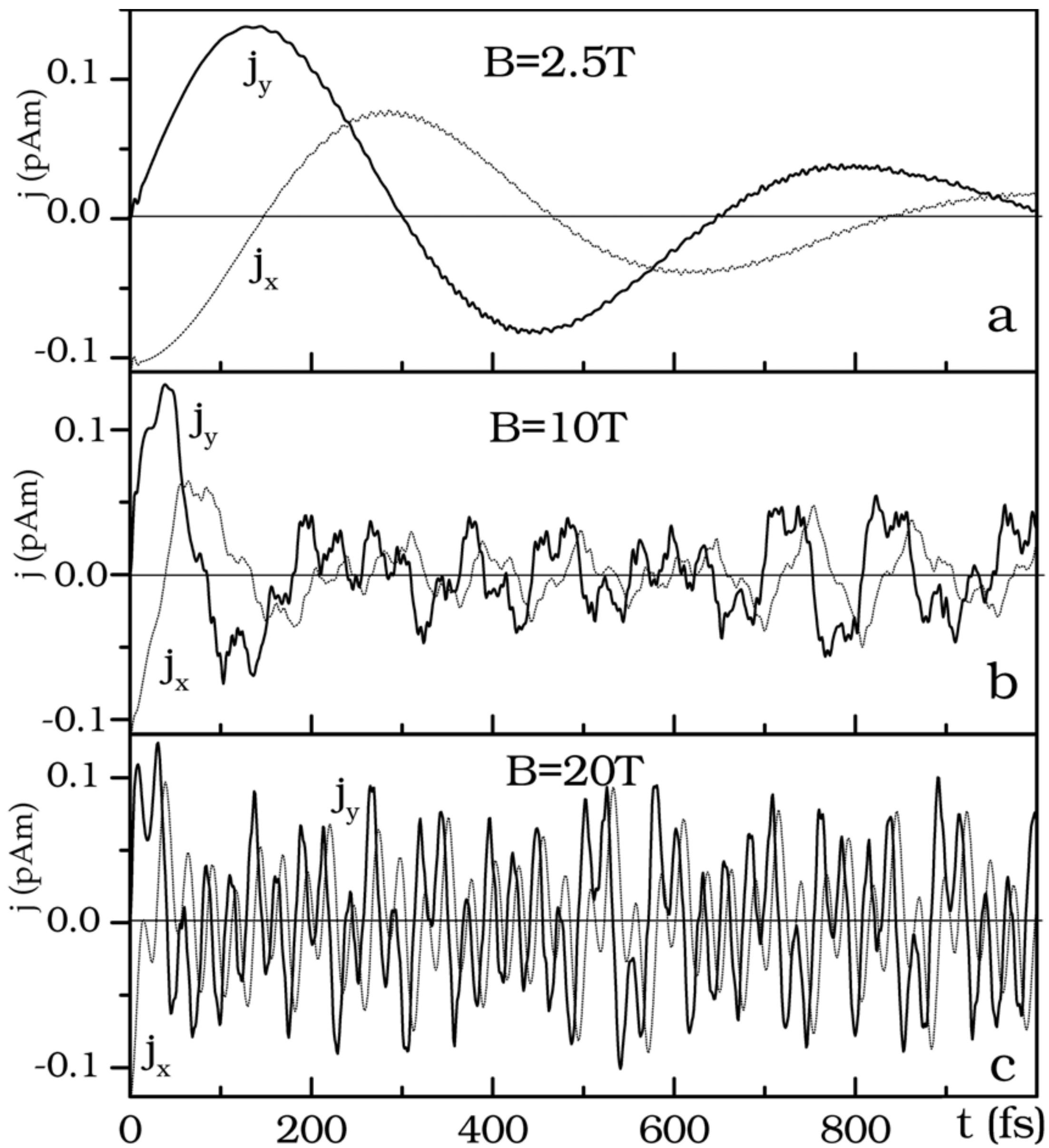
Energies

$$E_{ns} = s\hbar\omega\sqrt{n}$$

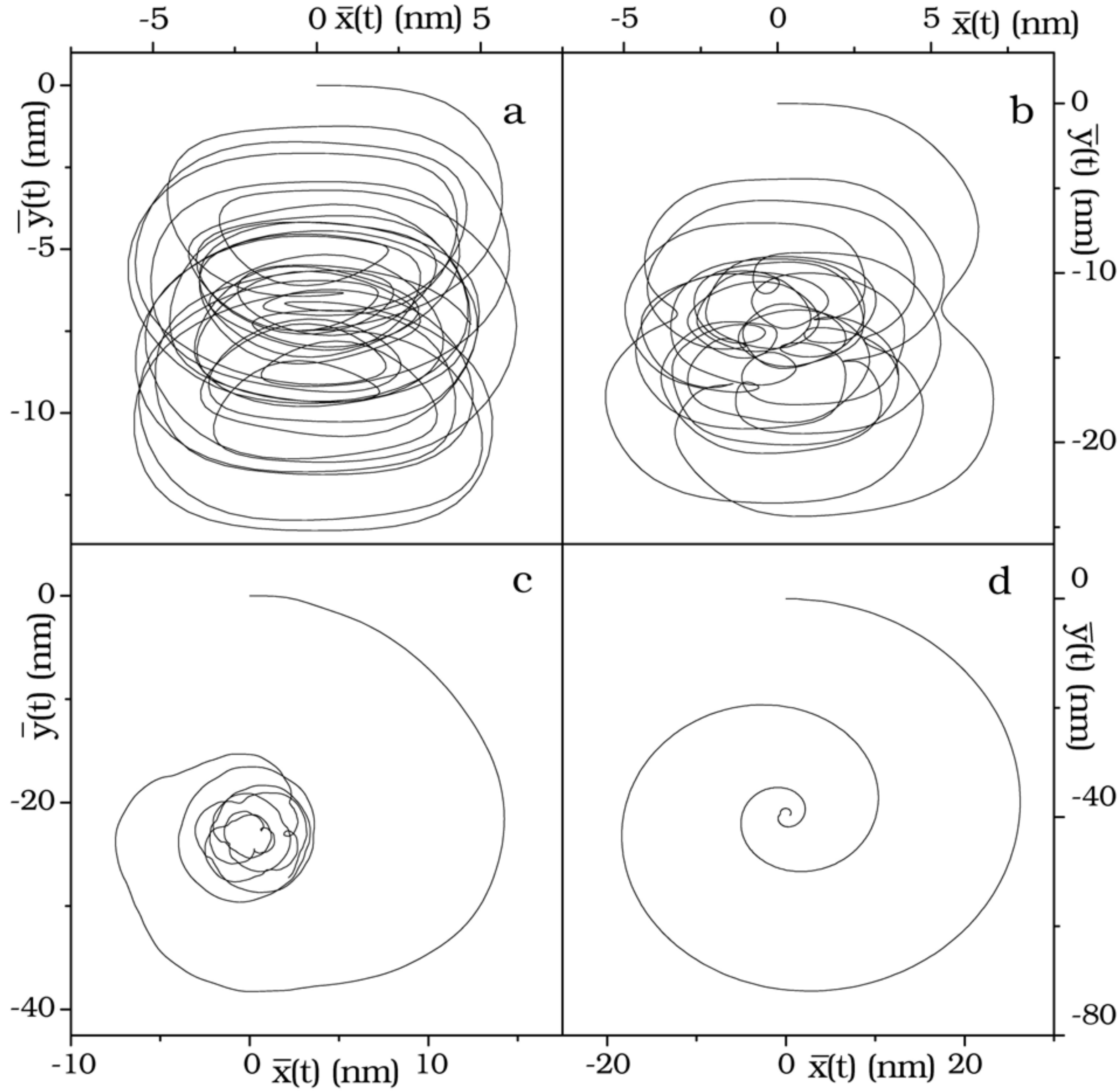
$$\omega = \sqrt{\frac{2eB}{\hbar}}u$$

$$|\mathrm{n}\rangle = \frac{\mathrm{e}^{ik_x x}}{\sqrt{4\pi}}\begin{pmatrix} -s|n-1\rangle \\ |n\rangle \end{pmatrix}$$

$$\langle \mathbf{r}|n\rangle = \frac{1}{\sqrt{LC_n}}\exp\left(-\frac{1}{2}\xi^2\right)\mathrm{H}_n(\xi)$$



Trajectories for given B and different k_{0x}



Moral

Electron in a solid with a non-zero momentum „zitters”.

This is a consequence of the periodic potential