Adiabatic approximation and various Berry curvatures in spin-orbit coupled systems

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Motivation

Quantum simulation

- Classical computer simulation of quantum system takes exponential time
- Hypothetical quantum computer does not
- Universal quantum computer still far away
- Dedicated quantum simulator possible
- Good candidate: Cold atoms

- Quantum simulation with ultracold atoms:
- Hubbard model (superfluid-Mott insulator transition)
- synthetic gauge fields (relativistic dispersion)
- strongly-correlated states (quantum Hall, spin liquids)

Trapped atoms – electrically neutral species

- No direct analogy with magnetic phenomena by electrons in solids, such as the Quantum Hall Effect, no Lorentz force
- A method to create an artificial magnetic field or artificial magnetic flux is required

Quantum simulation

- For quantum simulation a realization of the dynamics governed by the specified Hamiltonian is needed
- Adiabatic approximation — a way to construct an effective Hamiltonian

Adiabatic approximation in simple systems

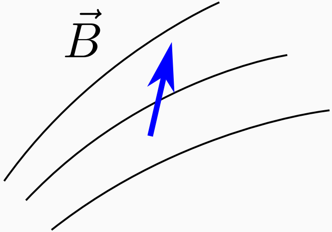
Hamiltonian

$$H(t) = \vec{B}(\boldsymbol{r}(t)) \cdot \vec{\sigma}$$

$\boldsymbol{r}$ is a parameter, motion $\boldsymbol{r}(t)$ is classical.

Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \Psi = H(t) \Psi$$



Adiabatic approximation

Eigenstates of $\vec{B} \cdot \vec{\sigma}$ are $\chi_\pm$ with eigenvalues $\pm|\vec{B}|$.

Adiabatic approximation: $\Psi = \psi \chi_\pm(\boldsymbol{r}(t))$

Resulting dynamics

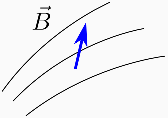
$$\mathrm{i}\hbar \frac{\partial}{\partial t} \psi = H_{\mathrm{eff}} \psi$$

The effective Hamiltonian

$$H_{\mathrm{eff}} = \pm|\vec{B}| - \mathcal{A}^{(t)}$$

with

$$\mathcal{A}^{(t)} = \mathrm{i}\hbar \chi_\pm^\dagger \frac{\partial}{\partial t} \chi_\pm$$



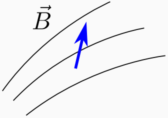
We can write

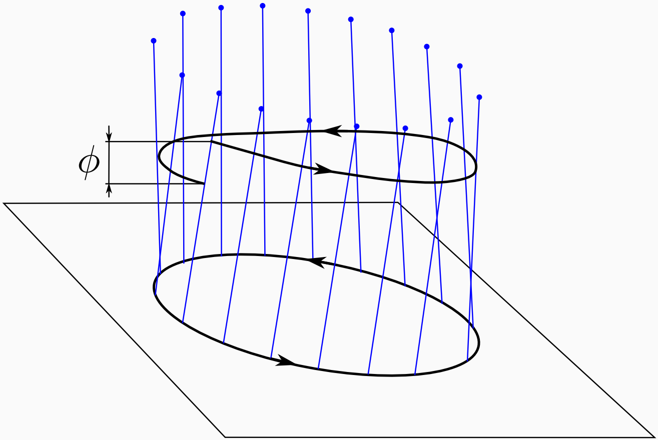
$$\mathcal{A}^{(t)} = \boldsymbol{\mathcal{A}}^{(r)} \cdot \dot{\boldsymbol{r}}, \qquad \boldsymbol{\mathcal{A}}^{(r)} = \mathrm{i}\hbar\chi_{\pm}^{\dagger}\boldsymbol{\nabla}^{(r)}\chi_{\pm}$$

If $\boldsymbol{r}(t)$ makes a closed loop, then $\mathcal{A}^{(t)}$ contributes to a phase (Berry's phase)

$$\phi = \int_0^t \boldsymbol{\mathcal{A}}^{(r)} \cdot \dot{\boldsymbol{r}}\,\mathrm{d}t = \oint \boldsymbol{\mathcal{A}}^{(r)} \cdot \mathrm{d}\boldsymbol{r}$$

Phase is nonzero if $\boldsymbol{\nabla}^{(r)} \times \boldsymbol{\mathcal{A}}^{(r)} \neq 0$

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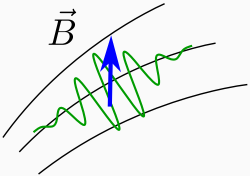
Hamiltonian

$$H = \frac{\hbar^2}{2m}\boldsymbol{k}^2 + \vec{B}(\boldsymbol{r}) \cdot \vec{\sigma}$$

Here $\boldsymbol{k} = -\mathrm{i}\boldsymbol{\nabla}$

Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi = H\Psi$$



$\vec{B}(\boldsymbol{r}) \cdot \vec{\sigma}$ has eigenvectors $\chi_{\pm}(\boldsymbol{r})$

Adiabatic approximation: $\Psi(\boldsymbol{r}) = \psi(\boldsymbol{r})\chi_{\pm}(\boldsymbol{r})$

The effective Hamiltonian

$$H_{\text{eff}} = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{\mathcal{A}}^{(r)})^2 \pm |\vec{B}| + \mathcal{V}^{(r)}$$

where

$$\boldsymbol{\mathcal{A}}^{(r)} = \mathrm{i}\chi_{\pm}^{\dagger}\boldsymbol{\nabla}^{(r)}\chi_{\pm}$$

is the Mead-Berry connection and

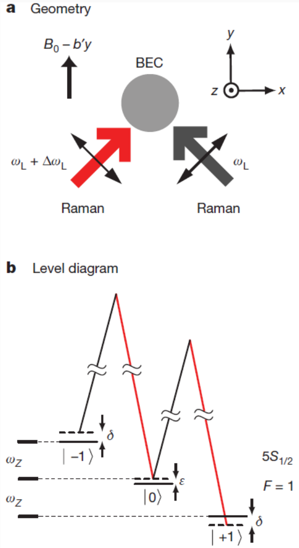
$$\mathcal{V}^{(r)} = -\frac{\hbar^2}{2m}\chi_{\pm}^{\dagger}\boldsymbol{\nabla}^{(r)}\chi_{\mp} \cdot \chi_{\mp}^{\dagger}\boldsymbol{\nabla}^{(r)}\chi_{\pm}$$

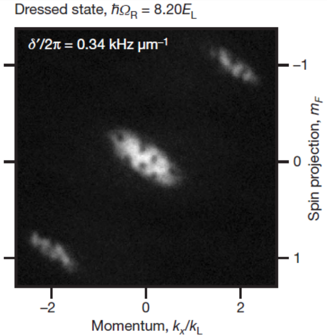
is the Born-Huang potential.

- The vector potential $\boldsymbol{\mathcal{A}}^{(r)}$ appears because the eigenvectors depend on the position
- $\boldsymbol{\mathcal{A}}^{(r)}$ has geometric nature
- The Berry connection $\boldsymbol{\mathcal{A}}^{(r)}$ is related to a curvature $\Theta^{(r,r)}$ as

$$\Theta_{jl}^{(r,r)} = \nabla_j^{(r)} \mathcal{A}_l^{(r)} - \nabla_l^{(r)} \mathcal{A}_j^{(r)}$$

Experimental realization





Y.-J. Lin, R. L. Compton, K. Jiménez-García, J. V. Porto and I. B. Spielman, Nature, **462**, 628 (2009).

General equations for adiabatic approximation

Hamiltonian with position-dependent spin-orbit coupling

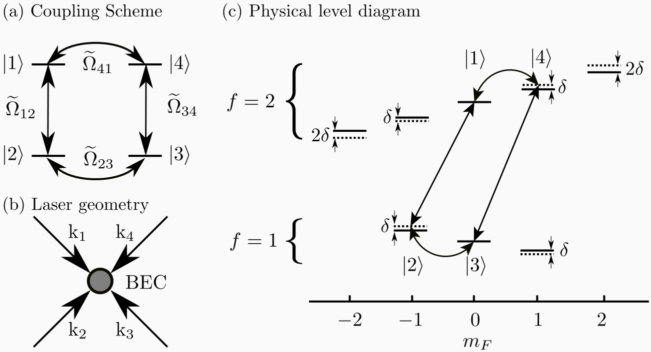
$$H = \frac{\hbar^2}{2m}(\boldsymbol{k} - \boldsymbol{A}(\boldsymbol{r}))^2 + V(\boldsymbol{r})$$

where $\boldsymbol{A}$ and V are 2×2 matrices:

$$\begin{aligned} V(\boldsymbol{r}) &= \vec{v}(\boldsymbol{r}) \cdot \vec{\sigma} + v_0(\boldsymbol{r}) I \\ A_j(\boldsymbol{r}) &= \vec{a}_j(\boldsymbol{r}) \cdot \vec{\sigma} \end{aligned}$$

Postion-dependent spin-orbit coupling for ultracold atoms

S.-W. Su, S.-C. Gou, I.-K. Liu, I. B. Spielman, L. Santos, A. Acus, A. Mekys, J. Ruseckas, and G. Juzeliūnas, New. J. Phys. **17**, 033045 (2015).



We can write

$$H = \frac{\hbar^2}{2m}\boldsymbol{k}^2 + \vec{B}\cdot\vec{\sigma} + W(\boldsymbol{r})I$$

where

$$B^j = -\frac{\hbar^2}{2m}\sum_l \{k_l, a_l^j\} + v^j$$

and

$$W = \frac{\hbar^2}{2m}\sum_{j,l}[a_l^j]^2 + v_0$$

Let us define a unitary operator U, which diagonalizes the term $\vec{B} \cdot \vec{\sigma}$.

The wavefunction in the diagonal basis

$$\tilde{\Psi} = U^{\dagger}\Psi$$

The Schrödinger equation in the new basis

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\tilde{\Psi} = \tilde{H}\tilde{\Psi}$$

where

$$\tilde{H} = U^{\dagger} H U = \frac{\hbar^2}{2m}\tilde{\boldsymbol{k}}^2 + \tilde{\vec{B}} \cdot \tilde{\vec{\sigma}} + W(\tilde{\boldsymbol{r}}) I$$

and

$$\tilde{\boldsymbol{r}} = U^{\dagger}\boldsymbol{r}U\,, \qquad \tilde{\boldsymbol{k}} = U^{\dagger}\boldsymbol{k}U\,, \qquad \tilde{\vec{\sigma}} = U^{\dagger}\vec{\sigma}\,U$$

Adiabatic approximation: $\tilde{\Psi} = \psi \mathcal{P}_\pm$, where

$$\mathcal{P}_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \mathcal{P}_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The effective Hamiltonian

$$H_{\text{eff}} = \mathcal{P}_\pm^\dagger \tilde{H} \mathcal{P}_\pm$$

In the effective Hamiltonian the following operators appear:

$$\begin{aligned} \boldsymbol{r}_\text{c} &= \mathcal{P}_\pm^\dagger \tilde{\boldsymbol{r}} \mathcal{P}_\pm = \mathcal{P}_\pm^\dagger U^\dagger \boldsymbol{r} U \mathcal{P}_\pm \\ \boldsymbol{k}_\text{c} &= \mathcal{P}_\pm^\dagger \tilde{\boldsymbol{k}} \mathcal{P}_\pm = \mathcal{P}_\pm^\dagger U^\dagger \boldsymbol{k} U \mathcal{P}_\pm \end{aligned}$$

Covariant operators

Covariant operators

- $\boldsymbol{r}_\mathrm{c}$ describes the motion of the center of a wavepacket
- $\boldsymbol{k}_\mathrm{c}$ corresponds the average operator $\boldsymbol{k}$ of a wavepacket
- $\boldsymbol{k}_\mathrm{c}$ does not correspond to the kinetic momentum, because in a system with SOC the kinetic momentum operator is $\hbar(\boldsymbol{k} - \boldsymbol{A})$

Covariant operators can be written as

$$\boldsymbol{r}_{\mathrm{c}} = \boldsymbol{r} - \boldsymbol{\mathcal{A}}^{(k)}$$
$$\boldsymbol{k}_{\mathrm{c}} = \boldsymbol{k} - \boldsymbol{\mathcal{A}}^{(r)}$$

where

$$\boldsymbol{\mathcal{A}}^{(k)} = -\mathcal{P}_{\pm}^{\dagger} U^{\dagger} [\boldsymbol{r}, U] \mathcal{P}_{\pm}$$
$$\boldsymbol{\mathcal{A}}^{(r)} = -\mathcal{P}_{\pm}^{\dagger} U^{\dagger} [\boldsymbol{k}, U] \mathcal{P}_{\pm}$$

Operators $\boldsymbol{\mathcal{A}}^{(k)}$ and $\boldsymbol{\mathcal{A}}^{(r)}$ correspond to Berry connetions

The effective Hamiltonian can be written as

$$H_{\text{eff}} = \frac{\hbar^2}{2m}\boldsymbol{k}_{\text{c}}^2 + W(\boldsymbol{r}_{\text{c}}) + \mathcal{V}$$

where

$$\mathcal{V} = \mathcal{P}_{\pm}^{\dagger}\vec{\tilde{B}}\cdot\vec{\tilde{\sigma}}\mathcal{P}_{\pm} + \mathcal{V}^{(r)} + \mathcal{V}^{(k)}$$

with

$$\mathcal{V}^{(r)} = \frac{\hbar^2}{2m}\mathcal{P}_{\pm}U^{\dagger}[\boldsymbol{k}, U]\mathcal{P}_{\mp}\cdot\mathcal{P}_{\mp}U^{\dagger}[\boldsymbol{k}, U]\mathcal{P}_{\pm}$$

$$\mathcal{V}^{(k)} = \sum_{j,l} w_{jl}^{(2)}\mathcal{P}_{\pm}U^{\dagger}[r_j, U]\mathcal{P}_{\mp}\mathcal{P}_{\mp}U^{\dagger}[r_l, U]\mathcal{P}_{\pm}$$

Here we assumed, that the potential $W(\boldsymbol{r})$ is at most quadratic:

$$W(\boldsymbol{r}) = w^{(0)} + \sum_{j} w_j^{(1)} r_j + \sum_{j,l} w_{jl}^{(2)} r_j r_l$$

Commutators:

$$
\begin{aligned}
[(r_c)_j, (r_c)_l] =& \mathrm{i}\Theta_{jl}^{(k,k)} \\
[(k_c)_j, (k_c)_l] =& \mathrm{i}\Theta_{jl}^{(r,r)} \\
[(r_c)_j, (k_c)_l] =& \mathrm{i}\delta_{j,l} + \mathrm{i}\Theta_{jl}^{(k,r)}
\end{aligned}
$$

where various Berry curvatures are given by

$$
\begin{aligned}
\Theta_{jl}^{(k,k)} =& \mathrm{i}[r_j, \mathcal{A}_l^{(k)}] - \mathrm{i}[r_l, \mathcal{A}_j^{(k)}] \\
\Theta_{jl}^{(r,r)} =& \mathrm{i}[k_j, \mathcal{A}_l^{(r)}] - \mathrm{i}[k_l, \mathcal{A}_j^{(r)}] \\
\Theta_{jl}^{(k,r)} =& \mathrm{i}[r_j, \mathcal{A}_l^{(r)}] - \mathrm{i}[k_l, \mathcal{A}_j^{(k)}] \\
\Theta_{jl}^{(r,k)} =& \mathrm{i}[k_j, \mathcal{A}_l^{(k)}] - \mathrm{i}[r_l, \mathcal{A}_j^{(r)}]
\end{aligned}
$$

Heisenberg equations for the covariant operators

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_\mathrm{c} = \frac{1}{\mathrm{i}\hbar}[\boldsymbol{k}_\mathrm{c}, H_\mathrm{eff}]$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}_\mathrm{c} = \frac{1}{\mathrm{i}\hbar}[\boldsymbol{r}_\mathrm{c}, H_\mathrm{eff}]$$

contain Berry curvature terms:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_\mathrm{c} =& -\frac{1}{\hbar}\boldsymbol{\nabla} W(\boldsymbol{r}_\mathrm{c}) + \frac{1}{\mathrm{i}\hbar}[\boldsymbol{k}_\mathrm{c}, \mathcal{V}] \\ &+ \frac{\hbar}{2m}\sum_{j,l} \boldsymbol{e}_j \left\{\Theta_{jl}^{(r,r)}, (k_\mathrm{c})_l\right\} + \frac{1}{2\hbar}\sum_{j,l} \boldsymbol{e}_j \left\{\Theta_{jl}^{(r,k)}, \nabla_l W(\boldsymbol{r}_\mathrm{c})\right\}\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}_\mathrm{c} =& \frac{\hbar}{m}\boldsymbol{k}_\mathrm{c} + \frac{1}{\mathrm{i}\hbar}[\boldsymbol{r}_\mathrm{c}, \mathcal{V}] \\ &+ \frac{\hbar}{2m}\sum_{j,l} \boldsymbol{e}_j \left\{\Theta_{jl}^{(k,r)}, (k_\mathrm{c})_l\right\} + \frac{1}{2\hbar}\sum_{j,l} \boldsymbol{e}_j \left\{\Theta_{jl}^{(k,k)}, \nabla_l W(\boldsymbol{r}_\mathrm{c})\right\}\end{aligned}$$

We neglect the commutator between position and momentum:

$$B^j = -\frac{\hbar^2}{m}\sum_l a_l^j(\boldsymbol{r})k_l + v^j(\boldsymbol{r})$$

Eigenvectors $\chi_\pm(\boldsymbol{r},\boldsymbol{k})$ of the matrix $\vec{B}\cdot\vec{\sigma}$ prametrically depend on the numbers $\boldsymbol{r}$ and $\boldsymbol{k}$.

Berry connections:

$$\boldsymbol{\mathcal{A}}^{(k)} = \mathrm{i}\chi_\pm^\dagger \boldsymbol{\nabla}^{(r)}\chi_\pm\,, \qquad \boldsymbol{\mathcal{A}}^{(r)} = -\mathrm{i}\chi_\pm^\dagger \boldsymbol{\nabla}^{(k)}\chi_\pm$$

Berry curvatures:

$$\begin{aligned}
\Theta_{jl}^{(k,k)} &= -\,\nabla_j^{(k)}\mathcal{A}_l^{(k)} + \nabla_l^{(k)}\mathcal{A}_j^{(k)} \\
\Theta_{jl}^{(r,r)} &= \nabla_j^{(r)}\mathcal{A}_l^{(r)} - \nabla_l^{(r)}\mathcal{A}_j^{(r)} \\
\Theta_{jl}^{(k,r)} &= -\,\nabla_j^{(k)}\mathcal{A}_l^{(r)} - \nabla_l^{(r)}\mathcal{A}_j^{(k)} \\
\Theta_{jl}^{(r,k)} &= \nabla_j^{(r)}\mathcal{A}_l^{(k)} + \nabla_l^{(k)}\mathcal{A}_j^{(r)}
\end{aligned}$$

Scalar potentials:

$$\begin{aligned}
\mathcal{V}^{(r)} &= -\,\frac{\hbar^2}{2m}\chi_\pm^\dagger \boldsymbol{\nabla}^{(r)}\chi_\mp \cdot \chi_\mp^\dagger \boldsymbol{\nabla}^{(r)}\chi_\pm \\
\mathcal{V}^{(k)} &= -\sum_{j,l} w_{jl}^{(2)}\chi_\pm^\dagger \nabla_j^{(k)}\chi_\mp\, \chi_\mp^\dagger \nabla_l^{(k)}\chi_\pm
\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_\mathrm{c} =& -\frac{1}{\hbar}\boldsymbol{\nabla}\, W(\boldsymbol{r}_\mathrm{c}) - \frac{1}{\hbar}\boldsymbol{\nabla}^{(r)}\mathcal{V} \\ &+ \frac{\hbar}{m}\sum_{j,l} \boldsymbol{e}_j \Theta_{jl}^{(r,r)} (k_\mathrm{c})_l + \frac{1}{\hbar}\sum_{j,l} \boldsymbol{e}_j \Theta_{jl}^{(r,k)} \nabla_l W(\boldsymbol{r}_\mathrm{c}) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}_\mathrm{c} =& \frac{\hbar}{m}\boldsymbol{k}_\mathrm{c} + \frac{1}{\hbar}\boldsymbol{\nabla}^{(k)}\mathcal{V} \\ &+ \frac{\hbar}{m}\sum_{j,l} \boldsymbol{e}_j \Theta_{jl}^{(k,r)} (k_\mathrm{c})_l + \frac{1}{\hbar}\sum_{j,l} \boldsymbol{e}_j \Theta_{jl}^{(k,k)} \nabla_l W(\boldsymbol{r}_\mathrm{c})\end{aligned}$$

In semiclassical approximation the terms containing the Berry curvatures Θ and scalar potentials $\mathcal{V}$ are small compared to the first term. In the zeroth-order approximation $\mathrm{d}\boldsymbol{k}_\mathrm{c}/\mathrm{d}t \approx \boldsymbol{\nabla} W(\boldsymbol{r}_\mathrm{c})/\hbar$ and $\mathrm{d}\boldsymbol{r}_\mathrm{c}/\mathrm{d}t \approx \hbar\boldsymbol{k}_\mathrm{c}/m$.

In the first-order approxmation

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_\mathrm{c} =& -\frac{1}{\hbar}\boldsymbol{\nabla} W(\boldsymbol{r}_\mathrm{c}) - \frac{1}{\hbar}\boldsymbol{\nabla}^{(r)}\mathcal{V} \\
&+ \sum_{j,l} \boldsymbol{e}_j \left(\Theta_{jl}^{(r,r)} \frac{\mathrm{d}}{\mathrm{d}t}(r_\mathrm{c})_l + \Theta_{jl}^{(r,k)} \frac{\mathrm{d}}{\mathrm{d}t}(k_\mathrm{c})_l \right) \\
\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}_\mathrm{c} =& \frac{\hbar}{m}\boldsymbol{k}_\mathrm{c} + \frac{1}{\hbar}\boldsymbol{\nabla}^{(k)}\mathcal{V} \\
&- \sum_{j,l} \boldsymbol{e}_j \left(\Theta_{jl}^{(k,r)} \frac{\mathrm{d}}{\mathrm{d}t}(r_\mathrm{c})_l + \Theta_{jl}^{(k,k)} \frac{\mathrm{d}}{\mathrm{d}t}(k_\mathrm{c})_l \right)
\end{aligned}$$

Spin-orbit coupling in one dimension

One-dimensional spiral

Let us consider the system with the Hamiltonian

$$H = H_0 - Fx$$

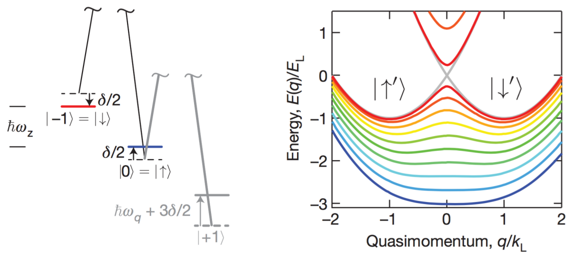
where

$$H_0 = \frac{\hbar^2}{2m}(k - a\sigma_3)^2 + \frac{\hbar\Omega}{2}[\cos(x/\lambda)\sigma_1 + \sin(x/\lambda)\sigma_2]$$

Experimental realization

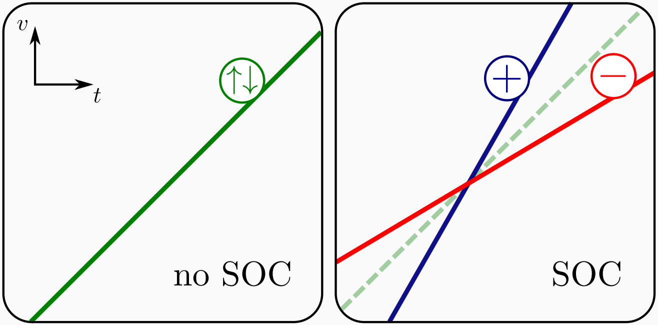
Hamiltonian H_0 has been realized experimentally

Y.-J. Lin, K. Jiménez-García and I. B. Spielman, Nature **471**, 83–86 (2011).



$$H = \frac{1}{2m}(p - \chi\sigma_y)^2 + \frac{\Omega}{2}\sigma_z$$

Response to a force: effective mass



Exact solution

Dispersion

$$E_{k,\pm} = \frac{\hbar^2}{m}\left(\frac{k^2}{2} + \frac{k_0^2}{2} \pm \sqrt{(k_0 k)^2 + (\kappa a)^2}\right)$$

where

$$k_0 = a + \frac{1}{2\lambda}\,, \qquad \kappa = \frac{\Omega}{2a}\frac{m}{\hbar}$$

Effective mass

$$\frac{m}{m^*_\pm} = 1 \pm \frac{k_0^2}{\kappa a} \approx 1 \pm \frac{1}{\kappa}\left(a + \frac{1}{\lambda}\right)$$

Semiclassical dynamics follows the equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_{\mathrm{c}} = \frac{F}{\hbar}(1 - \Theta^{(r,k)})$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}_{\mathrm{c}} = \frac{\hbar}{m}\boldsymbol{k}_{\mathrm{c}}(1 + \Theta^{(k,r)}) + \frac{1}{\hbar}\nabla^{(k)}\mathcal{V}$$

In the limit $1/\lambda a \ll 1$ and $|k| \ll \kappa$ the equations become

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{k}_{\mathrm{c}} = \frac{F}{\hbar}\left(1 \pm \frac{1}{2\lambda\kappa}\right)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}_{\mathrm{c}} = \frac{\hbar}{m}\boldsymbol{k}_{\mathrm{c}}\left(1 \pm \frac{1}{2\lambda\kappa} \pm \frac{a}{\kappa}\right)$$

Closed equation for the center of mass motion

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{x}_{\mathrm{c}} = \frac{F}{m}\left(1 \pm \frac{1}{\kappa}\left(a + \frac{1}{\lambda}\right)\right)$$

Summary

Summary

- In general, adiabatic approximation results in position-space, momentum-space and phase-space Berry curvatures.
- The the phase-space Berry curvature is directly related to the effective mass.
- The measurement of the effective mass is a direct probe of the phase-space Berry curvature in the system.
- J. Armaitis, J. Ruseckas, E. Anisimovas, *Phase space curvature in spin-orbit coupled ultracold atom systems*, arXiv:1702.03298 [cond-mat.quant-gas] (2017).

Thank you for your attention!