

Many-body Physics Homework 1

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Problem 1 Consider the 1D harmonic oscillator Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$. Define the ladder operator $\hat{a} = \sqrt{\frac{m\omega}{2}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)$. The Hamiltonian can be written as $\hat{H} = \omega\hat{a}^\dagger\hat{a}$. Note that we neglect the zero point energy in this problem. For any complex number α , define a coherent state by

$$|\alpha\rangle = e^{-|\alpha|^2} e^{\alpha\hat{a}^\dagger} |0\rangle.$$

They satisfy

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle.$$

An explicit expression for $|\alpha\rangle$ is $|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |0\rangle$, although it is not needed in this problem. One can further check that coherent states are not orthogonal:

$$\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta}.$$

But they still form a complete basis, in the sense that there is a resolution of identity:

$$\int \frac{d^2\alpha}{\pi} |\alpha\rangle\langle\alpha| = 1.$$

1. Consider the propagator in the coherent state basis: $U(\alpha_f, t_f; \alpha_i, t_i) = \langle\alpha_f|e^{-i\hat{H}(t_f-t_i)}|\alpha_i\rangle$. Derive an expression of U in terms of a discretized path integral over paths $\alpha(t)$.

2. Take the continuum limit and show that the Lagrangian is

$$L = i\alpha^*\dot{\alpha} - \omega|\alpha|^2.$$

3. Show that the Lagrangian (5) is the same as the phase-space Lagrangian $L = p\dot{x} - \frac{p^2}{2m} - \frac{1}{2}m\omega^2x^2$ (may be up to a total time derivative term).

Solution

1. We make the Trotter decomposition:

$$\begin{aligned} \langle\alpha_f|e^{-iH(t_f-t_i)}|\alpha_i\rangle &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N \langle\alpha_j|e^{-i\Delta t H}|\alpha_{j-1}\rangle \\ &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N e^{-i\Delta t \omega \alpha_{j-1}^* \alpha_{j-1}} \langle\alpha_j|\alpha_{j-1}\rangle \\ &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N e^{-i\Delta t \omega \alpha_{j-1}^* \alpha_{j-1}} e^{-\frac{1}{2}(|\alpha_j|^2+|\alpha_{j-1}|^2)+\alpha_j^* \alpha_{j-1}}, \end{aligned} \quad (1)$$

where $\Delta\tau = (t_f - t_i)/N$, $\alpha_N = \alpha_f$, and $\alpha_0 = \alpha_i$.

2. To continue, we can use the condition that α_j and α_{j-1} is close to each other and make the following derivation:

$$\begin{aligned} \langle\alpha_f|e^{-iH(t_f-t_i)}|\alpha_i\rangle &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N e^{-i\Delta t \omega \alpha_{j-1}^* \alpha_{j-1}} e^{-\alpha_j^* \alpha_j + \alpha_j^* \alpha_{j-1}} \\ &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N e^{-i\Delta t \omega \alpha_{j-1}^* \alpha_{j-1} - \alpha_j^* (\alpha_j - \alpha_{j-1})} \\ &= \lim_{N\rightarrow\infty} \prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \prod_{j=1}^N e^{i\Delta t (\alpha_j^* (\alpha_j - \alpha_{j-1}) / \Delta t - \omega \alpha_{j-1}^* \alpha_{j-1})} \\ &= \lim_{N\rightarrow\infty} \left(\prod_{j=1}^{N-1} \int \frac{d\alpha_j}{\pi} \right) e^{i \sum_j \Delta t (\alpha_j^* (\alpha_j - \alpha_{j-1}) / \Delta t - \omega \alpha_{j-1}^* \alpha_{j-1})}, \end{aligned}$$

so after taking the continuous limit, we get

$$\langle \alpha_f | e^{-iH(t_f - t_i)} | \alpha_i \rangle = \int \mathcal{D}\alpha e^{i \int_{t_i}^{t_f} dt (i\alpha^* \dot{\alpha} - \omega |\alpha|^2)}. \quad (2)$$

So the Lagrangian is

$$L = i\alpha^* \dot{\alpha} - \omega |\alpha|^2. \quad (3)$$

3. By putting

$$\alpha = \sqrt{\frac{m\omega}{2}} \left(x + ip/m\omega \right) \quad (4)$$

into (3), we get

$$\begin{aligned} L &= i \frac{m\omega}{2} \left(x - \frac{ip}{m\omega} \right) \left(\dot{x} + \frac{i\dot{p}}{m\omega} \right) - \omega \frac{m\omega}{2} \left(x - \frac{ip}{m\omega} \right) \left(x + \frac{ip}{m\omega} \right) \\ &= i \frac{m\omega}{2} \left(x - \frac{ip}{m\omega} \right) \left(\dot{x} + \frac{i\dot{p}}{m\omega} \right) - \frac{p^2}{2m} - \frac{1}{2} m\omega^2 x^2. \end{aligned}$$

By integration by parts, we have

$$\dot{p} \left(x - \frac{ip}{m\omega} \right) = \frac{d}{dt} \left(px - \frac{ip^2}{m\omega} \right) - p \left(\dot{x} - \frac{i\dot{p}}{m\omega} \right),$$

and thus

$$\begin{aligned} & i \frac{m\omega}{2} \left(x - \frac{ip}{m\omega} \right) \left(\dot{x} + \frac{i\dot{p}}{m\omega} \right) \\ &= i \frac{m\omega}{2} \left(x\dot{x} - \frac{i}{m\omega} p\dot{x} + \frac{i}{m\omega} \left(\frac{d}{dt} \left(px - \frac{ip^2}{m\omega} \right) - p \left(\dot{x} - \frac{i\dot{p}}{m\omega} \right) \right) \right) \\ &= \frac{im\omega}{2} \left(-\frac{2i}{m\omega} p\dot{x} + \frac{d}{dt} \left(x^2 - \frac{p^2}{m^2\omega^2} \right) \right) \\ &= p\dot{x} + \text{total time derivative}. \end{aligned}$$

So we have

$$L = p\dot{x} - \frac{p^2}{2m} - \frac{1}{2} m\omega^2 x^2 + \text{total time derivative}. \quad (5)$$

Problem 2 A quantum particle in a magnetic field is described by the quantum Hamiltonian

$$\hat{H} = \frac{1}{2m} (\hat{\mathbf{p}} - A(\hat{\mathbf{x}}))^2 = \frac{1}{2m} [\hat{\mathbf{p}}^2 - \hat{\mathbf{p}}A(\hat{\mathbf{x}}) - A(\hat{\mathbf{x}})\hat{\mathbf{p}} + A(\hat{\mathbf{x}})^2].$$

We set $q = c = 1$ for simplicity.

1. Derive a discrete (Lagrangian) path integral for $U(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i)$, using the ordering of $\hat{\mathbf{p}}, A(\hat{\mathbf{x}})$ in (6).
2. The Hamiltonian can be equivalently written as

$$\hat{H} = \frac{1}{2m} [\hat{\mathbf{p}}^2 - 2\hat{\mathbf{p}}A(\hat{\mathbf{x}}) - i\nabla A(\hat{\mathbf{x}}) + A(\hat{\mathbf{x}})^2].$$

Derive a discrete (Lagrangian) path integral for U using this ordering.

3. Take the continuum limit and show that the first discrete integral leads to a continuum path integral with Lagrangian $L = \frac{1}{2} m \dot{\mathbf{x}}^2 + A(\mathbf{x})\dot{\mathbf{x}}$, and the second leads to $L = \frac{1}{2} m \dot{\mathbf{x}}^2 + A(\mathbf{x})\dot{\mathbf{x}} + \frac{i}{2m} \nabla A(\mathbf{x})$.

Solution

1. The discrete path integral is

$$\begin{aligned}\langle \mathbf{x}_f | e^{-iHt} | \mathbf{x}_i \rangle &= \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \int d^3 \mathbf{x}_j \prod_{j=1}^N \langle \mathbf{x}_j | e^{-i\Delta t H} | \mathbf{x}_{j-1} \rangle \\ &= \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \int d^3 \mathbf{x}_j \prod_{j=1}^N \langle \mathbf{x}_j | e^{-i\Delta t (\hat{\mathbf{p}}^2 - \hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{x}_{j-1}) - \mathbf{A}(\mathbf{x}_j) \cdot \hat{\mathbf{p}} + \mathbf{A}(\mathbf{x}_{j-1})^2) / 2m} | \mathbf{x}_{j-1} \rangle.\end{aligned}$$

Now we introduce a \mathbf{p} variable to eliminate the momentum operator:

$$\begin{aligned}&\langle \mathbf{x}_j | e^{-i\Delta t (\hat{\mathbf{p}}^2 - \hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{x}_{j-1}) - \mathbf{A}(\mathbf{x}_j) \cdot \hat{\mathbf{p}} + \mathbf{A}(\mathbf{x}_{j-1})^2) / 2m} | \mathbf{x}_{j-1} \rangle \\ &= \int d^3 \mathbf{p} \langle \mathbf{x}_j | \mathbf{p} \rangle \langle \mathbf{p} | e^{-i\Delta t (\hat{\mathbf{p}}^2 - \hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{x}_{j-1}) - \mathbf{A}(\mathbf{x}_j) \cdot \hat{\mathbf{p}} + \mathbf{A}(\mathbf{x}_{j-1})^2) / 2m} | \mathbf{x}_{j-1} \rangle \\ &= \int \frac{d^3 \mathbf{p}}{(2\pi)^3} e^{i\mathbf{p} \cdot \mathbf{x}_j} e^{-i\Delta t (\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{A}(\mathbf{x}_{j-1}) - \mathbf{A}(\mathbf{x}_j) \cdot \mathbf{p} + \mathbf{A}(\mathbf{x}_{j-1})^2) / 2m} e^{-i\mathbf{p} \cdot \mathbf{x}_{j-1}} \\ &= e^{-i\Delta t \mathbf{A}(\mathbf{x}_{j-1})^2 / 2m} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} e^{-\frac{1}{2} \frac{i\Delta t}{m} \mathbf{p}^2} e^{i\mathbf{p} \cdot (\mathbf{x}_j - \mathbf{x}_{j-1} + \frac{\Delta t}{2m} (\mathbf{A}(\mathbf{x}_j) + \mathbf{A}(\mathbf{x}_{j-1})))} \\ &= e^{-i\Delta t \mathbf{A}(\mathbf{x}_{j-1})^2 / 2m} \frac{1}{(2\pi)^3} \sqrt{\frac{(2\pi)^3}{(i\Delta t/m)^3}} e^{-\frac{1}{2} \frac{m}{i\Delta t} (\mathbf{x}_j - \mathbf{x}_{j-1} + \frac{\Delta t}{2m} (\mathbf{A}(\mathbf{x}_j) + \mathbf{A}(\mathbf{x}_{j-1})))^2} \\ &\approx \sqrt{\frac{-im^3}{(2\pi)^3 \Delta t^3}} e^{i\Delta t \frac{m}{2} \left(\frac{(\mathbf{x}_j - \mathbf{x}_{j-1})^2}{\Delta t^2} + \frac{\mathbf{x}_j - \mathbf{x}_{j-1}}{\Delta t} \cdot \frac{\mathbf{A}(\mathbf{x}_j) + \mathbf{A}(\mathbf{x}_{j-1})}{2} \right)}.\end{aligned}$$

Here in the last line we make the approximation that $\mathbf{A}(\mathbf{x}_j)$ and $\mathbf{A}(\mathbf{x}_{j-1})$ are close to each other, so the two \mathbf{A}^2 terms cancel with each other. So the final discrete path integral is

$$\begin{aligned}\langle \mathbf{x}_f | e^{-iHt} | \mathbf{x}_i \rangle &= \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \left(\frac{-im^3}{(2\pi)^3 \Delta t^3} \right)^{N/2} \int d^3 \mathbf{x}_j \\ &\quad \cdot e^{\sum_{j=1}^N i\Delta t \left(\frac{m}{2} \frac{(\mathbf{x}_j - \mathbf{x}_{j-1})^2}{\Delta t^2} + \frac{\mathbf{x}_j - \mathbf{x}_{j-1}}{\Delta t} \cdot \frac{\mathbf{A}(\mathbf{x}_j) + \mathbf{A}(\mathbf{x}_{j-1})}{2} \right)}.\end{aligned}\tag{6}$$

2. The derivation is largely the same, but now in each time step, the $-2\hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{x})$ term results in $-2\hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{x}_{j-1})$, and the result is

$$\begin{aligned}\langle \mathbf{x}_f | e^{-iHt} | \mathbf{x}_i \rangle &= \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \left(\frac{-im^3}{(2\pi)^3 \Delta t^3} \right)^{N/2} \int d^3 \mathbf{x}_j \\ &\quad \cdot e^{\sum_{j=1}^N i\Delta t \left(\frac{m}{2} \frac{(\mathbf{x}_j - \mathbf{x}_{j-1})^2}{\Delta t^2} + \frac{\mathbf{x}_j - \mathbf{x}_{j-1}}{\Delta t} \cdot \mathbf{A}(\mathbf{x}_{j-1}) + \frac{i}{2m} \nabla \cdot \mathbf{A}(\mathbf{x}_{j-1}) \right)}.\end{aligned}\tag{7}$$

3. We make the following replacements:

$$\frac{(\mathbf{x}_j - \mathbf{x}_{j-1})^2}{\Delta t^2} \longrightarrow \dot{\mathbf{x}}^2, \quad \sum_j \Delta t = \int dt,$$

and from (6) we get

$$\langle \mathbf{x}_f | e^{-iHt} | \mathbf{x}_i \rangle = \int \mathcal{D}\mathbf{x} e^{i \int_{t_i}^{t_f} dt \left(\frac{1}{2} m \dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{A} \right)},\tag{8}$$

and from (7) we get

$$\langle \mathbf{x}_f | e^{-iHt} | \mathbf{x}_i \rangle = \int \mathcal{D}\mathbf{x} e^{i \int_{t_i}^{t_f} dt \left(\frac{1}{2} m \dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{A} + \frac{i}{2m} \nabla \cdot \mathbf{A} \right)}.\tag{9}$$

So for the first path integral the Lagrangian is

$$L = \frac{1}{2} m \dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{A},\tag{10}$$

while for the second, it is

$$L = \frac{1}{2} m \dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{A} + \frac{i}{2m} \nabla \cdot \mathbf{A}.\tag{11}$$

Problem 3 Consider the propagator $U(x_f, t_f; x_i, t_i)$ for a harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2$.

1. Compute U by generalizing the free particle calculation from class.
2. Write down the imaginary time evolution operator $U(x_f, \tau_f; x_i, \tau_i)$ by analytical continuation.
3. From the decay of $U(0, \beta; 0, 0)$ in the limit $\beta \rightarrow \infty$, determine the ground state energy. The following mathematical result may be useful: define C_N as the tridiagonal $N \times N$ matrix

$$C_N = \begin{pmatrix} 2 \cos x & -1 & 0 & \cdots \\ -1 & 2 \cos x & -1 & \cdots \\ 0 & -1 & 2 \cos x & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

then we have $\det C_N = \frac{\sin(N+1)x}{\sin x}$.

Solution

1. The path integral can be derived similar to what has been done above:

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \int \prod_{j=1}^{N-1} dx_j e^{i\Delta t \sum_{j=1}^N \left(\frac{m}{2} \frac{(x_j - x_{j-1})^2}{\Delta t^2} - \frac{1}{2} m \omega^2 x_{j-1}^2 \right)}. \quad (12)$$

Again, we do the decomposition

$$x = x_{cl} + y, \quad (13)$$

and the path integral becomes

$$\begin{aligned} & \langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle \\ &= e^{iS_{cl}} \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \int \prod_{j=1}^{N-1} dy_j e^{i\Delta t \sum_{j=1}^N \left(\frac{m}{2} \frac{(y_j - y_{j-1})^2}{\Delta t^2} - \frac{1}{2} m \omega^2 y_{j-1}^2 \right)}, \end{aligned}$$

where $y_0 = y_N = 0$. Thus the kernel of the Gaussian integral is

$$\mathbf{A} = \frac{m}{\Delta t} \begin{pmatrix} 2 - \omega^2 \Delta t^2 & -1 & & \\ -1 & 2 - \omega^2 \Delta t^2 & -1 & \\ & -1 & \ddots & \\ & & \ddots & -1 & 2 - \omega^2 \Delta t^2 \end{pmatrix},$$

and the path integral is

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = e^{iS_{cl}} \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \left(\frac{(2\pi)^{N-1}}{\det(-i\mathbf{A})} \right)^{1/2}. \quad (14)$$

We find when N is large,

$$\begin{aligned} & \det \begin{pmatrix} 2 - \omega^2 \Delta t^2 & -1 & & \\ -1 & 2 - \omega^2 \Delta t^2 & -1 & \\ & -1 & \ddots & \\ & & \ddots & -1 & 2 - \omega^2 \Delta t^2 \end{pmatrix} \\ &= \det \begin{pmatrix} 2 \cos(\omega \Delta t) & -1 & & \\ -1 & 2 \cos(\omega \Delta t) & -1 & \\ & -1 & \ddots & \\ & & \ddots & -1 & 2 \cos(\omega \Delta t) \end{pmatrix} = \frac{\sin(N+1)\omega \Delta t}{\sin \omega \Delta t} = \frac{\sin \omega(t_f - t_i)}{\omega \Delta t}. \end{aligned}$$

So

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = e^{iS_{\text{cl}}} \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \left(\frac{(2\pi)^{N-1}}{\left(\frac{-im}{\Delta t} \right)^{N-1} \frac{\sin \omega(t_f - t_i)}{\omega \Delta t}} \right)^{1/2}.$$

Simplifying this equation, we get

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = \sqrt{\frac{m\omega}{2\pi i \sin \omega(t_f - t_i)}} e^{iS_{\text{cl}}}. \quad (15)$$

2. The Wick rotation is $\tau = it$. So

$$\begin{aligned} \sin \omega(t_f - t_i) &= \sin(-i\omega(\tau_f - \tau_i)) = -i \sinh(\omega(\tau_f - \tau_i)) \\ &= \frac{e^{\omega(\tau_f - \tau_i)} - e^{-\omega(\tau_f - \tau_i)}}{2i}. \end{aligned}$$

Similarly S_{cl} should be changed into

$$S_{\text{cl, im}} = -i \int d\tau \left(-\frac{1}{2} \left(\frac{dx_{\text{cl}}}{d\tau} \right)^2 - \frac{1}{2} m\omega^2 x_{\text{cl}}^2 \right).$$

Thus after the Wick rotation, we get

$$U(x_f, \tau_f; x_i, \tau_i) = \sqrt{\frac{m\omega}{2\pi \sinh(\omega(\tau_f - \tau_i))}} e^{-\int_{\tau_i}^{\tau_f} d\tau \left(\frac{1}{2} m \left(\frac{dx_{\text{cl}}}{d\tau} \right)^2 + \frac{1}{2} m\omega^2 x_{\text{cl}}^2 \right)}. \quad (16)$$

3. In this case the classical configuration is $x_{\text{cl}} = 0$: that's the trajectory with the boundary conditions $x_f = x_i = 0$. So we have

$$U(0, \beta; 0, 0) = \sqrt{\frac{m\omega}{2\pi \sinh(\omega(\tau_f - \tau_i))}} \sim \text{const} \times \sqrt{\frac{1}{e^{\omega(\tau_f - \tau_i)}}} \sim e^{-\frac{1}{2}\omega(t_f - t_i)}. \quad (17)$$

Therefore the ground state energy (which is the coefficient α in the $e^{-\alpha t}$ damping) is $\omega/2$.

Problem 4 Consider a single particle in a periodic potential: $\hat{H}_0 = \frac{\mathbf{p}^2}{2m} + V(\hat{\mathbf{x}})$, where $V(\mathbf{x} + \mathbf{a}) = V(\mathbf{x})$ for Bravais lattice vector \mathbf{a} . According to Bloch's theorem, the eigenstates are of the form $\psi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}(\mathbf{x})$ where $u_{n\mathbf{k}}(\mathbf{x})$ are periodic functions ($u_{n\mathbf{k}}(\mathbf{x} + \mathbf{a}) = u_{n\mathbf{k}}(\mathbf{x})$). Here \mathbf{k} is the lattice momentum in the Brillouin zone (BZ) and n is the band index. Denote the corresponding energy eigenvalue by $\epsilon_n(\mathbf{k})$. We do not need to know explicitly the Bloch wavefunctions $\psi_{m\mathbf{k}}$ and $\epsilon_n(\mathbf{k})$, so will keep them general.

In this problem we will study the semiclassical dynamics of a wave packet, of the form $\int_{\text{BZ}} c(\mathbf{k}) \psi_{n\mathbf{k}}(\mathbf{x})$. Here the wave packet is composed entirely of states from a single band n , and there is a large gap Δ separating n from neighboring bands, so we can ignore the other bands. From now on we drop the band index n , and denote $|\psi_{n\mathbf{k}}\rangle$ by $|\mathbf{k}\rangle$, $|u_{n\mathbf{k}}\rangle$ by $|u_{\mathbf{k}}\rangle$.

1. It is useful to analyze the system in the presence of a weak harmonic potential, and a weak (uniform) electric field:

$$\hat{H} = \hat{H}_0 + \frac{1}{2\alpha} \hat{\mathbf{x}}^2 - \mathbf{E} \cdot \hat{\mathbf{x}}$$

Construct a path integral in the \mathbf{k} -space for the propagator $\langle \mathbf{k}_f | e^{-i\hat{H}} | \mathbf{k}_i \rangle$ for electron in one band, and show that the effective Lagrangian takes the form

$$L_{\text{eff}} = \mathcal{A}(\mathbf{k}) \cdot \dot{\mathbf{k}} + \mathcal{F}(\dot{\mathbf{k}}, \mathbf{k}).$$

where $\mathcal{A}(\mathbf{k}) = i \langle u_{\mathbf{k}} | \nabla_{\mathbf{k}} | u_{\mathbf{k}} \rangle$ is the "Berry connection" of the band. Find out $\mathcal{F}(\dot{\mathbf{k}}, \mathbf{k})$. Hint: To describe electron dynamics in one band, the resolution of identity should only involve states in the band.

2. Find $\boldsymbol{\pi}$, the momentum canonically conjugate to \mathbf{k} , and compute the effective Hamiltonian $H_{\text{eff}}(\mathbf{k}, \boldsymbol{\pi})$.

- Find the position \mathbf{x} in terms of $\mathbf{k}, \boldsymbol{\pi}$ by differentiating H_{eff} with respect to \mathbf{E} .
- Find the classical equations of motion for H_{eff} and express them in terms of \mathbf{x}, \mathbf{k} . Taking the limit of vanishing harmonic potential $\alpha \rightarrow \infty$, derive the semiclassical equations of motion

$$\begin{aligned}\dot{\mathbf{x}} &= \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) - \mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k}) \\ \dot{\mathbf{k}} &= \mathbf{E}\end{aligned}$$

Here $\boldsymbol{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}$ is the "Berry curvature". Notice that there is an "anomalous velocity" term in $\dot{\mathbf{x}}$ coming from Berry phase effect. This term is neglected in many standard textbooks (e.g. Ashcroft and Mermin)

- As an example, consider a 2D particle in a uniform perpendicular magnetic field B . This system can be analyzed in terms of Bloch states if we work in a periodic gauge with a unit cell of area $\frac{2\pi}{B}$, again setting electric charge unit and speed of light to 1 (we do not need the specific form of this gauge). The resulting band structure consists of perfectly flat bands (Landau levels) with $\epsilon(\mathbf{k}) = \text{const.}$, and $\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}_0$ also a constant. Let us consider the dynamics of electrons in one Landau level. Find $\boldsymbol{\Omega}_0$ in terms of B by comparing the semi-classical equations (12) to the behavior of a classical particle in electric and magnetic fields.
- The integral of the Berry curvature over a closed surface is always quantized in multiples of 2π . In particular, this is true for the integral of the Berry curvature over the 2D Brillouin zone: $\int d^2\mathbf{k} \boldsymbol{\Omega}(\mathbf{k}) = 2\pi C$, where the integer C is known as the "Chern number" of the band. Find the Chern number of the Landau level.

Solution

- We do the Trotter decomposition again:

$$\langle \mathbf{k}_f | e^{-iHt} | \mathbf{k}_i \rangle = \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \int \frac{V}{(2\pi)^3} d^3\mathbf{k}_j \cdot \prod_{j=1}^N \langle \mathbf{k}_j | e^{-i\Delta t H} | \mathbf{k}_{j-1} \rangle, \quad \mathbf{k}_0 = \mathbf{k}_i, \quad \mathbf{k}_N = \mathbf{k}_f.$$

Each time step is given by

$$\begin{aligned}& \langle \mathbf{k}_j | e^{-i\Delta t (H_0 + \hat{\mathbf{x}}^2/2\alpha - \mathbf{E} \cdot \hat{\mathbf{x}})} | \mathbf{k}_{j-1} \rangle \\&= \langle \mathbf{k}_j | e^{-i\Delta t (\hat{\mathbf{x}}^2/2\alpha - \mathbf{E} \cdot \hat{\mathbf{x}})} | \mathbf{k}_{j-1} \rangle e^{-\Delta t \epsilon_{\mathbf{k}_{j-1}}} \\&= e^{-\Delta t \epsilon_{\mathbf{k}_{j-1}}} \int d^3\mathbf{r} u_{\mathbf{k}_j}^*(\mathbf{r}) e^{-i\mathbf{k}_j \cdot \mathbf{r}} e^{-i\Delta t (\mathbf{r}^2/2\alpha - \mathbf{E} \cdot \mathbf{r})} u_{\mathbf{k}_{j-1}}(\mathbf{r}) e^{i\mathbf{k}_{j-1} \cdot \mathbf{r}} \\&= e^{-\Delta t \epsilon_{\mathbf{k}_{j-1}}} \int d^3\mathbf{r} u_{\mathbf{k}_j}^*(\mathbf{r}) u_{\mathbf{k}_{j-1}}(\mathbf{r}) e^{-\frac{1}{2} \frac{i\Delta t}{\alpha} \mathbf{r}^2 + i\mathbf{r} \cdot (\Delta t \mathbf{E} + \mathbf{k}_{j-1} - \mathbf{k}_j)}.\end{aligned}$$

Due to the strong variation of the potential in each unit cell, $u_{\mathbf{k}}(\mathbf{r})$ varies much quicker than $e^{i\mathbf{k} \cdot \mathbf{r}}$.¹ Thus, we can separate the two scales and have

$$\begin{aligned}& \int d^3\mathbf{r} u_{\mathbf{k}_j}^*(\mathbf{r}) u_{\mathbf{k}_{j-1}}(\mathbf{r}) e^{-\frac{1}{2} \frac{i\Delta t}{\alpha} \mathbf{r}^2 + i\mathbf{r} \cdot (\Delta t \mathbf{E} + \mathbf{k}_{j-1} - \mathbf{k}_j)} \\&= \frac{1}{V_{\text{u.c.}}} \int_{\text{u.c.}} d^3\mathbf{r} u_{\mathbf{k}_j}^*(\mathbf{r}) u_{\mathbf{k}_{j-1}}(\mathbf{r}) \int d^3\mathbf{r} e^{-\frac{1}{2} \frac{i\Delta t}{\alpha} \mathbf{r}^2 + i\mathbf{r} \cdot (\Delta t \mathbf{E} + \mathbf{k}_{j-1} - \mathbf{k}_j)},\end{aligned}$$

and the Gaussian integral on the RHS can be evaluated as

$$\begin{aligned}& \int d^3\mathbf{r} e^{-\frac{1}{2} \frac{i\Delta t}{\alpha} \mathbf{r}^2 + i\mathbf{r} \cdot (\Delta t \mathbf{E} + \mathbf{k}_{j-1} - \mathbf{k}_j)} \\&= \sqrt{\frac{(2\pi)^3}{(i\Delta t/\alpha)^3}} e^{\frac{1}{2} \frac{\alpha}{i\Delta t} (i(\Delta t \mathbf{E} + \mathbf{k}_{j-1} - \mathbf{k}_j))^2} \\&= \sqrt{\frac{(2\pi)^3}{(i\Delta t/\alpha)^3}} e^{\frac{i\alpha}{2} (\mathbf{E} - \dot{\mathbf{k}})^2 \Delta t}.\end{aligned}$$

¹Another way to derive the semiclassical equations is to consider a wave packet. In that case, the envelope varies *slower* than $e^{i\mathbf{k} \cdot \mathbf{r}}$.

Thus

$$\begin{aligned}
\langle \mathbf{k}_f | e^{-iHt} | \mathbf{k}_i \rangle &= \lim_{N \rightarrow \infty} \mathcal{N} \prod_{j=1}^{N-1} \int d^3 \mathbf{k}_j e^{-i\Delta t \epsilon_{\mathbf{k}_{j-1}}} e^{\frac{i\Delta t \alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2} \langle u_{\mathbf{k}_j} | u_{\mathbf{k}_{j-1}} \rangle \\
&= \lim_{N \rightarrow \infty} \mathcal{N} \prod_{j=1}^{N-1} \int d^3 \mathbf{k}_j e^{-i\Delta t \epsilon_{\mathbf{k}_{j-1}}} e^{\frac{i\Delta t \alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2} (1 - \Delta t \dot{\mathbf{k}} \cdot \langle u_{\mathbf{k}_j} | \nabla_{\mathbf{k}_j} | u_{\mathbf{k}_j} \rangle) \\
&= \lim_{N \rightarrow \infty} \mathcal{N} \prod_{j=1}^{N-1} \int d^3 \mathbf{k}_j e^{-i\Delta t \epsilon_{\mathbf{k}_{j-1}} + \frac{i\Delta t \alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2 - \Delta t \dot{\mathbf{k}} \cdot \langle u_{\mathbf{k}_j} | \nabla_{\mathbf{k}_j} | u_{\mathbf{k}_j} \rangle} \\
&= \lim_{N \rightarrow \infty} \left(\mathcal{N} \prod_{j=1}^{N-1} \int d^3 \mathbf{k}_j \right) e^{i\Delta t (\sum_j -\epsilon_{\mathbf{k}_{j-1}} + \frac{\alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2 + i\dot{\mathbf{k}} \cdot \langle u_{\mathbf{k}_j} | \nabla_{\mathbf{k}_j} | u_{\mathbf{k}_j} \rangle)}.
\end{aligned}$$

Putting all normalization factors into the measure, we get

$$\begin{aligned}
\langle \mathbf{k}_f | e^{-iHt} | \mathbf{k}_i \rangle &= \int \mathcal{D}\mathbf{k} e^{i \int_t^f dt L_{\text{eff}}}, \\
L_{\text{eff}} &= \dot{\mathbf{k}} \cdot \mathcal{A} + \frac{\alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2 - \epsilon_{\mathbf{k}}.
\end{aligned} \tag{18}$$

So we find

$$\mathcal{F}(\mathbf{k}, \dot{\mathbf{k}}) = \frac{\alpha}{2} (\dot{\mathbf{k}} - \mathbf{E})^2 - \epsilon_{\mathbf{k}}. \tag{19}$$

2. We have

$$\boldsymbol{\pi} = \frac{\partial L_{\text{eff}}}{\partial \dot{\mathbf{k}}} = \mathcal{A} + \alpha (\dot{\mathbf{k}} - \mathbf{E}). \tag{20}$$

So

$$\begin{aligned}
H_{\text{eff}} &= \dot{\mathbf{k}} \cdot \boldsymbol{\pi} - L_{\text{eff}} \\
&= \frac{1}{2} \alpha \dot{\mathbf{k}}^2 - \frac{1}{2} \alpha \mathbf{E}^2 + \epsilon_{\mathbf{k}}.
\end{aligned}$$

Replacing $\dot{\mathbf{k}}$ by $\boldsymbol{\pi}$, we get

$$\begin{aligned}
H_{\text{eff}} &= \frac{1}{2} \alpha \left(\frac{\boldsymbol{\pi} - \mathcal{A}}{\alpha} + \mathbf{E} \right)^2 - \frac{1}{2} \alpha \mathbf{E}^2 + \epsilon_{\mathbf{k}} \\
&= \frac{(\boldsymbol{\pi} - \mathcal{A})^2}{2\alpha} + (\boldsymbol{\pi} - \mathcal{A}) \cdot \mathbf{E} + \epsilon_{\mathbf{k}}.
\end{aligned}$$

So the answer is

$$H_{\text{eff}} = \frac{(\boldsymbol{\pi} - \mathcal{A})^2}{2\alpha} + (\boldsymbol{\pi} - \mathcal{A}) \cdot \mathbf{E} + \epsilon_{\mathbf{k}}. \tag{21}$$

3. We can interpret $-\boldsymbol{\pi}$ as some sort of “position”, because

$$[\mathbf{k}, \boldsymbol{\pi}] = 1 \Leftrightarrow [-\boldsymbol{\pi}, \mathbf{k}] = 1,$$

so we replace $\boldsymbol{\pi}$ by $-\mathbf{x}$, and thus in the $\alpha \rightarrow \infty$ limit, we have

$$H_{\text{eff}} = -(\mathbf{x} + \mathcal{A}) \cdot \mathbf{E} + \epsilon_{\mathbf{k}}. \tag{22}$$

4. We have

$$\dot{\mathbf{x}} = \frac{\partial H_{\text{eff}}}{\partial \mathbf{k}} = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} - \nabla_{\mathbf{k}} (\mathbf{E} \cdot \mathcal{A}).$$

By vector analysis formula, and by the condition that \mathbf{E} is a constant, we have

$$\nabla_{\mathbf{k}} (\mathbf{E} \cdot \mathcal{A}) = \mathbf{E} \times (\nabla_{\mathbf{k}} \times \mathcal{A}),$$

so finally we get

$$\dot{\mathbf{x}} = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} - \mathbf{E} \times \boldsymbol{\Omega}, \tag{23}$$

where

$$\boldsymbol{\Omega} = \nabla_{\mathbf{k}} \times \mathcal{A}. \tag{24}$$

Also

$$\dot{\mathbf{k}} = -\frac{\partial H_{\text{eff}}}{\partial \mathbf{x}} = \mathbf{E}. \tag{25}$$

5. From (23) and (25) we have²

$$\dot{\mathbf{x}} = -\mathbf{E} \times \boldsymbol{\Omega} = -\dot{\mathbf{k}} \times \boldsymbol{\Omega},$$

and therefore

$$\boldsymbol{\Omega} \times \dot{\mathbf{x}} = -\Omega^2 \dot{\mathbf{k}} + (\boldsymbol{\Omega} \cdot \dot{\mathbf{k}}) \boldsymbol{\Omega}. \quad (26)$$

On the other hand, the classical EOM is (here $e = 1$)

$$\dot{\mathbf{p}} = -\dot{\mathbf{x}} \times \mathbf{B}. \quad (27)$$

So

$$\boldsymbol{\Omega} = \Omega_0 \hat{\mathbf{z}}, \quad \Omega_0 = \frac{1}{B}. \quad (28)$$

6. The size of the first Brillouin zone is

$$\frac{(2\pi)^2}{2\pi/B} = 2\pi B.$$

So

$$2\pi C = \int d^2\mathbf{k} \, \Omega = 2\pi B \cdot \Omega_0 = 2\pi,$$

and thus the Chern number of the Landau level is 1.

²Here we assume there is a very weak electric field \mathbf{E} , so we can put (25) and (23) into one equation, and then we let $\mathbf{E} \rightarrow 0$.