Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field

Rajath Shashidhara
2012B5A7589P
rajath.shashidhara@gmail.com

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Dr. Tapomoy Guha Sarkar

Department of Physics
Birla Institute of Technology and Science, Pilani
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Abstract

Study of quantum hall effect in 2D square lattice driven by oscillatory magnetic field perpendicular to the plane. The time-dependent hamiltonian is solved in fourier space using Brillouin-Wigner perturbation theory, in the high frequency limit. Investigation of localization/delocalization transitions of time-averaged wavefunctions and calculation of hall conductivity of the system using TKNN invariant. Comparison of the results with the effective static hamiltonian picture carried out in the previous work.

Acknowledgements

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Declaration

I, Rajath Shashidhara, declare that this thesis titled, 'Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field' and the work presented in it is my original work. I affirm that all references are clearly attributed and any collaboration with others has been duly acknowledged.

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Certificate

This is to certify that the thesis titled, 'Hall conductivity of Aubry-André system driven by rapidly oscillating magnetic field' and submitted by Rajath Shashidhara 2012B5A7589P in partial fulfillment of the requirements of BITS F421T embodies the work done by him under my supervision.

Supervisor

Dr. Tapomoy Guha Sarkar
Department of Physics
Birla Institute of Technology and Science, Pilani

Date: November 17, 2016

Contents

Chapter 1

Introduction

Part I

Background

Chapter 2

Geometric Phase

Physical measurements or observations are extracted from quantum mechanical systems in the form of expectation values of hermitian operators $\langle\psi|\hat{A}|\psi\rangle$. Eigenvectors of the hamiltonian are only specified up to a phase factor. Expectation values and thereby, the physical observations are unaltered by a transformation of the form $\psi \rightarrow e^{i\phi}\psi$. This guage choice can be eliminated by formulating quantum mechanics in terms of guage invariant representations such as density matrices $\psi\psi^{\dagger}$. Expectation value of an operator $\hat{A}$ is recast as $\langle\hat{A}\rangle = tr(\psi\psi^{\dagger}\hat{A})$.

2.1 Definition

Prof. M V Berry studied the adiabatic evolution of a quantum system described by the hamiltonian $\hat{H}(\mathbf{R})$, parameterized by external factors $\mathbf{R}$ – such as magnetic field, electric field, etc [1]. The hamiltonian is varied by slowly changing $\mathbf{R}$ from time $t = 0$ to $t = T$ such that $\mathbf{R}(0) = \mathbf{R}(T)$. This evolution is a closed loop in the parameter space. Apart from the adiabatic assumption, we also assume that the energy spectrum is discrete and there are no level crossings or degeneracies in the energy spectrum. Using the guage freedom, we enforce single-valuedness on the eigenvectors of the hamiltonian in the parameter space. Under the assumptions stated above, eigenvectors of the hamiltonian can be uniquely identified as $|n(\mathbf{R})\rangle$ at each point in parameter space without any ambiguity. The schrodinger equation is stated in this notation as

$$\hat{H}(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle = E(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle \tag{2.1}$$

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle \tag{2.2}$$

In the case of static time-independent hamiltonian, any state expanded as a linear combination of stationary states is written as $|\psi(t)\rangle = \sum c_n e^{-\frac{iE_n(t)}{\hbar}}\,|n\rangle$. Taking cue from this, the expansion ansatz

$$|\psi(t)\rangle = \sum c_n(t) e^{-\frac{i}{\hbar}\int_0^t E_n(t)dt}\,|n(t)\rangle \tag{2.3}$$

is a valid generalization for a system with a time-dependent hamiltonian. When the ansatz is substituted into Eq. (2.2), we obtain

$$\dot{c}_m(t) = -c_m(t)\left\langle m(t)\,\middle|\,\frac{\partial}{\partial t}m(t)\right\rangle - \sum_n c_n(t)e^{i(\theta_n-\theta_m)}\frac{\langle m(t)|\dot{\hat{H}}|n(t)\rangle}{E_n - E_m} \tag{2.4}$$

where $\theta_n = \frac{-1}{\hbar}\int_0^t E_n(t')\,dt'$. In the adiabatic limit, the transition probability between states tends to zero. We ignore the second term in the general solution above to obtain the result

$$c_n(t) = e^{i\gamma_n(t)}\, c_n(0) \tag{2.5}$$

If we started in an eigenstate of the hamiltonian $|\psi(0)\rangle = |n(\mathbf{R}(0)\rangle$, then the state evolves as

$$|\psi(t)\rangle = e^{i\gamma_n(t)} e^{i\theta_n(\mathrm{R}(t))}\, |n(\mathbf{R}(t))\rangle \tag{2.6}$$

remaining in the nth eigenstate all along, only picking up phase factors. In the case of cyclic evolution, we write

$$|\psi(T)\rangle = e^{i\gamma_n(C)} e^{i\theta_n(T)}\, |\psi(0)\rangle \tag{2.7}$$

From Eq. (2.4), we note that

$$\gamma_n(C) = i\int_0^T \langle n(t)|\frac{\partial}{\partial t} n(t)\rangle\; dt = i\oint_c \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot d\mathbf{R} \tag{2.8}$$

$\gamma_n(C)$ is a real number and therefore $e^{i\gamma_n(C)}$ is a pure phase term. This simple fact can be demonstrated by taking the time-derivative of $\langle n(t)|n(t)\rangle = 1$.

$$\begin{gathered}
\langle n(t)|n(t)\rangle = 1 \\
\left[\frac{\partial}{\partial t}\langle n(t)|\right]|n(t)\rangle + \langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right] = 0 \\
\langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right] = -\left(\langle n(t)|\left[\frac{\partial}{\partial t}|n(t)\rangle\right]\right)^*
\end{gathered}$$

$\theta_n(T)$ is the familiar dynamical phase and $\gamma_n(C)$ is known as geometric phase or simply berry phase. While the dynamical phase is a time-dependent quantity, the geometric phase is a line integral, that only depends on path traversed in the parameter space. Another important observation is the fact that γ_n is a non-integrable quantity as it is not single valued - $\gamma_n(0) \neq \gamma_n(T)$ in the parameter space. Therefore, the geometric phase cannot be expressed as a field over the parameter space. By application of stokes theorem, the line integral can be convereted into a surface integral as shown below

$$\begin{aligned}
\gamma_n(C) &= i\oint_C \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot d\mathbf{R} \\
&= i\int_S \boldsymbol{\nabla}_{\boldsymbol{R}}\wedge\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot d\mathbf{S} \qquad (2.9)\\
&= i\int_S (\boldsymbol{\nabla}_{\boldsymbol{R}}\langle n(\mathbf{R})|)\wedge\boldsymbol{\nabla}_{\boldsymbol{R}}|n(\mathbf{R})\rangle\cdot d\mathbf{S} \\
&= i\int_S \sum_{m\neq n}\frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}(\mathbf{R})|m(\mathbf{R})\rangle\wedge\langle m(\mathbf{R})|\boldsymbol{\nabla}_{\boldsymbol{R}}\hat{H}(\mathbf{R})|n(\mathbf{R})\rangle}{(E_n(\mathbf{R})-E_m(\mathbf{R}))^2}\cdot d\mathbf{S} \qquad (2.10)
\end{aligned}$$

Eq. (2.10) has a remarkable property of being gauge independent. Any transformation of the form $|n(\mathbf{R})\rangle \to e^{i\delta(\mathrm{R})}|n(\mathbf{R})\rangle$, leaves Eq. (2.10) unchanged.

2.1.1 Anology to electromagnetism

Before we proceed, it is useful to define two important quantities called the berry connection and the berry curvature. *Berry connection* is defined as

$$\mathbf{A}_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \boldsymbol{\nabla}_{\boldsymbol{R}} | n(\mathbf{R}) \rangle \tag{2.11}$$

and the *Berry curvature* is given by

$$\mathbf{B}_n(\mathbf{R}) = i \, \boldsymbol{\nabla}_{\boldsymbol{R}} \wedge \langle n(\mathbf{R}) | \boldsymbol{\nabla}_{\boldsymbol{R}} | n(\mathbf{R}) \rangle = \boldsymbol{\nabla}_{\boldsymbol{R}} \wedge \mathbf{A}_n(\mathbf{R}) \tag{2.12}$$

Berry phase is conveniently expressed in terms of these quantities as

$$\gamma_n(C) = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot \, d\mathbf{R} = \int_S \mathbf{B}_n(\mathbf{R}) \cdot \, d\mathbf{S} \tag{2.13}$$

If we transform the states as $|n(\mathbf{R})\rangle \rightarrow e^{i\delta(\mathrm{R})} |n(\mathbf{R})\rangle$, then the berry connection transforms as $\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) - \boldsymbol{\nabla}_{\boldsymbol{R}} \delta(\mathbf{R})$, but the berry curvature remains unchanged. This shows an uncanny resemblence between magnetic vector potential and the berry connection and consequently the magnetic field strength and the berry curvature. However, it must be kept in mind that the berry connection and the berry curvature are defined over the parameter space (could be more than 4-dimensional) and not the real space.

Geometric phase was overlooked as physically irrelevant as the expectation values are independent of the phase of eigenfunctions. As opposed to the then prevalant notion, Prof. Berry, in his seminal paper, demonstrated that the geometric phase is in fact, physically observable [1, 2]. Several assumptions imposed by Prof. Berry in defining the geometric phase can be relaxed and definition of geometric phase has been generalized to nonadiabatic, noncyclic, nonunitary and nonabelian situations [3–6].

2.2 Bargmann invariants

Appendices

Appendix A

Brillouin-Wigner Perturbation Theory

When encountered with an analytically intractable quantum mechanical problem, perturbation techniques may be used to obtain approximate solutions. Formally, the problem can be stated as follows : Given a hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0$ is exactly solvable and $\hat{V}$ is the perturbation term, and the eigendecomposition of $\hat{H}_0$ —

$$\begin{aligned} \hat{H}_0 \left|n\right\rangle &= \epsilon_n \left|n\right\rangle \\ \left\langle m|n\right\rangle &= \delta_{mn} \\ \sum_m \left|m\right\rangle \left\langle m\right| &= 1 \end{aligned}$$

Brillouin-Wigner (BW) perturbation theory expresses $\{\left|\psi_n\right\rangle, \dots\}$ and $\{E_n, \dots\}$, such that $\hat{H}\left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$ in terms of $\hat{V}$ and $\{\left|n\right\rangle, \dots\}$. A simplistic exposition of BW theory is presented below.

To obtain the BW perturbative expansion, we begin with the eigenvalue equation.

$$\hat{H}\left|\psi_n\right\rangle = (\hat{H}_0 + \hat{V})\left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$$

The wavefunctions $\left|\psi_n\right\rangle$ are normalized as $\left\langle n|\psi_n\right\rangle = 1$, as discussed in [7]. On contracting with $\left\langle n\right|$,

$$\begin{aligned} \left\langle n|(\hat{H}_0 + \hat{V})|\psi_n\right\rangle &= E_n \left\langle n|\psi_n\right\rangle \\ \epsilon_n \left\langle n|\psi_n\right\rangle + \left\langle n|\hat{V}|\psi_n\right\rangle &= E_n \left\langle n|\psi_n\right\rangle \\ E_n &= \epsilon_n + \left\langle n|\hat{V}|\psi_n\right\rangle \end{aligned} \tag{A.1}$$

Rewriting the eigenvalue equation as

$$\begin{aligned} (E_n - \hat{H}_0)\left|\psi_n\right\rangle &= \hat{V}\left|\psi_n\right\rangle \\ &= 1\,\hat{V}\left|\psi_n\right\rangle \\ &= \sum_m \left|m\right\rangle \left\langle m\right|\hat{V}\left|\psi_n\right\rangle \\ &= \left|n\right\rangle \left\langle n|\hat{V}|\psi_n\right\rangle + (1 - \left|n\right\rangle \left\langle n\right|)\hat{V}\left|\psi_n\right\rangle \end{aligned}$$

Using Eq. A.1,

$$\begin{aligned} &= (E_n - \hat{H}_0)\left|n\right\rangle + (1 - \left|n\right\rangle \left\langle n\right|)\hat{V}\left|\psi_n\right\rangle \\ (E_n - \hat{H}_0)(\left|\psi_n\right\rangle - \left|n\right\rangle) &= (1 - \left|n\right\rangle \left\langle n\right|)\hat{V}\left|\psi_n\right\rangle \\ \left|\psi_n\right\rangle &= \left|n\right\rangle + (E_n - \hat{H}_0)^{-1}(1 - \left|n\right\rangle \left\langle n\right|)\hat{V}\left|\psi_n\right\rangle \end{aligned}$$

Define resolvent operator as $\hat{R}_n = (E_n - \hat{H}_0)^{-1} = \sum_n |n\rangle (E_n - \epsilon_n)^{-1} \langle n|$,

$$|\psi_n\rangle = |n\rangle + \hat{R}_n(1 - |n\rangle \langle n|)\hat{V} |\psi_n\rangle \tag{A.2}$$

The above iterative equation is the main result of BW perturbation theory. Solving Eq. (A.2) self-consistently with Eq. (A.1), solutions to the eigenvalue equation are obtained. No approximation has been used until this point, and exact solution can be obtained if iterated infinitely. In practice, approximate solution is obtained by truncating the iteration.

Further, Eq. (A.2) can be simplified by expanding the recurrence relation

$$\begin{aligned} |\psi_n\rangle &= |n\rangle + \hat{R}_n\hat{Q}_n\hat{V} |\psi_n\rangle \\ \text{where } \hat{Q}_n = 1 - |n\rangle \langle n|\,, & \\ &= |n\rangle + \hat{R}_n\hat{Q}_n\hat{V} |n\rangle + \hat{R}_n\hat{Q}_n\hat{V}\hat{R}_n\hat{Q}_n\hat{V} |n\rangle + \dots \\ &= \sum_{k=0}^{\infty} \{\hat{R}_n\hat{Q}_n\hat{V}\}^k |n\rangle \\ &= (1 - \{\hat{R}_n\hat{Q}_n\hat{V}\})^{-1} |n\rangle \end{aligned} \tag{A.3}$$

When higher order term contributions are diminishingly small, truncating the series produces approximate solutions to the problem.

Unlike Rayleigh-Schrodinger (RS) perturbation theory, BW theory does not rely on power series expansion requiring strict analyticity and does not require seperate treatment of degenerate case. RS theory is an approximation to BW theory obtained by power series expansion of $(E_n - \epsilon_m)^{-1}$ in the resolvent operator [8]. [9] provides an excellent comparison between RS and BW perturbation theories including situations where BW perturbation technique is more applicable.

Recent efforts to extend the theory to many-body systems has led to systematization of BW theory in terms of model space and effective hamiltonian formalism. This new representation requires the introduction of a model space with respect to a set of reference states. Any complete set of orthonormal states of hilbert space is chosen as a set of reference states. Usually, eigenstates of the unperturbed hamiltonian $\hat{H}_0$ is chosen as a set of reference states. The hilbert space is partitioned into model space and orthogonal space, by choosing one state from the set of reference states as model state [1].

Let R $\equiv \{|\phi_n\rangle \dots\}$ is the set of reference states, $|\phi_0\rangle \in$ R is the model state, then $P = |\phi_0\rangle \langle\phi_0|$ is the corresponding projection operator of the model space and $Q = 1 - P$ is the projection operator corresponding to orthogonal space. A state $|\psi\rangle$ in the hilbert space can be projected onto the model space using operator P, $|\phi\rangle = P |\psi\rangle$ and a wavefunction $|\phi\rangle$ in model space can be reconstructed in hilbert space using the wave operator Ω as $|\psi\rangle = \Omega |\phi\rangle$. Provided the eigenvalue equation $\hat{H} |\psi\rangle = E |\psi\rangle$, then $|\phi\rangle = P |\psi\rangle$ satisfies the equation $\hat{H}_{eff} |\phi\rangle = E |\phi\rangle$, where

$$\hat{H}_{eff} = P\hat{H}\Omega P \tag{A.4}$$

[1] In this treatment, a single reference state is chosen as the model function. See [8] for multi-reference partitioning.

$$\begin{aligned}\hat{H}_{eff}\,|\phi\rangle &= P\hat{H}\Omega P\,|\phi\rangle \\ &= P\hat{H}\Omega PP\,|\psi\rangle \\ &= P\hat{H}\,|\psi\rangle \\ &= E\,P\,|\psi\rangle \\ &= E\,|\phi\rangle\end{aligned}$$

Therefore, the eigenvalues of the effective hamiltonian are equal to the eigenvalues of the original hamiltonian and the eigenfunctions of the original hamiltonian can be obtained by application of the wave operator Ω on the eigenfunctions of the effective hamiltonian $|\psi\rangle = \Omega\,|\phi\rangle$.

How do we obtain the wave operator Ω ? Operating Q on the eigenvalue equation,

$$\begin{aligned}Q\hat{H}\,|\psi\rangle &= E\,Q\,|\psi\rangle \\ Q\,|\psi\rangle &= \frac{Q\hat{H}}{E}\,|\psi\rangle\end{aligned}$$

Therefore,

$$\begin{aligned}|\psi\rangle &= (P+Q)\,|\psi\rangle \\ &= P\,|\psi\rangle + Q\,|\psi\rangle \\ &= P\,|\psi\rangle + \frac{Q\hat{H}}{E}\,|\psi\rangle \qquad \text{(A.5)} \\ P\,|\psi\rangle &= \left(1 - \frac{Q\hat{H}}{E}\right)|\psi\rangle \\ |\psi\rangle &= \left(1 - \frac{Q\hat{H}}{E}\right)^{-1} P^2\,|\psi\rangle \qquad \text{(A.6)}\end{aligned}$$

Eq. (A.5) has the familiar iterative form as Eq. (A.2) with the choice of $P = |n\rangle\langle n|$. From Eq. (A.6),

$$\Omega = \left(1 - \frac{Q\hat{H}}{E}\right)^{-1} P \qquad \text{(A.7)}$$

The inverse operation in the wave operator can be expanded to obtain the perturbative expansion.

Above presentation of partitioning and effective hamiltonian formalism of BW theory is described in detail in [8].

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