Dynamics of the effective mass and the anomalous velocity



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SUE THE BASTARDS











Outline

The conventional wisdom The conventional wisdom is wrong! When the conventional wisdom is not so wrong Beyond the conventional wisdom Experiments and possible experiments The moral(s) of the story

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Effective mass and Bloch oscillations

The anomalous velocity



Effective mass and Bloch oscillations

The anomalous velocity

Effective mass "theorem"

























Wavepacket spreading



Wavepacket spreading



Wavepacket spreading

















> Wavepacket spreading Zener tunneling Scattering processes





$$t_{Bloch} = \frac{h}{bF} = \frac{h}{beE}$$

$$b = 0.5nm$$
$$E = \frac{170 \ kV}{cm} = \frac{17 \ V}{\mu m}$$
$$t_{Bloch} \approx 500 \ fs$$

Semiconductor superlattices



Waschke et al., Phys. Rev. Lett. 70, 3319 (1993)

Optical lattices



I. Bloch, M. Grenier (2005)

Ultracold atoms: small spread in momentum Adiabatic loading: wavepacket in one band Acceleration of the lattice: inertial force in the lattice frame Turn off the lattice: measure the velocity at any desired time



FIG. 3. Mean atomic velocity $\langle v \rangle$ as a function of the acceleration time t_a for three values of the potential depth: (a) $U_0 = 1.4E_R$, (b) $U_0 = 2.3E_R$, (c) $U_0 = 4.4E_R$. The negative values of Ft_a were measured by changing the sign of F. Solid lines: theoretical prediction.

Dehan et al., Phys. Rev. Lett. 76, 4508 (1996) Peik et al., Phys. Rev. A55, 2989 (1997)

Acceleration of a BEC: Denschlag et al, J. Phys. B35, 3095 (2002)



Effective mass and Bloch oscillations

The anomalous velocity






2D atomic lattices



Chequerboard Triangular Dimer
 Image: Dimer</

$$V(x,y) = -\frac{V_{\bar{X}}}{2}\cos(k_R(x+y)+\theta) - \frac{V_X}{2}\cos(k_R(x+y)) - \frac{V_Y}{2}\cos(k_R(x-y)) - \frac{V$$

Tarruell et al., Nature 483, 202 (2012)



 $V_X = 0.25E_R$ $V_{\bar{X}} = 3.5E_R$ $V_Y = 1.0E_R$









$$\phi_{n\mathbf{k}}(\mathbf{r}) = \frac{u_{n\mathbf{k}}(\mathbf{r})}{2\pi} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})=u_{n\mathbf{k}}(\mathbf{r})$$



$$\phi_{n\mathbf{k}}(\mathbf{r}) = \frac{u_{n\mathbf{k}}(\mathbf{r})}{2\pi} e^{i\mathbf{k}\cdot\mathbf{r}}$$
$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

$$i\frac{\partial u_{n\mathbf{k}}(\mathbf{r})}{\partial \mathbf{k}} = \sum_{m} u_{m\mathbf{k}}(\mathbf{r})\xi_{mn}(\mathbf{k})$$

$$\xi_{mn}(\mathbf{k}) = \frac{\hbar}{im} \frac{\mathbf{p}_{mn}(\mathbf{k})}{E_{mn}(\mathbf{k})}$$



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Berry phase

$$\phi_{n\mathbf{k}}(\mathbf{r}) = \frac{u_{n\mathbf{k}}(\mathbf{r})}{2\pi} e^{i\mathbf{k}\cdot\mathbf{r}}$$
$$u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

$$i\frac{\partial u_{n\mathbf{k}}(\mathbf{r})}{\partial \mathbf{k}} = \sum_{m} u_{m\mathbf{k}}(\mathbf{r})\xi_{mn}(\mathbf{k})$$

$$\xi_{mn}(\mathbf{k}) = \frac{\hbar}{im} \frac{\mathbf{p}_{mn}(\mathbf{k})}{E_{mn}(\mathbf{k})}$$

 $\xi_{nn}(\mathbf{k})$



Berry curvature

$$\phi_{n\mathbf{k}}(\mathbf{r}) = \frac{u_{n\mathbf{k}}(\mathbf{r})}{2\pi} e^{i\mathbf{k}\cdot\mathbf{r}}$$
$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

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$$\xi_{mn}(\mathbf{k}) = \frac{\hbar}{im} \frac{\mathbf{p}_{mn}(\mathbf{k})}{E_{mn}(\mathbf{k})}$$

$$\Omega_n(\mathbf{k}) = \frac{\partial}{\partial \mathbf{k}} \times \xi_{nn}(\mathbf{k})$$









 $\langle \mathbf{k} \rangle \rightarrow \langle \mathbf{k} \rangle + \frac{\mathbf{F}}{\hbar} t$



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 $\frac{d\langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g$

 $\mathbf{v}_{g} = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$

 $\langle \mathbf{k} \rangle \rightarrow \langle \mathbf{k} \rangle + \frac{\mathbf{F}}{\hbar} t$ k_y (2π/b) k_x (2π/b)

 $\frac{d\langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g + \mathbf{v}_a$

 $\mathbf{v}_{g} = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$

 $\mathbf{v}_a = \frac{1}{\hbar} \langle \mathbf{\Omega}(\mathbf{k}) \rangle \times \mathbf{F}$



Effective mass and Bloch oscillations

The anomalous velocity

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 $\frac{d^2 \langle r^a \rangle}{dt^2} = \left(\frac{1}{\hbar} \frac{\partial^2 \boldsymbol{\omega}(\mathbf{k})}{\partial k^a \partial k^b}\right) F^b$

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$$= \left[\frac{1}{m^*(\mathbf{k})}\right]^{ab} F^b$$

$$\mathbf{v}_{a} = \frac{1}{\hbar} \langle \mathbf{\Omega}(\mathbf{k}) \rangle \times \mathbf{F}$$

Outline

The conventional wisdom

The conventional wisdom is wrong!

When the conventional wisdom is not so wrong

Beyond the conventional wisdom

Experiments and possible experiments

The moral(s) of the story







$$H = H_o - xF$$
$$H_o = \frac{p^2}{2m} + V(x)$$
$$V(x) = V(x+b)$$



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Bloch states

$$\langle \psi(t) | a | \psi(t) \rangle \equiv \frac{d^2}{dt^2} \langle \psi(t) | x | \psi(t) \rangle$$



$$= H_o - xF$$

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Bloch states

H

$$\langle \psi(t) | a | \psi(t) \rangle \equiv \frac{d^2}{dt^2} \langle \psi(t) | x | \psi(t) \rangle = \frac{1}{m} \frac{d}{dt} \langle \psi(t) | p | \psi(t) \rangle$$



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$$= \frac{d}{dt} \left\langle \psi(t) \, | \, p \, | \, \psi(t) \right\rangle = \frac{1}{i\hbar} \left\langle \psi(t) \, | \left[\, p, H \right] | \, \psi(t) \right\rangle$$



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$$\frac{d}{dt} \left\langle \psi(t) \left| p \right| \psi(t) \right\rangle = \frac{1}{i\hbar} \left\langle \psi(t) \left| \left[p, H \right] \right| \psi(t) \right\rangle = \frac{1}{i\hbar} \left\langle \psi(t) \left| \left[p, H_o \right] \right| \psi(t) \right\rangle + F$$









D. Pfirsch and E. Spenke, Z. Physik 137, 309 (1954)






apply F: initially.... $\frac{d\langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g + \mathbf{v}_a$ $\frac{d^2 \langle r^a \rangle}{dt^2} = \left(\frac{1}{\hbar} \frac{\partial^2 \omega(\mathbf{k})}{\partial k^a \partial k^b}\right) F^b$ k_y (2π/b) k_x (2π/b) $= \left[\frac{1}{m^*(\mathbf{k})}\right]^{ab} F^b$

 $\mathbf{v}_g = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$

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apply **F**: initially....



$$\frac{d\langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g + \mathbf{v}_a$$

$$\frac{d^2 \left\langle r^a \right\rangle}{dt^2} = \frac{F^a}{m}$$

$$\mathbf{v}_{g} = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$$

 $\mathbf{v}_a = \frac{1}{\hbar} \langle \mathbf{\Omega}(\mathbf{k}) \rangle \times \mathbf{F}$

apply **F**: initially....



 $\frac{d\langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g$

 $\frac{d^2 \left\langle r^a \right\rangle}{dt^2} = \frac{F^a}{m}$

 $\mathbf{v}_g = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$





period(s) inversely proportional
to energy difference(s)



decay time increases with smaller spread in k ...and with increasing m and b







The conventional wisdom The conventional wisdom is wrong! When the conventional wisdom is not so wrong Beyond the conventional wisdom Experiments and possible experiments The moral(s) of the story





describes a wave packet moving with the effective mass, as long as Zener tunneling can be neglected

$$\xi_{n'n}(\mathbf{k}) = \frac{\hbar}{im} \frac{\mathbf{p}_{n'n}(\mathbf{k})}{E_{n'n}(\mathbf{k})}$$

for $n' \neq n$

$$\overline{n\mathbf{k}} = |n\mathbf{k}\rangle + \sum_{n'\neq n} \frac{\xi_{n'n}(\mathbf{k}) \cdot \mathbf{F}}{E_{n'n}(\mathbf{k})} |n'\mathbf{k}\rangle + \cdots$$

$$\langle \mathbf{k} \rangle \rightarrow \langle \mathbf{k} \rangle + \frac{\mathbf{F}}{\hbar} t \qquad \qquad \frac{d \langle \mathbf{r} \rangle}{dt} = \mathbf{v}_g + \mathbf{v}_a$$
$$\frac{d^2 \langle r^a \rangle}{dt^2} = \left(\frac{1}{\hbar} \frac{\partial^2 \omega(\mathbf{k})}{\partial k^a \partial k^b}\right) F^b$$
$$= \left[\frac{1}{m^*(\mathbf{k})}\right]^{ab} F^b$$

$$\mathbf{v}_g = \left\langle \frac{\partial \boldsymbol{\omega}(\mathbf{k})}{\partial \mathbf{k}} \right\rangle$$

$$\mathbf{v}_a = \frac{1}{\hbar} \langle \mathbf{\Omega}(\mathbf{k}) \rangle \times \mathbf{F}$$

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$$|\Psi(t)\rangle = |\Psi_n(t)\rangle + \sum_{n'\neq n} |\Psi_{n'}(t)\rangle$$

$$|\Psi(0)\rangle = \int d\mathbf{k} c_n(\mathbf{k}) e^{-i\phi_n(\mathbf{k},0)} |n\mathbf{k}\rangle$$



$$\left| \boldsymbol{\psi}_{n}(t) \right\rangle = \int d\mathbf{k} \ c_{n}(\kappa) e^{-i\phi_{n}(\mathbf{k},t)} \left[n\mathbf{k} \right\rangle$$
$$= \int d\mathbf{k} \ c_{n}(\kappa) e^{-i\phi_{n}(\mathbf{k},t)} \left[\left| n\mathbf{k} \right\rangle + \sum_{n' \neq n} \frac{\xi_{n'n}(\mathbf{k}) \cdot \mathbf{F}}{E_{n'n}(\mathbf{k})} \left| n'\mathbf{k} \right\rangle + \cdots \right]$$

$$|\psi(t)\rangle = |\psi_n(t)\rangle + \sum_{n'\neq n} |\psi_{n'}(t)\rangle$$



$$\left\langle a(t) \right\rangle \approx \frac{F}{m} \int dk \left| c_n(\kappa) \right|^2 \left(\frac{m}{m_n^*(k)} + \frac{2}{m} \sum_{n' \neq n} \frac{E_{n'n}(k)}{E_{n'n}^2(\kappa)} \operatorname{Re}\left[p_{nn'}(k) p_{n'n}(\kappa) e^{i\gamma_{nn'}(\kappa,t)} \right] \right)$$

$$\kappa = k - \frac{Ft}{\hbar}$$

$$\gamma_{nn'}(\kappa,t) = \frac{1}{\hbar} \int_0^t E_{nn'}(\kappa + \frac{1}{\hbar} Ft') dt'$$

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The moral(s) of the story

Mathieu potential:

$$V(x) = sE_R \sin^2\left(\frac{\pi x}{b}\right)$$
$$E_R = \frac{\hbar^2 \pi^2}{2mb^2}$$

Gaussian wavepacket initially in centre of lowest band:



F. Duque Gomez and J.E. Sipe, Phys. Rev. A85, 053412 (2012)



$$s = 8$$
 $\sigma = 0.3 \frac{\pi}{b}$ $\tilde{F} \equiv \frac{bF}{\pi E_R} = 0.143$



Gaussian wavepacket initially in centre of lowest band:



simple effective mass prediction
 approximate analytic expression
 full numerical solution



$$s = 8$$
 $\sigma = 0.3 \frac{\pi}{b}$ $\tilde{F} \equiv \frac{bF}{\pi E_R} = 0.143$



...still <1% Zener tunneling into other bands

Experiments

Rockson Chang et al., Phys. Rev. Lett. 112, 170404 (2014)



S = 9.4, F/m = 11.7 μ m/ms²



Experiments in 2D systems?

Y. Fang, Federico Duque-Gomez, and J.E. Sipe, Phys. Rev. A90, 053407 (2014)



Load a wave packet in a band and apply a force

Experiments in 2D systems?

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Load a wave packet in a band and apply a force Simple effective mass picture

$$v_R = h / mb$$
 $\tau_B = h / bF$



Simple effective mass + anomalous velocity picture





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see the "emergence" of mass,



see the "emergence" of mass,

and other "single particle" quasi-particle properties



 $|\psi(0)\rangle = \int dk \ c(k) |nk\rangle$ Bloch states



$$\kappa = \mathbf{k} - \frac{\mathbf{F}t}{\hbar}$$

$$|\Psi(0)\rangle = \int dk \ c(k)|nk\rangle$$

Bloch states

$$\left[\frac{1}{m^*(t)}\right] = \int_{BZ} d\mathbf{k} \left|c(\kappa)\right|^2 \left(\left[\frac{1}{m^{(n)}(\mathbf{k},t)}\right] - K_{sym}^{(n)}(\mathbf{k},t)\right)$$



$$\begin{bmatrix} \frac{1}{m^{*}(t)} \end{bmatrix} = \int_{BZ} d\mathbf{k} |c(\kappa)|^{2} \left(\begin{bmatrix} \frac{1}{m^{(n)}(\mathbf{k},t)} \end{bmatrix} - K_{sym}^{(n)}(\mathbf{k},t) \right)$$
$$\Omega(t) = \int_{BZ} d\mathbf{k} |c(\kappa)|^{2} \left(\Omega^{(n)}(\mathbf{k}) - \Lambda^{(n)}(\mathbf{k},t) \right)$$



$$\begin{bmatrix} \frac{1}{m^{*}(t)} \end{bmatrix} = \int_{BZ} d\mathbf{k} |c(\kappa)|^{2} \left(\begin{bmatrix} \frac{1}{m^{(n)}(\mathbf{k},t)} \end{bmatrix} - K_{sym}^{(n)}(\mathbf{k},t) \right)$$
$$\Omega(t) = \int_{BZ} d\mathbf{k} |c(\kappa)|^{2} \left(\Omega^{(n)}(\mathbf{k}) - \Lambda^{(n)}(\mathbf{k},t) \right)$$
$$\mathbf{a}_{anomalous}(t) = \int_{BZ} d\mathbf{k} |c(\kappa)|^{2} \left(-K_{antisym}^{(n)}(\mathbf{k},t) \right)$$


period(s) inversely proportional
to energy difference(s)



Attosecond control of pulses should allow the study of the emergence of "single-particle" quasi-particle properties

What about materials like graphene?

How affected by electron-electron, electron-phonon interactions?





