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:

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

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

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

1. Consider the propagator in the coherent state basis: $U\left(\alpha_f, t_f; \alpha_i, t_i\right) = \left\langle\alpha_f \left| e^{-i\hat{H}(t_f-t_i)} \right| \alpha_i\right\rangle$. 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:

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

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:

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

so after taking the continuous limit, we get

$$\langle\alpha_f|\mathrm{e}^{-\mathrm{i}H(t_f-t_i)}|\alpha_i\rangle = \int \mathcal{D}\alpha \mathrm{e}^{\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t(\mathrm{i}\alpha^*\dot{\alpha}-\omega|\alpha|^2)}. \tag{2}$$

So the Lagrangian is

$$L = \mathrm{i}\alpha^*\dot{\alpha} - \omega|\alpha|^2. \tag{3}$$

3. By putting

$$\alpha = \sqrt{\frac{m\omega}{2}}(x + \mathrm{i}p/m\omega) \tag{4}$$

into (3), we get

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

By integration by parts, we have

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

and thus

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

So we have

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

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

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

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

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

   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

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

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

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

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

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

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

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

3. We make the following replacements:

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

and from (6) we get

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

and from (7) we get

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

So for the first path integral the Lagrangian is

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

while for the second, it is

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

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 $\beta \to \infty$, 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:

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

Again, we do the decomposition

$$x = x_{\mathrm{cl}} + y, \tag{13}$$

and the path integral becomes

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

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

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

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

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

Simplifying this equation, we get

$$\langle x_f|\mathrm{e}^{-\mathrm{i}H(t_f-t_i)}|x_i\rangle = \sqrt{\frac{m\omega}{2\pi\mathrm{i}\sin\omega(t_f-t_i)}}\mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}}. \tag{15}$$

2. The Wick rotation is $\tau = \mathrm{i}t$. So

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

Similarly S_{cl} should be changed into

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

Thus after the Wick rotation, we get

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

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

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

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

Problem 4 Consider a single particle in a periodic potential: $\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})$, where $V(\mathbf{x}+\mathbf{a}) = V(\mathbf{x})$ for Bravais lattice vector a. According to Bloch's theorem, the eigenstates are of the form $\psi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}u_{nk}(\mathbf{x})$ where $u_{nk}(\mathbf{x})$ are periodic functions ($u_{n\mathbf{k}}(\mathbf{x}+a) = u_{n\mathbf{k}}(\mathbf{x})$). 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 $\int_{\mathrm{BZ}} c(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{x})$. 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. 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 $\left\langle \mathbf{k}_f \left| e^{-i\hat{H}} \right| \mathbf{k}_i \right\rangle$ for electron in one band, and show that the effective Lagrangian takes the form

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

   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 $H_{\mathrm{eff}}(\mathbf{k},\boldsymbol{\pi})$.

3. Find the position $\mathbf{x}$ in terms of $\mathbf{k}, \boldsymbol{\pi}$ by differentiating H_{eff} with respect to $\mathbf{E}$.

4. 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 $\alpha \to \infty$, derive the semiclassical equations of motion

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

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)

5. 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 $\varepsilon(\mathbf{k}) = \text{const.}$, and $\Omega(\mathbf{k}) = \Omega_0$ also a constant. Let us consider the dynamics of electrons in one Landau level. Find Ω_0 in terms of B by comparing the semi-classical equations (12) to the behavior of a classical particle in electric and magnetic fields.

6. 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: $\int \mathrm{d}^2\mathbf{k}\Omega(\mathbf{k}) = 2\pi C$, where the integer C is known as the "Chern number" of the band. Find the Chern number of the Landau level.

Solution

1. We do the Trotter decomposition again:

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

Each time step is given by

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

The semi-classical dynamics only works when $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ is "concentrated" enough in the reciprocal space, which means $u_{\boldsymbol{k}}(\boldsymbol{r})$ should be very smooth compared with $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$ (or otherwise the picture of an electron with a certain momentum traveling in the material is simply wrong). Thus, we have

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

and the Gaussian integral on the RHS can be evaluated as

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

Thus

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

Putting all normalization factors into the measure, we get

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

So we find

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

2. We have

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

So

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

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

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

So the answer is

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

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

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

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

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

4. We have

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

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

$$\boldsymbol{\nabla}_{\boldsymbol{k}}(\boldsymbol{E}\cdot\boldsymbol{A}) = \boldsymbol{E}\times(\boldsymbol{\nabla}_{\boldsymbol{k}}\times\boldsymbol{\mathcal{A}}),$$

so finally we get

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

where

$$\boldsymbol{\Omega} = \boldsymbol{\nabla}_{\boldsymbol{k}}\times\boldsymbol{\mathcal{A}}.\tag{24}$$

Also

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

5. From (23) and (25) we have[1]

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

and therefore

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

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

$$\dot{\boldsymbol{p}} = -\dot{\boldsymbol{x}} \times \boldsymbol{B}. \tag{27}$$

So

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

6. The size of the first Brillouin zone is

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

So

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

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

[1] Here we assume there is a very weak electric field $\boldsymbol{E}$, so we can put (25) and (23) into one equation, and then we let $\boldsymbol{E} \to 0$.