Advanced quantum mechanics

Chapter 1 – Effective dynamics of quantum systems

Sylvain Nascimbene

M2 ICFP – École Normale Supérieure

Outline

1. Effective dynamics of quantum systems
   - Effective description and separation of energy scales
   - Adiabatic particle motion and Berry phase
   - Resonant coupling to a continuum
   - From effective Hamiltonians to open quantum systems

Chapter 1 – Effective descriptions

The Schrödinger equation describes, in principle, the full dynamics of an isolated system. In practice, the microscopic description is often neither necessary nor useful:

- some degrees of freedom are inaccessible to measurement,
- they evolve on very different time scales,
- or they are only weakly coupled to the degrees of freedom of interest.

We look for a reduced description that keeps the relevant physics:

- eliminate weakly coupled excited states: effective Hamiltonians;
- follow slowly varied eigenstates: Berry phase;
- couple a discrete state to a continuum: irreversible decay;
- a small system coupled to a large environment: Lindblad equation for its density matrix.

Separation of energy scales

Split the Hilbert space into

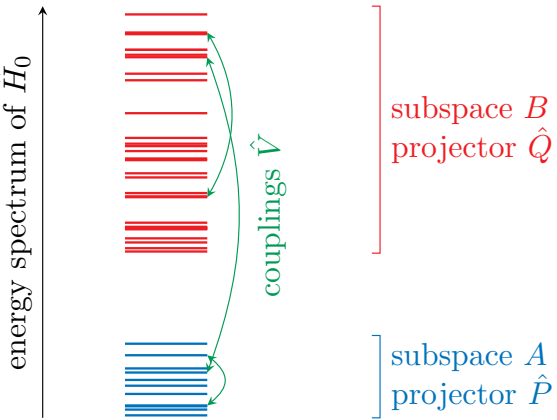
- a subspace A of states we keep, projector $\hat{P}$;
- a subspace B that can be eliminated, projector $\hat{Q} = 1 - \hat{P}$.

Block decomposition in $A \oplus B$:

$$\hat{H} = \begin{pmatrix} \hat{H}_{AA} & \hat{H}_{AB} \\ \hat{H}_{BA} & \hat{H}_{BB} \end{pmatrix},$$

$\hat{H}_{AA} = \hat{P}\hat{H}\hat{P}$, $\hat{H}_{AB} = \hat{P}\hat{H}\hat{Q}$, $\hat{H}_{BB} = \hat{Q}\hat{H}\hat{Q}$, $\hat{H}_{BA} = \hat{H}_{AB}^{\dagger}$.

Goal: an effective Schrödinger equation for $\hat{P}|\psi\rangle$, valid when the energy scales of A and B are well separated.



Formal expression of the effective Hamiltonian

Project $\hat{H}|\psi\rangle = E|\psi\rangle$ onto A and B:

$$E\hat{P}|\psi\rangle = \hat{H}_{AA}\hat{P}|\psi\rangle + \hat{H}_{AB}\hat{Q}|\psi\rangle, \qquad E\hat{Q}|\psi\rangle = \hat{H}_{BA}\hat{P}|\psi\rangle + \hat{H}_{BB}\hat{Q}|\psi\rangle.$$

For E away from the spectrum of B, solve the second equation,

$$\hat{Q}|\psi\rangle = \frac{1}{E - \hat{Q}\hat{H}\hat{Q}}\,\hat{Q}\hat{H}\hat{P}|\psi\rangle,$$

and insert it in the first one: $\hat{H}_{\text{eff}}(E)\,\hat{P}|\psi\rangle = E\,\hat{P}|\psi\rangle$ with

Effective Hamiltonian

$$\hat{H}_{\text{eff}}(E) = \hat{P}\hat{H}\hat{P} + \hat{P}\hat{H}\hat{Q}\,\frac{1}{E - \hat{Q}\hat{H}\hat{Q}}\,\hat{Q}\hat{H}\hat{P}$$

- Exact, but parametrized by E: the eigen-energies solve $\det[E - \hat{H}_{\text{eff}}(E)] = 0$.
- $1/(E - \hat{Q}\hat{H}\hat{Q})$: resolvent of the eliminated subspace, describing the virtual propagation through B.

Perturbative expansion

$\hat{H} = \hat{H}_0 + \hat{V}$; $\hat{H}_0$: A and B uncoupled, quasi-degenerate around E_A, E_B, with $\hbar\Delta = E_A - E_B$.

Second order. For E in the range of A, $1/(E - \hat{Q}\hat{H}\hat{Q}) = 1/(\hbar\Delta) + \mathcal{O}(\hat{V})$:

$$\hat{H}_{\text{eff}} = \hat{P}\hat{H}_0\hat{P} + \hat{P}\hat{V}\hat{P} + \frac{\hat{P}\hat{V}\hat{Q}\hat{V}\hat{P}}{\hbar\Delta} + \mathcal{O}(\hat{V}^3)$$

Single state $|\psi_0\rangle$: standard 2nd-order perturbation theory,
$E = E_0 + \langle\psi_0|\hat{V}|\psi_0\rangle + \langle\psi_0|\hat{V}\hat{Q}\frac{1}{E_0 - \hat{Q}\hat{H}_0\hat{Q}}\hat{Q}\hat{V}|\psi_0\rangle$.

$(*)$ **Third order** ($\hat{P}\hat{H}_0\hat{P} = E_A\hat{P}$, $\hat{Q}\hat{H}_0\hat{Q} = E_B\hat{Q}$). The resolvent depends on $E - E_A = \mathcal{O}(\hat{V})$:

$$\frac{1}{E - \hat{Q}\hat{H}\hat{Q}} = \frac{1}{\hbar\Delta + E - E_A - \hat{Q}\hat{V}\hat{Q}} \simeq \frac{1}{\hbar\Delta} + \frac{\hat{Q}\hat{V}\hat{Q} - (E - E_A)}{(\hbar\Delta)^2}.$$

Replacing $E - E_A \to \hat{P}\hat{V}\hat{P}$, symmetrized to keep $\hat{H}_{\text{eff}}$ Hermitian:

$$\hat{H}^{(3)}_{\text{eff}} = \frac{1}{(\hbar\Delta)^2}\left(\hat{P}\hat{V}\hat{Q}\hat{V}\hat{Q}\hat{V}\hat{P} - \frac{1}{2}\{\hat{P}\hat{V}\hat{P}, \hat{P}\hat{V}\hat{Q}\hat{V}\hat{P}\}\right).$$

(∗) Landau levels

Charged particle in the xy plane, uniform field $\mathbf{B} = B\mathbf{e}_z$:

$$\hat{H}_0 = \frac{[\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}})]^2}{2m}, \qquad \nabla \times \mathbf{A} = B\mathbf{e}_z.$$

Guiding center $\hat{\mathbf{R}}$ and cyclotron coordinate $\hat{\mathbf{r}}_\mathrm{c}$:

$$\hat{\mathbf{r}} = \hat{\mathbf{R}} + \hat{\mathbf{r}}_\mathrm{c}, \qquad \hat{\mathbf{r}}_\mathrm{c} = \frac{1}{qB}\,\mathbf{e}_z \times [\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}})], \qquad \partial_t \hat{\mathbf{r}}_\mathrm{c} = \omega_\mathrm{c}\,\hat{\mathbf{r}}_\mathrm{c} \times \mathbf{e}_z, \quad \omega_\mathrm{c} = \frac{qB}{m}.$$

Two independent conjugate pairs ($\ell_\mathrm{c} = \sqrt{\hbar/qB}$: magnetic length):

$$[\hat{X}, \hat{Y}] = -\mathrm{i}\ell_\mathrm{c}^2, \qquad [\hat{x}_\mathrm{c}, \hat{y}_\mathrm{c}] = \mathrm{i}\ell_\mathrm{c}^2.$$

$$\hat{H}_0 = \frac{\hbar\omega_\mathrm{c}}{2\ell_\mathrm{c}^2}\left(\hat{x}_\mathrm{c}^2 + \hat{y}_\mathrm{c}^2\right) \quad \Rightarrow \quad E_{n_\mathrm{c}} = \hbar\omega_\mathrm{c}\left(n_\mathrm{c} + \tfrac{1}{2}\right)$$

$\hat{H}_0$ does not involve $\hat{\mathbf{R}}$: each n_c is a highly degenerate flat band, the n_cth Landau level.
What is the dynamics induced by a weak potential $V(\hat{\mathbf{r}})$ within the lowest Landau level?

(∗) Projection onto the lowest Landau level

$\hat{P}$: projector on $n_c = 0$. At first order, $\hat{H}_{\text{eff}} = \hat{P}\hat{H}_0\hat{P} + \hat{P}\hat{V}\hat{P}$, with

$$\hat{V}_{\text{eff}} = \hat{P}\, V(\hat{\mathbf{R}} + \hat{\mathbf{r}}_c)\, \hat{P} = \int \tilde{V}(\mathbf{q})\, e^{i\mathbf{q}\cdot\hat{\mathbf{R}}}\, \hat{P} e^{i\mathbf{q}\cdot\hat{\mathbf{r}}_c} \hat{P}\, d^2q, \qquad V(\mathbf{r}) = \int \tilde{V}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} d^2q.$$

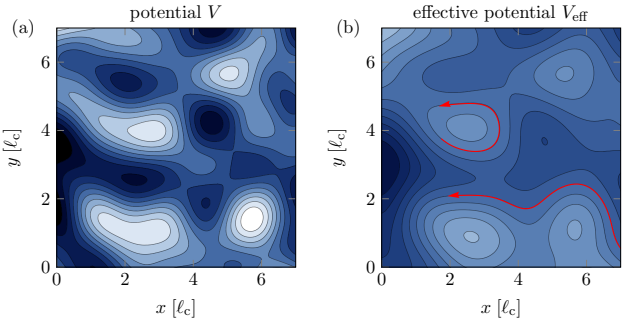
Gaussian cyclotron ground state: $\langle n_c = 0 | e^{i\mathbf{q}\cdot\hat{\mathbf{r}}_c} | n_c = 0\rangle = e^{-(q\ell_c)^2/4}$, a low-pass filter:

$$\hat{H}_{\text{eff}} = \hat{P}\left[\frac{\hbar\omega_c}{2} + V_{\text{eff}}(\hat{\mathbf{R}})\right]\hat{P}, \qquad V_{\text{eff}} = V * K, \quad K(\mathbf{R}) = \frac{1}{\pi\ell_c^2} e^{-(R/\ell_c)^2}$$

The cyclotron motion averages V over a region of size ℓ_c: variations on scales $\ll \ell_c$ are suppressed.

Kinetic energy frozen, but $\hat{X}$ and $\hat{Y}$ do not commute: the guiding center remains dynamical.

(∗) Hall drift of guiding centers



Heisenberg equation with $[\hat{X}, \hat{Y}] = -\mathrm{i}\ell_c^2$:

$$\partial_t \hat{\mathbf{R}} = \frac{1}{\mathrm{i}\hbar}[\hat{\mathbf{R}}, \hat{H}_{\text{eff}}] = \frac{1}{qB}\,\mathbf{e}_z \times \nabla V_{\text{eff}}(\hat{\mathbf{R}}).$$

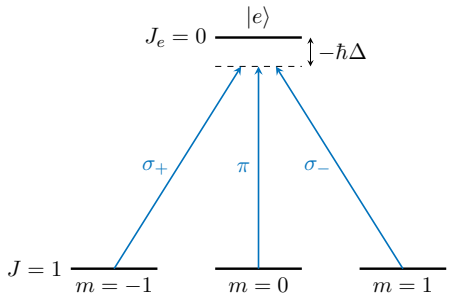
Semiclassically, the guiding center drifts along the equipotential lines of V_{eff}.

Uniform field: $V = -q\mathbf{E}\cdot\mathbf{r}$ is unchanged by the convolution,

$$\partial_t \hat{\mathbf{R}} = \frac{\mathbf{E}\times\mathbf{B}}{B^2}$$

the Hall drift: quantum version of the $\mathbf{E}\times\mathbf{B}$ drift.

Two-photon transitions: atom–light coupling



Ground manifold $J = 1$ ($\hat{P}$), excited state $|e\rangle$ with $J_e = 0$ ($\hat{Q} = |e\rangle\langle e|$), at energy $\hbar\omega_0$.

Field $\mathbf{E}(t) = \mathcal{E}\,\boldsymbol{\epsilon}\,\mathrm{e}^{-\mathrm{i}\omega t} + \text{c.c.}$, coupling $\hat{V} = -\hat{\mathbf{d}}\cdot\mathbf{E}(t)$.

Wigner–Eckart, in the Cartesian basis $|i\rangle = |m = 0\rangle_i$:

$$\hat{\mathbf{d}} = d\sum_{i=x,y,z}\mathbf{e}_i\left(|e\rangle\langle i| + |i\rangle\langle e|\right), \qquad |m\rangle_z = \sum_i (\mathbf{e}_m)_i |i\rangle.$$

Rotating-wave approximation + frame rotating at ω, with $\Omega = -d\mathcal{E}/\hbar$, $\Delta = \omega - \omega_0$:

$$\hat{H}_0 = -\hbar\Delta\,\hat{Q}, \qquad \hat{V} = \hbar\Omega|e\rangle\langle\boldsymbol{\epsilon}^*| + \hbar\Omega^*|\boldsymbol{\epsilon}^*\rangle\langle e|,$$

where $|\mathbf{v}\rangle = \sum_i v_i|i\rangle$.

- Light couples $|e\rangle$ to a single bright state $|\boldsymbol{\epsilon}^*\rangle$; the orthogonal plane is dark.
- $\boldsymbol{\epsilon} = \mathbf{e}_q$: $|\boldsymbol{\epsilon}^*\rangle = |m = -q\rangle_z$ (selection rule: σ^+ couples $m = -1$).

Adiabatic elimination: the light shift

For $|\Omega| \ll |\Delta|$, $|e\rangle$ is only virtually populated. Here $\hat{P}\hat{V}\hat{P} = 0$, $E_A = 0$, $\hat{H}^{(0)}_{BB} = -\hbar\Delta$:

$$\hat{H}^{(2)}_{\text{eff}} = \hat{P}\hat{V}\hat{Q}\,\frac{1}{E_A - \hat{H}^{(0)}_{BB}}\,\hat{Q}\hat{V}\hat{P} = \frac{1}{\hbar\Delta}\,\hat{P}\hat{V}\hat{Q}\hat{V}\hat{P}.$$

Light shift (AC Stark shift)

$$\hat{H}_{\text{eff}} = \frac{\hbar|\Omega|^2}{\Delta}\,|\boldsymbol{\epsilon}^*\rangle\langle\boldsymbol{\epsilon}^*|$$

- Virtual process: $|\boldsymbol{\epsilon}^*\rangle \to |e\rangle \to |\boldsymbol{\epsilon}^*\rangle$. Dark states are unaffected.
- Red detuning ($\Delta < 0$) lowers the energy of the bright state: basis of optical trapping (optical tweezers).
- The complex conjugate $\boldsymbol{\epsilon}^*$ matters for elliptical or circular polarizations: absorption is driven by the positive-frequency part of the field.

Raman coupling between two ground states

Zeeman field: $\hat{H}_Z = \hbar\omega_Z \sum_m m|m\rangle_z\langle m|_z$ ($|\omega_Z| \ll |\Delta|$). Two beams $\boldsymbol{\epsilon}_1 = \mathbf{e}_0$ (π), $\boldsymbol{\epsilon}_2 = \mathbf{e}_{+1}$ (σ^+): bright states $|\boldsymbol{\epsilon}_1^*\rangle = |0\rangle_z$, $|\boldsymbol{\epsilon}_2^*\rangle = |-1\rangle_z$; $|+1\rangle_z$ stays dark.
Frequencies ω_1, $\omega_2 = \omega_1 + \delta$; frame rotating at ω_1, $\Delta = \omega_1 - \omega_0$:

$$\hat{V}(t) = \hbar\left(\Omega_1|e\rangle\langle\boldsymbol{\epsilon}_1^*| + \Omega_2 e^{-i\delta t}|e\rangle\langle\boldsymbol{\epsilon}_2^*| + \text{h.c.}\right).$$

$\hat{H}_{\text{eff}} = \hat{H}_Z + \hat{H}_{\text{eff}}^{(2)}$: light shifts $\hbar|\Omega_j|^2/\Delta$, plus a coupling

$$\frac{\hbar\Omega_1^*\Omega_2}{\Delta} e^{-i\delta t}|\boldsymbol{\epsilon}_1^*\rangle\langle\boldsymbol{\epsilon}_2^*| + \text{h.c.}: \quad |-1\rangle_z \to |e\rangle \to |0\rangle_z, \quad \Omega_{2\text{ph}} = \frac{\Omega_1^*\Omega_2}{\Delta}.$$

Static two-level Hamiltonian (after removing $e^{\mp i\delta t}$)

$$\hat{H}_{\text{eff}} = E_1|\boldsymbol{\epsilon}_1^*\rangle\langle\boldsymbol{\epsilon}_1^*| + E_2|\boldsymbol{\epsilon}_2^*\rangle\langle\boldsymbol{\epsilon}_2^*| + (\hbar\Omega_{2\text{ph}}|\boldsymbol{\epsilon}_1^*\rangle\langle\boldsymbol{\epsilon}_2^*| + \text{h.c.}), \quad E_1 = \frac{\hbar|\Omega_1|^2}{\Delta}, \; E_2 = \hbar(\delta - \omega_Z) + \frac{\hbar|\Omega_2|^2}{\Delta}$$

Resonance at $\delta = \omega_Z + (|\Omega_1|^2 - |\Omega_2|^2)/\Delta$ (differential light shift): Rabi oscillations at $|\Omega_{2\text{ph}}|$, with $\Delta m = +1$.

Adiabatic following of a local internal state

Particle with an internal degree of freedom whose local eigenstates vary in space. If the internal state stays locked to a non-degenerate local eigenstate $|\phi(\mathbf{r})\rangle$:

$$|\Psi\rangle = \int \psi(\mathbf{r})\,|\mathbf{r}\rangle \otimes |\phi(\mathbf{r})\rangle\,\mathrm{d}^3 r, \qquad \hat{P} = \int |\mathbf{r}\rangle\langle\mathbf{r}| \otimes \hat{\Pi}(\mathbf{r})\,\mathrm{d}^3 r, \quad \hat{\Pi}(\mathbf{r}) = |\phi(\mathbf{r})\rangle\langle\phi(\mathbf{r})|.$$

Adiabaticity: transitions to the other local internal states are neglected.

Example: spinful particle in an inhomogeneous magnetic field.

$$\hat{H}_0 = -g\mu_\mathrm{B}\hat{\mathbf{J}}\cdot\mathbf{B}(\mathbf{r}), \qquad g > 0 \quad \text{(ground state along } \mathbf{B}\text{; opposite to the electron convention)}$$

Strong and slowly varying field: the spin stays in the local ground state

$$|\phi(\mathbf{r})\rangle = |m = J\rangle_{\mathbf{n}(\mathbf{r})}, \qquad \mathbf{n}(\mathbf{r}) = \frac{\mathbf{B}(\mathbf{r})}{B(\mathbf{r})}, \qquad E_0(\mathbf{r}) = -g\mu_\mathrm{B} J B(\mathbf{r}).$$

Question: effective dynamics of $\psi(\mathbf{r})$ within this position-dependent subspace?

Projected kinetic energy: the Berry connection

The kinetic energy $\hat{V} = -\frac{\hbar^2}{2m}\nabla^2$ also acts on $|\phi(\mathbf{r})\rangle$. Projecting onto $\langle \mathbf{r}| \otimes \langle \phi(\mathbf{r})|$:

$$-\frac{\hbar^2}{2m}\Big[\nabla^2\psi + 2\langle\phi|\nabla|\phi\rangle \cdot \nabla\psi + \langle\phi|\nabla^2|\phi\rangle\,\psi\Big].$$

Normalization $\langle\phi|\phi\rangle = 1$ at all $\mathbf{r} \Rightarrow \langle\phi|\nabla|\phi\rangle$ is purely imaginary:

Berry connection (real vector field)

$$\mathbf{A}(\mathbf{r}) = \mathrm{i}\hbar\langle\phi(\mathbf{r})|\nabla|\phi(\mathbf{r})\rangle$$

Comparing with the expansion of $\frac{1}{2m}\left[\frac{\hbar}{\mathrm{i}}\nabla - \mathbf{A}\right]^2\psi$:

Effective Hamiltonian

$$\hat{H}_{\text{eff}} = \frac{[\hat{\mathbf{p}} - \mathbf{A}(\hat{\mathbf{r}})]^2}{2m} + U(\hat{\mathbf{r}}), \qquad U = E_0 + W, \qquad W = \frac{\hbar^2}{2m}\big\|\hat{Q}\nabla|\phi\rangle\big\|^2, \quad \hat{Q} = \mathbb{1} - \hat{\Pi}.$$

An effective spinless particle in a geometric vector potential $\mathbf{A}$ and a scalar potential U (including the geometric scalar potential $W \geq 0$).

Gauge structure and Berry phase

A is not gauge invariant. Arbitrary smooth phase redefinition, with $|\Psi\rangle$ unchanged:

$$|\phi(\mathbf{r})\rangle \to \mathrm{e}^{\mathrm{i}\alpha(\mathbf{r})}|\phi(\mathbf{r})\rangle, \quad \psi(\mathbf{r}) \to \mathrm{e}^{-\mathrm{i}\alpha(\mathbf{r})}\psi(\mathbf{r}) \quad \Longrightarrow \quad \mathbf{A} \to \mathbf{A} - \hbar\nabla\alpha,$$

the gauge transformation law of an electromagnetic vector potential.

Gauge-invariant quantities:

Berry curvature and Berry phase

$$\mathbf{\Omega}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}), \qquad \gamma(\mathcal{C}) = \frac{1}{\hbar}\oint_{\mathcal{C}} \mathbf{A}\cdot \mathrm{d}\mathbf{l} = \frac{1}{\hbar}\int_{\mathcal{S}} \mathbf{\Omega}\cdot \mathrm{d}\mathbf{S}, \quad \mathcal{C} = \partial\mathcal{S}$$

Adiabatic transport around $\mathcal{C}$: the state acquires $\mathrm{e}^{\mathrm{i}\gamma}$, with $\gamma = \mathrm{i}\oint_{\mathcal{C}}\langle\phi|\nabla|\phi\rangle\cdot\mathrm{d}\mathbf{l}$, gauge invariant modulo 2π ($|\phi\rangle$ single-valued). Stokes requires **A** smooth on $\mathcal{S}$.

Analogy with the Aharonov–Bohm effect: **A** $\leftrightarrow$ vector potential, $\mathbf{\Omega} \leftrightarrow$ magnetic field, $\gamma \leftrightarrow$ Aharonov–Bohm phase [1].

Difference: **A** and $\mathbf{\Omega}$ emerge from the geometry of the internal Hilbert space, not from an electromagnetic field acting on the orbital motion.

Berry phase of a spinful particle

Polar angles (θ, φ) of $\mathbf{n}(\mathbf{r})$. Spin 1/2, with the gauge choice

$$|\tfrac{1}{2}\rangle_{\mathbf{n}} = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)\mathrm{e}^{\mathrm{i}\varphi} \end{pmatrix} \quad \Longrightarrow \quad \mathbf{A} = -\hbar \sin^2\left(\frac{\theta}{2}\right) \nabla\varphi, \qquad \mathbf{\Omega} = -\frac{\hbar}{2} \nabla\theta \times (\sin\theta \, \nabla\varphi) \, .$$

This gauge is singular at $\theta = \pi$ (φ undefined, $\sin^2(\theta/2) = 1$): a *Dirac string*, to be avoided by $\mathcal{S}$.
Spin J: $|m = J\rangle_{\mathbf{n}}$ is the symmetric product of $2J$ spins 1/2 along $\mathbf{n}$ $\Rightarrow$ curvature $\times 2J$:

$$\mathbf{\Omega} = -J\hbar \, \nabla\theta \times (\sin\theta \, \nabla\varphi) \, , \qquad \gamma(\mathcal{C}) = -J \int_{\mathcal{S}} \sin\theta \, \nabla\theta \times \nabla\varphi \cdot \mathrm{d}\mathbf{S}.$$

$\gamma(\mathcal{C}) = -J \, \Omega(\mathcal{C})$, $\Omega(\mathcal{C})$: signed solid angle swept by $\mathbf{n}$ on the unit sphere

- As the particle moves, $\mathbf{n}$ traces a path on the Bloch sphere: the phase measures the enclosed solid angle.
- $\Omega(\mathcal{C})$ is counted with the orientation inherited from $\mathcal{S}$: negative if swept with the opposite orientation. This sign cannot be inferred from the swept area alone.

Engineering a synthetic magnetic monopole

Quadrupolar magnetic field, divergence-free, vanishing only at the origin:

$$\mathbf{B}(\mathbf{r}) = b'(x, y, -2z), \qquad b' > 0.$$

On a closed surface $\mathcal{S}$ enclosing the origin, $\mathbf{n}$ covers the unit sphere once, $|\Omega| = 4\pi$.
Sign. $\mathbf{r} \mapsto (x, y, -2z)$ has determinant $-2 < 0$: orientation reversed, degree -1. Explicitly, sphere of radius R, polar angles (α, β): $\varphi = \beta$ and

$$\cos\theta = \frac{-2\cos\alpha}{\sqrt{\sin^2\alpha + 4\cos^2\alpha}} \quad \Longrightarrow \quad \Omega = \int_0^{2\pi} \mathrm{d}\beta \int_0^{\pi} \sin\theta \, \frac{\mathrm{d}\theta}{\mathrm{d}\alpha} \, \mathrm{d}\alpha = -2\pi \Big[\cos\theta \Big]_{\alpha=0}^{\alpha=\pi} = -4\pi.$$

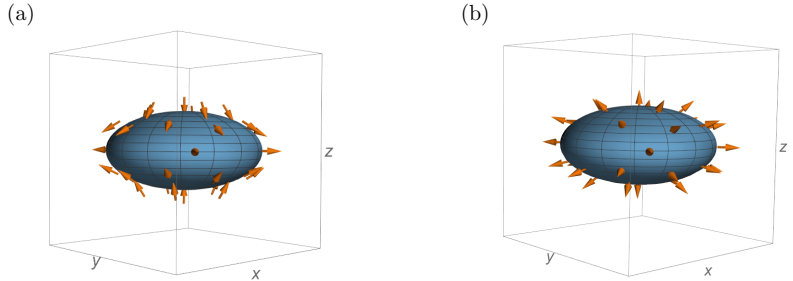
North pole of $\mathcal{S} \mapsto$ south pole of the Bloch sphere.

Flux of the Berry curvature through any surface enclosing the origin

$$\int_{\mathcal{S}} \boldsymbol{\Omega} \cdot \mathrm{d}\mathbf{S} = \hbar\gamma = -J\hbar\,\Omega = 4\pi J\hbar > 0 \quad \text{(outward)}$$

The two minus signs compensate. Reversing b' maps $\mathbf{n} \to -\mathbf{n}$ and flips the monopole charge.

Origin of the monopole



(a) Quadrupolar field: surface of constant $|\mathbf{B}|$ and field orientation. (b) Berry curvature on the same surface: outward, with nonzero total flux.

- At $\mathbf{r} = \mathbf{0}$, $\mathbf{B} = \mathbf{0}$: the direction $\mathbf{n}$ is undefined, $|\phi(\mathbf{r})\rangle$ cannot be defined smoothly — a degeneracy of the internal Hamiltonian.
- Away from degeneracies, $\nabla \cdot \mathbf{\Omega} = 0$, as for a magnetic field. A nonzero total flux appears only if the enclosed region contains such a singular point.
- Realized with ultracold atoms carrying a magnetic moment in a quadrupolar field [2].

Short-time dynamics: Fermi's golden rule

Discrete state $|\psi_0\rangle$ of $\hat{H}_0$ (energy E_0), coupled by a weak $\hat{V}$ to a continuum $|\psi_f\rangle$ (energies E_f):

$$\hat{U}(t) = \hat{U}_0(t) + \frac{1}{\mathrm{i}\hbar}\int_0^t \hat{U}_0(t-\tau)\hat{V}\hat{U}(\tau)\,\mathrm{d}\tau.$$

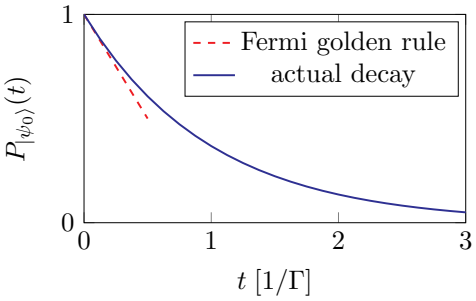
Lowest order, $\hat{U}(\tau) \to \hat{U}_0(\tau) = \mathrm{e}^{-\mathrm{i}\hat{H}_0\tau/\hbar}$:

$$P_{\psi_f}(t) = \frac{|\langle\psi_f|\hat{V}|\psi_0\rangle|^2 t^2}{\hbar^2}\,\mathrm{sinc}^2\left(\frac{(E_0-E_f)t}{2\hbar}\right).$$

Long times, yet $\Gamma t \ll 1$: $t\,\mathrm{sinc}^2(\cdots) \to 2\pi\hbar\,\delta(E_0-E_f)$ (smooth ρ_E and matrix elements over $\hbar/t$):

Fermi's golden rule

$$P_{\psi_0}(t) \simeq 1-\Gamma t, \qquad \Gamma = \frac{2\pi}{\hbar}\overline{|\langle\psi_f|\hat{V}|\psi_0\rangle|^2}\,\rho_E(E_0)$$



Only the initial rate, not an exponential law. Obtaining $P_{\psi_0}(t) \simeq \mathrm{e}^{-\Gamma t}$ requires the back-action of the continuum on $|\psi_0\rangle$ → resolvent.

The resolvent and the retarded Green function

$$\hat{G}(z) = \frac{1}{z - \hat{H}}, \qquad z \in \mathbb{C},$$

analytic away from the (real) spectrum of $\hat{H}$: eigenvalues $\to$ poles, continua $\to$ branch cuts.

Retarded Green function: $\mathrm{i}\hbar\partial_t \hat{U}_+(t) = \hat{H}\hat{U}_+(t) + \mathrm{i}\hbar\,\delta(t)$, with $\hat{U}_+(t) = 0$ for $t < 0$, i.e. $\hat{U}_+(t) = \hat{U}(t)\Theta(t)$.

Its Fourier transform is the resolvent just above the real axis ($\eta \to 0^+$ ensures convergence):

$$\hat{G}(E + \mathrm{i}\eta) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty} \hat{U}_+(t)\,\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\eta)t/\hbar}\,\mathrm{d}t = \frac{1}{E + \mathrm{i}\eta - \hat{H}}.$$

Inversion, with $z = E + \mathrm{i}\eta$ running on the line $\mathrm{Im}\, z = \eta$:

$$\hat{U}_+(t) = \int_{\mathcal{C}_+} \mathrm{e}^{-\mathrm{i}zt/\hbar}\,\hat{G}(z)\,\frac{\mathrm{d}z}{2\mathrm{i}\pi},$$

where $\mathcal{C}_+$ is the line $\mathrm{Im}\, z = \eta$, traversed from $+\infty$ to $-\infty$.

Integration contour and analytic structure

Closing the contour. $|e^{-izt/\hbar}| = e^{t\ \mathrm{Im}\, z/\hbar}$:

- $t > 0$: close below (counterclockwise):

$$\hat{U}_+(t) = \sum_j \operatorname*{Res}_{z=z_j} \left[e^{-izt/\hbar} \hat{G}(z) \right];$$

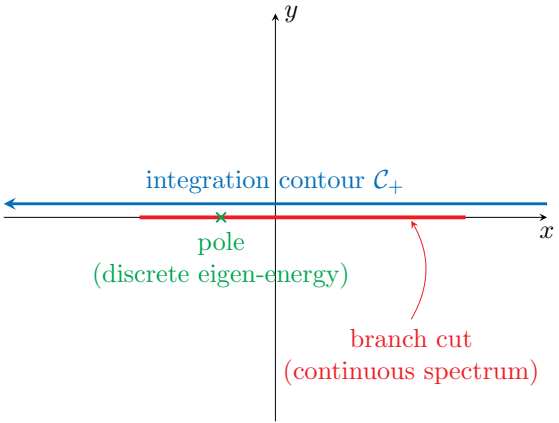
- $t < 0$: close above, no singularity: $\hat{U}_+(t) = 0$.
  η encodes causality.

Spectral decomposition ($\langle \psi_E | \psi_{E'} \rangle = \delta(E - E')$):

$$\hat{G}(z) = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{z - E_n} + \int \frac{|\psi_E\rangle\langle\psi_E|}{z - E}\, \mathrm{d}E.$$

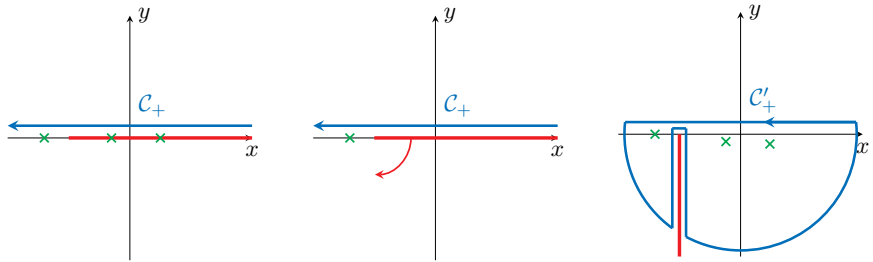
On the continuum, two different boundary values:

$$\frac{1}{E - E' \pm i\eta} = \mathcal{P}\frac{1}{E - E'} \mp i\pi\delta(E - E').$$



Poles (green crosses): discrete eigenvalues, residue $|\phi_n\rangle\langle\phi_n|$. Branch cut (red): continuous spectrum. Contour $\mathcal{C}_+$ in blue.

Resonance pole: analytic continuation



Survival amplitude: $A(t) = \langle\psi_0|\hat{U}_+(t)|\psi_0\rangle = \displaystyle\int_{\mathcal{C}_+} \mathrm{e}^{-\mathrm{i}zt/\hbar}\langle\psi_0|\hat{G}(z)|\psi_0\rangle \frac{\mathrm{d}z}{2\mathrm{i}\pi}$.

- (a)→(b): with $\hat{V}$, the pole E_0 embedded in the continuum disappears from the physical sheet.
- (c): continuing $\hat{G}'(z)$ through the cut reveals a resonance pole $E'_0 = E_0 + \hbar\,(\Delta_0 - \mathrm{i}\Gamma_0/2)$ — *not* an eigenvalue of $\hat{H}$, whose spectrum remains real.
- Deforming $\mathcal{C}_+ \to \mathcal{C}'_+$ and neglecting the branch-cut contribution (broad continuum):

$$A(t) \simeq Z_0\,\mathrm{e}^{-\mathrm{i}(E_0/\hbar+\Delta_0)t}\,\mathrm{e}^{-\Gamma_0 t/2} \underset{Z_0\simeq 1}{\Longrightarrow} P_{\psi_0}(t) \simeq \mathrm{e}^{-\Gamma_0 t}.$$

Projected resolvent and effective Hamiltonian

$\hat{P} = |\psi_0\rangle\langle\psi_0|$, $\hat{Q} = \mathbb{1} - \hat{P}$. Same block elimination as for the effective Hamiltonian, exact:

$$\hat{P}\hat{G}(z)\hat{P} = \hat{P}\frac{1}{z - \hat{H}_{\text{eff}}(z)}\hat{P}, \qquad \hat{H}_{\text{eff}}(z) = \hat{P}\hat{H}\hat{P} + \hat{P}\hat{V}\hat{Q}\frac{1}{z - \hat{Q}\hat{H}\hat{Q}}\hat{Q}\hat{V}\hat{P}.$$

Poles: $z = \langle\psi_0|\hat{H}_{\text{eff}}(z)|\psi_0\rangle$ (self-consistent); near E_0, the resonance pole $z_0 \equiv E_0'$.

Close to the continuum, $z = E + \mathrm{i}\eta$:

$$\hat{H}_{\text{eff}}(E + \mathrm{i}\eta) = \hat{P}\hat{H}\hat{P} + \hbar\hat{\Delta}(E) - \frac{\mathrm{i}\hbar}{2}\hat{\Gamma}(E),$$

$$\hbar\hat{\Delta}(E) = \hat{P}\hat{V}\hat{Q}\,\mathcal{P}\left(\frac{1}{E - \hat{Q}\hat{H}\hat{Q}}\right)\hat{Q}\hat{V}\hat{P}, \qquad \hat{\Gamma}(E) = \frac{2\pi}{\hbar}\hat{P}\hat{V}\hat{Q}\,\delta(E - \hat{Q}\hat{H}\hat{Q})\,\hat{Q}\hat{V}\hat{P}.$$

- $\hat{H}_{\text{eff}}$ is non-Hermitian on the real axis: the eliminated continuum acts as a reservoir ($\hat{H}$ itself stays Hermitian).
- Kramers–Kronig: $\hat{\Delta}(E) = \frac{1}{2\pi}\int \mathcal{P}\left(\frac{1}{E - E'}\right)\hat{\Gamma}(E')\,\mathrm{d}E'$ — shift and rate are the real and imaginary parts of a single self-energy.

Broad-continuum approximation: exponential decay

If $\hat{\Delta}(E)$, $\hat{\Gamma}(E)$ vary slowly over the resonance width: evaluate them at E_0 (on-shell or broad-continuum approximation), and to second order in $\hat{V}$ ($\hat{Q}\hat{H}\hat{Q} \to \hat{Q}\hat{H}_0\hat{Q}$):

$$\hbar\Delta_0 = \int |\langle\psi_k|\hat{V}|\psi_0\rangle|^2\, \mathcal{P}\frac{1}{E_0 - E_k}\,\mathrm{d}k, \qquad \Gamma_0 = \frac{2\pi}{\hbar}\int |\langle\psi_k|\hat{V}|\psi_0\rangle|^2\, \delta(E_0 - E_k)\,\mathrm{d}k :$$

the second-order Lamb shift and Fermi's golden rule. From $\frac{1}{E_0 - E_k + \mathrm{i}\eta} = \mathcal{P}\frac{1}{E_0 - E_k} - \mathrm{i}\pi\delta(E_0 - E_k)$: virtual (off-resonant) transitions shift the level, on-shell transitions make it decay.

Breit–Wigner resolvent:

$$\langle\psi_0|\hat{G}(E + \mathrm{i}\eta)|\psi_0\rangle \simeq \frac{1}{E - E_0 - \hbar\Delta_0 + \mathrm{i}\hbar\Gamma_0/2}$$

$$\langle\psi_0|\hat{U}(t)|\psi_0\rangle \simeq \mathrm{e}^{-\mathrm{i}(E_0/\hbar + \Delta_0)t}\,\mathrm{e}^{-\Gamma_0 t/2}, \qquad P_{\psi_0}(t) \simeq \mathrm{e}^{-\Gamma_0 t} :$$

the golden-rule rate is the imaginary part of the resonance pole.

Fails when $\Delta(E)$, $\Gamma(E)$ vary over the width: band edge, sharp resonance, photonic bandgap $\to$ keep $\hat{H}_{\mathrm{eff}}(z)$ self-consistently, non-exponential decay.

The Wigner–Weisskopf model

Exactly solvable [3]: a discrete state $|\phi\rangle$ coupled to a continuum $|\psi_E\rangle$, $\langle\psi_E|\psi_{E'}\rangle = \delta(E - E')$,

$$\hat{H}_0 = E_0|\phi\rangle\langle\phi| + \int_{E_{\min}}^{E_{\max}} E|\psi_E\rangle\langle\psi_E|\,\mathrm{d}E, \qquad \hat{V} = \int_{E_{\min}}^{E_{\max}} [V_0(E)|\psi_E\rangle\langle\phi| + V_0^*(E)|\phi\rangle\langle\psi_E|]\,\mathrm{d}E.$$

The density of states is absorbed in the energy normalization: $|V_0|^2$ is an energy.

Since $\hat{Q}\hat{V}\hat{Q} = 0$:

$$\langle\phi|\hat{H}_{\text{eff}}(z)|\phi\rangle = E_0 + \int_{E_{\min}}^{E_{\max}} \frac{|V_0(E)|^2}{z - E}\,\mathrm{d}E \underset{V_0(E)=V_0}{=} E_0 + |V_0|^2 \log\left(\frac{E_{\min} - z}{E_{\max} - z}\right).$$

Exact projected resolvent

$$\langle\phi|\hat{G}(z)|\phi\rangle = \frac{1}{z - E_0 - |V_0|^2 \log\left(\frac{E_{\min} - z}{E_{\max} - z}\right)}$$

Contains the full dynamics: poles → dressed states or resonances; branch cut $[E_{\min}, E_{\max}]$ → continuum. $\langle\phi|\hat{U}(t)|\phi\rangle$ follows from a single contour integral.

Infinite band: exact exponential decay

Symmetric limit $E_{\min} = -E_{\max} \to -\infty$ (otherwise the real part diverges logarithmically):

$$\log\left(\frac{E_{\min} - z}{E_{\max} - z}\right) \longrightarrow -\mathrm{i}\pi \quad (\mathrm{Im}\, z > 0), \qquad +\mathrm{i}\pi \quad (\mathrm{Im}\, z < 0)\,:$$

a jump of $2\mathrm{i}\pi$ across the real axis, i.e. the branch cut. On the physical sheet:

$$\langle\phi|\hat{G}(z)|\phi\rangle = \frac{1}{z - E_0 + \mathrm{i}\hbar\Gamma/2}, \qquad \Gamma = \frac{2\pi}{\hbar}|V_0|^2 \quad \text{(Fermi's golden rule)}.$$

- A rational function: its analytic continuation $\hat{G}'(z)$ through the cut is the same formula $\to$ resonance pole $z_0 = E_0 - \mathrm{i}\hbar\Gamma/2$ on the second sheet.
- Not to be confused with $\hat{G}(z)$ evaluated below the cut, $1/(z - E_0 - \mathrm{i}\hbar\Gamma/2)$, whose pole lies in the upper half plane and is never reached.

$$\langle\phi|\hat{U}(t)|\phi\rangle = \mathrm{e}^{-\mathrm{i}E_0 t/\hbar}\,\mathrm{e}^{-\Gamma t/2}, \qquad P_\phi(t) = \mathrm{e}^{-\Gamma t} \quad \text{exactly.}$$

No Lamb shift: the continuum is perfectly symmetric and unbounded.

Finite bandwidth: Lamb shift and validity

Level outside the continuum ($E_0 < E_{\min}$): no resonant state, $\Gamma_0 = 0$, but

$$\Delta_0 = \frac{|V_0|^2}{\hbar} \int_{E_{\min}}^{E_{\max}} \frac{\mathrm{d}E}{E_0 - E} = \frac{|V_0|^2}{\hbar} \log \left| \frac{E_{\min} - E_0}{E_{\max} - E_0} \right| < 0 :$$

the level is repelled by the continuum and remains a true discrete eigenstate.

Level inside the continuum ($E_{\min} < E_0 < E_{\max}$), weak coupling and broad continuum:

$$\Delta_0 = \frac{|V_0|^2}{\hbar} \mathcal{P} \int_{E_{\min}}^{E_{\max}} \frac{\mathrm{d}E}{E_0 - E} = \frac{|V_0|^2}{\hbar} \log \left| \frac{E_0 - E_{\min}}{E_{\max} - E_0} \right|, \qquad \Gamma_0 = \frac{2\pi}{\hbar} |V_0|^2 = \Gamma,$$

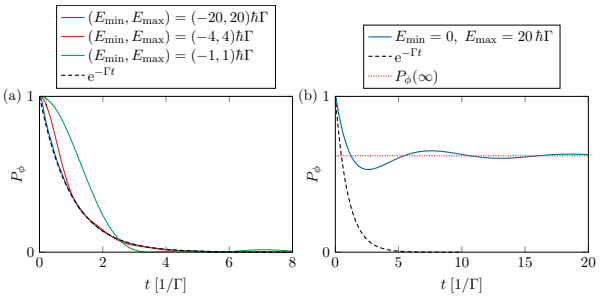
resonance pole $z_0 \simeq E_0 + \hbar\Delta_0 - \mathrm{i}\hbar\Gamma_0/2$ on the second sheet: a metastable state.

Validity: resonance far from the band edges

$$\hbar|\Delta_0|, \ \hbar\Gamma_0 \ll \min(E_0 - E_{\min}, E_{\max} - E_0)$$

Otherwise the energy dependence of the self-energy matters and the Breit–Wigner description breaks down.

Beyond the exponential regime



$P_\phi(t)$ for E_0 (a) in the middle, (b) at the lower edge of the continuum. Dashed: $e^{-\Gamma t}$ (infinite band). Dotted: plateau $P_\phi(\infty)$.

Branch points at $E_{\min}$, $E_{\max}$ contribute besides the pole:

- intermediate times: pole, $P_\phi \simeq e^{-\Gamma_0 t}$;
- very long times: branch cut, algebraic decay.

Exponential decay is an intermediate-time regime.

Real pole outside the continuum, with a significant weight for a level outside or within $\sim |V_0|^2$ of an edge: a dressed bound state E_b,

$$E_b - E_0 - |V_0|^2 \log \left| \frac{E_{\min} - E_b}{E_{\max} - E_b} \right| = 0,$$

which never decays: $P_\phi(\infty) = |Z_b|^2 > 0$, with Z_b the residue of the pole.

A solvable band-edge model: the dressed bound state

Continuum $[E_{\min}, E_{\max}] = [0, W]$, discrete state at the edge, $E_0 = 0$:

$$\Sigma(z) = |V_0|^2 \int_0^W \frac{\mathrm{d}E}{z - E} = |V_0|^2 \log \frac{z}{z - W}.$$

Bound state $z = E_b = -\epsilon$: $\epsilon = |V_0|^2 \log\left(\frac{\epsilon + W}{\epsilon}\right)$ has exactly one solution, for arbitrarily weak coupling.
A real eigenvalue outside the continuum: no decay.
Perturbation theory fails: $|V_0|^2 \mathcal{P} \int_0^W \mathrm{d}E/(0 - E)$ diverges at the edge. Cured self-consistently, for $|V_0|^2 \ll W$:

$$\epsilon \simeq |V_0|^2 \log \frac{W}{|V_0|^2} \qquad \text{(first order in } |V_0|^2\text{, enhanced by a large logarithm)}.$$

Residue:

$$Z_b = \frac{1}{1 - \Sigma'(E_b)} = \frac{\epsilon(\epsilon + W)}{\epsilon(\epsilon + W) + |V_0|^2 W} \underset{\epsilon \ll W}{\simeq} \frac{L}{L + 1}, \qquad L = \log \frac{W}{|V_0|^2}.$$

$P_\phi(\infty) = |Z_b|^2$: $Z_b \to 1$ only logarithmically. E.g. $W = 100\,|V_0|^2$: $\epsilon \simeq 3.41\,|V_0|^2$, $Z_b \simeq 0.78$, $P_\phi(\infty) \simeq 0.61$.

A solvable band-edge model: non-exponential decay

The weight $1 - Z_b$ in the continuum decays, with spectral density ($z = E + \mathrm{i}\eta$ inside the band)

$$\rho(E) = -\frac{1}{\pi}\,\mathrm{Im}\langle\phi|\hat{G}(E+\mathrm{i}\eta)|\phi\rangle = \frac{|V_0|^2}{\left[E + |V_0|^2 \log\dfrac{W-E}{E}\right]^2 + \pi^2|V_0|^4}.$$

- Not a Lorentzian: suppressed at the edge, $\rho(E) \simeq 1/[|V_0|^2 \log^2(W/E)]$. No pole close to the real axis: no exponential regime at all.
- Long times set by the window $E \lesssim \hbar/t$:

$$\left|A(t) - Z_b\, \mathrm{e}^{-\mathrm{i}E_b t/\hbar}\right| \sim \frac{\hbar}{|V_0|^2\, t\, \log^2(Wt/\hbar)}\,:$$

  plateau $|Z_b|^2$ approached as $1/t$ (up to logs), with oscillations at $\epsilon/\hbar$ (figure (b)).
- State **well inside the band**: a bound state still exists below the edge, but

$$\epsilon \simeq W\, \mathrm{e}^{-E_0/|V_0|^2}, \qquad Z_b \simeq \frac{W}{|V_0|^2}\, \mathrm{e}^{-E_0/|V_0|^2}\,:$$

  exponentially small: the Markovian, exponential description is recovered.

Spontaneous emission in free space

$\Gamma_0 = \frac{2\pi}{\hbar}\overline{|\langle\psi_f|\hat{V}|\psi_0\rangle|^2}\rho_E(E_0)$: the environment controls the decay through the density of states.

Atom with ground state $|g\rangle$ (S) and excited state $|e\rangle$ (P, set by the excitation polarization $\boldsymbol{\epsilon}_{\rm exc}$):

- initial state $|e, \mathbf{0}\rangle$: field in the vacuum;
- final states $|g, 1_{\mathbf{k},\boldsymbol{\epsilon}}\rangle$: one photon, wavevector $\mathbf{k}$, polarization $\boldsymbol{\epsilon} \perp \mathbf{k}$.

Electric-dipole coupling $\hat{V} = -\hat{\mathbf{d}} \cdot \hat{\mathbf{E}}$:

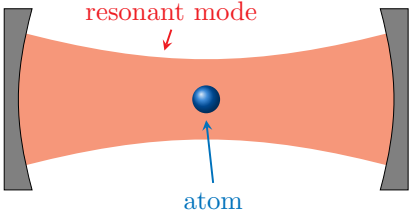
$$\langle e, \mathbf{0}|(-\hat{\mathbf{d}} \cdot \hat{\mathbf{E}})|g, 1_{\mathbf{k},\boldsymbol{\epsilon}}\rangle = -d\,\mathcal{E}_\omega\,\boldsymbol{\epsilon}^*_{\rm exc} \cdot \boldsymbol{\epsilon}, \qquad \mathcal{E}_\omega = \sqrt{\frac{\hbar\omega}{2\epsilon_0 V}}, \quad \omega = ck.$$

Density of states (two polarizations) $\rho_E(E) = \dfrac{VE^2}{\pi^2\hbar^3c^3}$, and $\overline{|\boldsymbol{\epsilon}^*_{\rm exc} \cdot \boldsymbol{\epsilon}|^2} = 1/3$:

$$\Gamma_0 = \frac{\omega_0^3 d^2}{3\pi\epsilon_0\hbar c^3}$$

$\hbar\Gamma_0 \ll \hbar\omega_0$ and ρ_E smooth on the scale $\hbar\omega_0$: broad continuum, exponential decay.

Purcell effect in an optical resonator



The resonator concentrates the density of states around ω_{cav} [4, 5].

Cavity mode with photon loss rate κ:

$$\rho_E(E) = \frac{1}{\pi}\frac{\hbar\kappa/2}{(E-\hbar\omega_{\mathrm{cav}})^2+(\hbar\kappa/2)^2}, \qquad \rho_E(\hbar\omega_0) \underset{\omega_{\mathrm{cav}}=\omega_0}{=} \frac{2}{\pi\hbar\kappa}.$$

$$\Gamma = \frac{4d^2}{\hbar^2\kappa}\left|\epsilon^*_{\mathrm{exc}}\cdot\mathbf{E}_{\mathrm{cav}}(\mathbf{r}_0)\right|^2 = \frac{2d^2\omega_0}{\epsilon_0\hbar\kappa V_{\mathrm{cav}}},$$

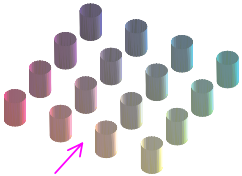
with the mode volume $V_{\mathrm{cav}}\,\epsilon_0 E_{\mathrm{cav}}(\mathbf{r}_0)^2 = \hbar\omega_0/2$ (parallel polarizations).

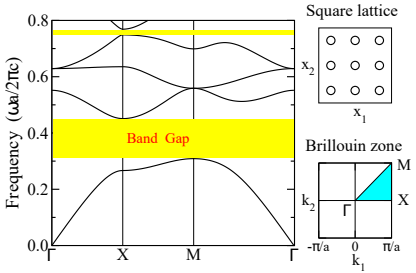
Purcell factor

$$\frac{\Gamma}{\Gamma_0} = \frac{3}{4\pi^2}\frac{\lambda_0^3}{V_{\mathrm{cav}}}\,Q, \qquad Q = \frac{\omega_0}{\kappa}$$

Observed from Rydberg atoms in microwave cavities [6] to quantum dots in microcavities [7]: single-photon sources [8].

Photonic bandgaps: inhibited emission and photon bound states

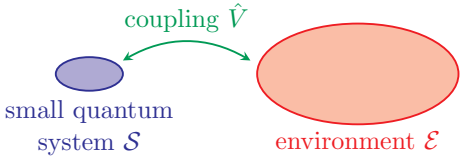




2D photonic crystal of dielectric rods: no propagating mode in the bandgaps (yellow).

- ω_0 **inside a gap**: no resonant photon mode, $\Gamma_0 = 0$: inhibited spontaneous emission [9, 10, 11, 12]. Virtual transitions still shift the level.
- ω_0 **close to a band edge**: rapidly varying density of states, the broad-continuum approximation fails. As in the band-edge Wigner–Weisskopf model: non-exponential decay, and a real pole outside the continuum, a photon bound state keeping part of the excitation near the emitter [13, 14, 15, 16, 17, 18].

Open quantum systems



So far: $\mathcal{H} = \mathcal{H}_A \oplus \mathcal{H}_B$; eliminating $\mathcal{H}_B$ gives an effective Hamiltonian in $\mathcal{H}_A$.

Now: a subsystem coupled to an environment,

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E, \qquad \hat{H} = \hat{H}_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \hat{H}_E + \hat{V}.$$

The environment is not an alternative state of $\mathcal{S}$, but additional degrees of freedom that become entangled with it.

State of the subsystem: reduced density operator (reminder in Appendix A)

$$\hat{\rho}_S = \mathrm{Tr}_E(\hat{\rho}).$$

In general, $\hat{\rho}_S$ follows neither a unitary Schrödinger equation, nor an evolution generated by a Hermitian effective Hamiltonian alone: relaxation and decoherence.

Same idea as before: eliminate unobserved degrees of freedom. But the environment has its own dynamics and keeps information on $\mathcal{S}$: not only energy shifts, but also dissipation and decoherence.

A two-level system coupled to a continuum

Two-level subsystem $\{|g\rangle, |e\rangle\}$, environment initially in $|0_E\rangle$, coupling

$$\hat{V} = \hbar \int \left[g_\omega \, \hat{\sigma}_- \otimes \hat{b}_\omega^\dagger + g_\omega^* \, \hat{\sigma}_+ \otimes \hat{b}_\omega \right] \mathrm{d}\omega, \qquad \hat{\sigma}_- = |g\rangle\langle e|, \quad \hat{\sigma}_+ = |e\rangle\langle g|,$$

$\hat{b}_\omega^\dagger$: creates an excitation in the environment mode of frequency ω. With $[\hat{b}_\omega, \hat{b}_{\omega'}^\dagger] = \delta(\omega - \omega')$, $|g_\omega|^2$ is a rate.

Starting from $|e\rangle \otimes |0_E\rangle$, the dynamics stays in the single-excitation sector

$$\mathcal{H}_1 = \mathrm{span}\{|e, 0_E\rangle\} \oplus \mathrm{span}\{|g, 1_\omega\rangle\}_\omega :$$

a discrete state coupled to a continuum, as in the previous section. Physically: $|e, 0_E\rangle \to |g, 1_\omega\rangle$ is the decay of $|e\rangle$ with emission of an excitation into the environment.

Weak coupling, broad continuum (resolvent):

$$\langle e, 0_E | \hat{U}(t) | e, 0_E \rangle \simeq \mathrm{e}^{-\mathrm{i}(E_e/\hbar + \Delta)t} \mathrm{e}^{-\Gamma t/2} \quad \Rightarrow \quad \rho_{ee}(t) = \langle e | \hat{\rho}_S(t) | e \rangle = \mathrm{e}^{-\Gamma t}.$$

Goal: an equation of motion for the density matrix $\hat{\rho}_S(t)$ itself.

The Wigner–Weisskopf model: memory kernel

ω now denotes the detuning from the atomic frequency ω_0; uniform coupling $g_\omega = g > 0$ for $-W/2 < \omega < W/2$. Exact ansatz:

$$|\Psi(t)\rangle = c_e(t)|e,0\rangle + \int_{-W/2}^{W/2} \mathrm{d}\omega\; c_\omega(t) \mathrm{e}^{-\mathrm{i}\omega t} |g, 1_\omega\rangle,$$

$$\dot{c}_e = -\mathrm{i}g \int_{-W/2}^{W/2} \mathrm{d}\omega\, c_\omega(t) \mathrm{e}^{-\mathrm{i}\omega t}, \qquad \dot{c}_\omega = -\mathrm{i}g\, c_e(t) \mathrm{e}^{\mathrm{i}\omega t} \;\Rightarrow\; c_\omega(t) = -\mathrm{i}g \int_0^t \mathrm{d}\tau\, c_e(\tau) \mathrm{e}^{\mathrm{i}\omega\tau}.$$

Closed, still exact, integro-differential equation:

$$\dot{c}_e(t) = -\int_0^t \mathrm{d}\tau\; K(t-\tau)\, c_e(\tau), \qquad K(s) = g^2 \int_{-W/2}^{W/2} \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega s} = g^2 W \,\mathrm{sinc}\left(\frac{Ws}{2}\right).$$

- The whole influence of the environment is encoded in the memory kernel $K(s)$.
- K decays over the correlation time $\tau_E \sim 1/W$.
- Its weight does not depend on W: $\int_{-\infty}^{\infty} K(s)\,\mathrm{d}s = 2\pi g^2$, so that $K(s) \xrightarrow[W\to\infty]{} 2\pi g^2\, \delta(s)$.

The Markov approximation

In terms of the delay $s = t - \tau$:

$$\dot{c}_e(t) = -\int_0^t \mathrm{d}s\; K(s)\, c_e(t-s).$$

Markov approximation: replace $c_e(t-s)$ by $c_e(t)$, and extend the integral to $s \to \infty$:

$$\dot{c}_e(t) = -\left[\int_0^\infty \mathrm{d}s\, K(s)\right] c_e(t) = -\frac{\Gamma}{2}\, c_e(t), \qquad \Gamma \equiv 2\pi g^2 \qquad \Rightarrow \qquad c_e(t) = \mathrm{e}^{-\Gamma t/2}.$$

- Γ: Fermi's golden rule. Broad continuum means precisely $W \gg \Gamma$.
- No Lamb shift, $\Delta = 0$: the band is symmetric about resonance.

Short times. Expanding the exact equation for $t \to 0$: quadratic (Zeno) behaviour

$$|c_e(t)|^2 \simeq 1 - K(0)\, t^2, \qquad K(0) = g^2 W,$$

which crosses over to the exponential decay only for $t \gtrsim \tau_E \sim 1/W$.
Any Markovian description is coarse-grained in time.

From amplitudes to the reduced density matrix

Arbitrary initial state $(c_g|g\rangle + c_e|e\rangle) \otimes |0\rangle$, with $|g,0\rangle$ stationary, and the survival amplitude

$$A(t) \equiv \langle e,0|\hat{U}(t)|e,0\rangle = \mathrm{e}^{-\mathrm{i}\omega_0 t} c_e(t), \qquad |\Psi(t)\rangle = c_g|g,0\rangle + c_e\, A(t)|e,0\rangle + c_e|g\rangle \otimes |\varphi(t)\rangle,$$

with $|\varphi(t)\rangle$ a one-excitation state of the environment, $\langle\varphi|\varphi\rangle = 1 - |A|^2$, $\langle 0|\varphi\rangle = 0$.

The environment ends up in two orthogonal states, $|0\rangle$ and $|\hat{\varphi}\rangle = |\varphi\rangle/\sqrt{1-|A|^2}$:

$$|\Psi(t)\rangle = |\chi_0(t)\rangle \otimes |0\rangle + |\chi_1(t)\rangle \otimes |\hat{\varphi}(t)\rangle, \qquad \begin{cases} |\chi_0\rangle = c_g|g\rangle + c_e\, A(t)|e\rangle & \text{no photon emitted} \\ |\chi_1\rangle = c_e\sqrt{1-|A(t)|^2}\,|g\rangle & \text{one photon emitted} \end{cases}$$

Partial trace: the cross terms vanish since $\langle\hat{\varphi}|0\rangle = 0$,

$$\hat{\rho}_S(t) = \mathrm{Tr}_E|\Psi(t)\rangle\langle\Psi(t)| = |\chi_0(t)\rangle\langle\chi_0(t)| + |\chi_1(t)\rangle\langle\chi_1(t)|.$$

A sum of two branches, without interference: the environment has kept a record of which branch occurred.

Kraus decomposition

$|\chi_{0,1}\rangle$ are linear in $|\psi_0\rangle = c_g|g\rangle + c_e|e\rangle$: $|\chi_i(t)\rangle = \hat{M}_i(t)|\psi_0\rangle$, with

$$\hat{M}_0 = |g\rangle\langle g| + A(t)|e\rangle\langle e|, \qquad \hat{M}_1 = \sqrt{1-|A(t)|^2}\,\hat{\sigma}_-.$$

Kraus decomposition (any initial $\hat{\rho}_S(0)$, environment in its vacuum)

$$\hat{\rho}_S(t) = \hat{M}_0(t)\,\hat{\rho}_S(0)\,\hat{M}_0^\dagger(t) + \hat{M}_1(t)\,\hat{\rho}_S(0)\,\hat{M}_1^\dagger(t), \qquad \hat{M}_0^\dagger\hat{M}_0 + \hat{M}_1^\dagger\hat{M}_1 = \mathbb{1}.$$

Trace preserving and completely positive: $\hat{\rho}_S(t)$ is a legitimate density matrix.

$$\rho_{ee}(t) = |A(t)|^2\rho_{ee}(0), \qquad \rho_{eg}(t) = A(t)\,\rho_{eg}(0), \qquad \rho_{gg}(t) = \rho_{gg}(0) + \left[1-|A(t)|^2\right]\rho_{ee}(0).$$

- $\hat{M}_1 \propto \hat{\sigma}_-$: an excitation is emitted into the environment, the quantum jump.
- $\hat{M}_0$: no emission. Not unitary ($|A| < 1$): microscopic origin of the non-Hermitian effective Hamiltonian.

Infinitesimal time step: the Lindblad equation

Markovian regime, $A(t) = \mathrm{e}^{-\mathrm{i}\omega_0 t}\mathrm{e}^{-\Gamma t/2}$. To first order in $\mathrm{d}t$:

$$\hat{M}_0 = \mathbb{1} - \left[\mathrm{i}\omega_0 + \frac{\Gamma}{2}\right]\hat{\sigma}_+\hat{\sigma}_-\mathrm{d}t = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\hat{H}_{\mathrm{eff}}\,\mathrm{d}t, \qquad \hat{M}_1 = \sqrt{\Gamma\,\mathrm{d}t}\;\hat{\sigma}_- = \sqrt{\mathrm{d}t}\;\hat{L},$$

$$\hat{H}_{\mathrm{eff}} = \hbar\omega_0\,\hat{\sigma}_+\hat{\sigma}_- - \frac{\mathrm{i}\hbar\Gamma}{2}\hat{\sigma}_+\hat{\sigma}_-, \qquad \hat{L} = \sqrt{\Gamma}\,\hat{\sigma}_- \quad \text{(jump operator)}.$$

The $\sqrt{\mathrm{d}t}$ scaling is the signature of the Markov limit: it makes the jump term first order in $\mathrm{d}t$.

With $\hat{H}_S = \hbar\omega_0\hat{\sigma}_+\hat{\sigma}_-$:

Lindblad equation

$$\partial_t\hat{\rho}_S = -\frac{\mathrm{i}}{\hbar}\left[\hat{H}_S, \hat{\rho}_S\right] + \hat{L}\hat{\rho}_S\hat{L}^\dagger - \frac{1}{2}\left\{\hat{L}^\dagger\hat{L}, \hat{\rho}_S\right\}$$

$\partial_t\rho_{ee} = -\Gamma\rho_{ee}$, $\partial_t\rho_{eg} = -\left(\frac{\Gamma}{2} + \mathrm{i}\omega_0\right)\rho_{eg}$: coherences decay twice as slowly as populations ($\rho_{eg} \propto A$, $\rho_{ee} \propto |A|^2$).

Band not centred on resonance: additional Lamb shift $\hat{H}_{\mathrm{LS}} = \hbar\Delta\,\hat{\sigma}_+\hat{\sigma}_-$.

The general Lindblad equation

Several irreversible channels (pairs of levels, photon polarizations...): one jump operator $\hat{L}_k$ each,

$$\partial_t \hat{\rho}_S = -\frac{\mathrm{i}}{\hbar}\left[\hat{H}_S, \hat{\rho}_S\right] + \sum_k \left(\hat{L}_k \hat{\rho}_S \hat{L}_k^\dagger - \frac{1}{2}\left\{\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}_S\right\}\right), \qquad \hat{H}_S = \hat{H}_S^\dagger.$$

- **Linear**, and **preserves Hermiticity** (each term is Hermitian).
- **Trace preserving**: $\mathrm{Tr}(\hat{L}_k \hat{\rho}_S \hat{L}_k^\dagger) = \mathrm{Tr}(\hat{L}_k^\dagger \hat{L}_k \hat{\rho}_S)$ cancels the anticommutator.
- **Completely positive**: with $\hat{H}_{\mathrm{eff}} = \hat{H}_S - \frac{\mathrm{i}\hbar}{2}\sum_k \hat{L}_k^\dagger \hat{L}_k$,

$$\hat{M}_0 = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\hat{H}_{\mathrm{eff}}\mathrm{d}t, \quad \hat{M}_k = \sqrt{\mathrm{d}t}\,\hat{L}_k : \quad \hat{\rho}_S(t+\mathrm{d}t) = \sum_i \hat{M}_i \hat{\rho}_S \hat{M}_i^\dagger, \quad \sum_i \hat{M}_i^\dagger \hat{M}_i = \mathbb{1} + O(\mathrm{d}t^2).$$

Over each $\mathrm{d}t$, a genuine Kraus map.

Conversely, this is the most general generator with these properties:
Gorini–Kossakowski–Sudarshan–Lindblad theorem. Microscopic derivation: next two slides, additional material.

(∗) Microscopic derivation: Born–Markov

$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{V}$. Interaction picture w.r.t. $\hat{H}_S + \hat{H}_E$, integrated once and traced over $\mathcal{E}$ (exact):

$$\partial_t \tilde{\rho}_S(t) = \frac{1}{\mathrm{i}\hbar} \mathrm{Tr}_E[\tilde{V}(t), \tilde{\rho}(0)] - \frac{1}{\hbar^2} \int_0^t \mathrm{Tr}_E \left[\tilde{V}(t), [\tilde{V}(\tau), \tilde{\rho}(\tau)]\right] \mathrm{d}\tau.$$

- **Initial product state** $\tilde{\rho}(0) = \tilde{\rho}_S(0) \otimes \hat{\rho}_E$, $\hat{\rho}_E$ stationary, and $\mathrm{Tr}_E(\tilde{V}\hat{\rho}_E) = 0$: first term vanishes.
- **Born approximation**: large reservoir, weak correlations, $\tilde{\rho}(t) \simeq \tilde{\rho}_S(t) \otimes \hat{\rho}_E$.
- **Markov approximation**: the reservoir correlation function, for $\hat{V} = \hat{S} \otimes \hat{R}$,

$$g(\tau) = \mathrm{Tr}_E \left[\tilde{R}(\tau)\tilde{R}(0)\hat{\rho}_E\right],$$

  decays over $\tau_E \ll \tau_S$ (evolution time of $\tilde{\rho}_S$): $\tilde{\rho}_S(t-\tau) \simeq \tilde{\rho}_S(t)$ and $\int_0^t \to \int_0^\infty$.

$\Rightarrow$ a time-local master equation, with coefficients set by $g(\pm\tau)$: the density-matrix analogue of the broad-continuum approximation.

Not yet manifestly positive: a further step, the secular approximation, is needed.

(∗) Secular approximation and Lindblad form

Transition operators: $\tilde{S}(t) = \sum_\omega e^{i\omega t}\hat{\mathfrak{S}}(\omega)$, with $\hat{\mathfrak{S}}(\omega) = \sum_{\omega_{nn'}=\omega} S_{nn'}|\psi_{n'}\rangle\langle\psi_n|$, $\omega_{nn'} = (E^S_{n'} - E^S_n)/\hbar$.
Secular approximation: drop terms oscillating at $\omega - \omega' \neq 0$ (separations $\gg$ dissipative rates). With

$$\Phi(\omega) = \int_0^\infty e^{-i\omega\tau} g(\tau)\, d\tau, \qquad \gamma(\omega) = \frac{2\,\mathrm{Re}\,\Phi(\omega)}{\hbar^2}, \qquad \hat{H}_{\mathrm{LS}} = \sum_\omega \frac{\mathrm{Im}\,\Phi(\omega)}{\hbar}\hat{\mathfrak{S}}^\dagger(\omega)\hat{\mathfrak{S}}(\omega),$$

$$\partial_t \hat{\rho}_S = \frac{1}{i\hbar}[\hat{H}_S + \hat{H}_{\mathrm{LS}}, \hat{\rho}_S] + \sum_\omega \left[\hat{L}_\omega \hat{\rho}_S \hat{L}_\omega^\dagger - \frac{1}{2}\left\{\hat{L}_\omega^\dagger \hat{L}_\omega, \hat{\rho}_S\right\}\right], \qquad \hat{L}_\omega = \sqrt{\gamma(\omega)}\,\hat{\mathfrak{S}}(\omega).$$

- Rates $\gamma(\omega) \geq 0$: $g(\tau)$ only has positive Fourier components.
- $\hat{H}_{\mathrm{eff}} = \hat{H}_S + \frac{1}{i\hbar}\sum_\omega \Phi(\omega)\hat{\mathfrak{S}}^\dagger\hat{\mathfrak{S}} \simeq \sum_m \Pi_m \hat{H}^{(m)}_{\mathrm{eff}}$: reservoir average of the resolvent effective Hamiltonians.
- Validity: weak coupling (Born), $\tau_E \ll \tau_S$ (Markov), well-separated transitions (secular).

Quantum trajectories

With $\hat{H}_{\text{eff}} = \hat{H}_S - \frac{i\hbar}{2}\sum_k \hat{L}_k^\dagger \hat{L}_k$, the Lindblad equation reads

$$\partial_t \hat{\rho}_S = \frac{1}{i\hbar}\left(\hat{H}_{\text{eff}}\hat{\rho}_S - \hat{\rho}_S \hat{H}_{\text{eff}}^\dagger\right) + \sum_k \hat{L}_k \hat{\rho}_S \hat{L}_k^\dagger :$$

a deterministic evolution that loses norm, plus jump terms restoring the lost probability.

Kraus operators over dt = outcomes of a measurement on the environment: nothing detected ($\hat{M}_0$), or a quantum of type k detected ($\hat{M}_k$). Following one sequence of outcomes:

Quantum trajectory (pure state $|\psi\rangle$)

1. between jumps: $i\hbar\,\partial_t|\psi\rangle = \hat{H}_{\text{eff}}|\psi\rangle$, renormalized at each step;
2. jump k during dt with probability $dp_k = dt\,\langle\psi|\hat{L}_k^\dagger \hat{L}_k|\psi\rangle$;
3. after the jump: $|\psi\rangle \to \hat{L}_k|\psi\rangle / \sqrt{\langle\psi|\hat{L}_k^\dagger \hat{L}_k|\psi\rangle}$.

Averaging over trajectories reproduces the Lindblad equation exactly, $\hat{\rho}_S(t) = \mathbb{E}_{\text{traj}}\left[|\psi(t)\rangle\langle\psi(t)|\right]$ [19, 20].

Example: a decaying field in an optical cavity

Cavity mode $\hat{H}_S = \hbar\omega\,\hat{a}^\dagger\hat{a}$; a single channel, loss of one photon:

$$\hat{L} = \sqrt{\kappa}\,\hat{a},$$

$$\partial_t\hat{\rho}_S = \frac{1}{\mathrm{i}\hbar}[\hat{H}_S, \hat{\rho}_S] + \kappa\left(\hat{a}\hat{\rho}_S\hat{a}^\dagger - \frac{1}{2}\left\{\hat{a}^\dagger\hat{a}, \hat{\rho}_S\right\}\right).$$

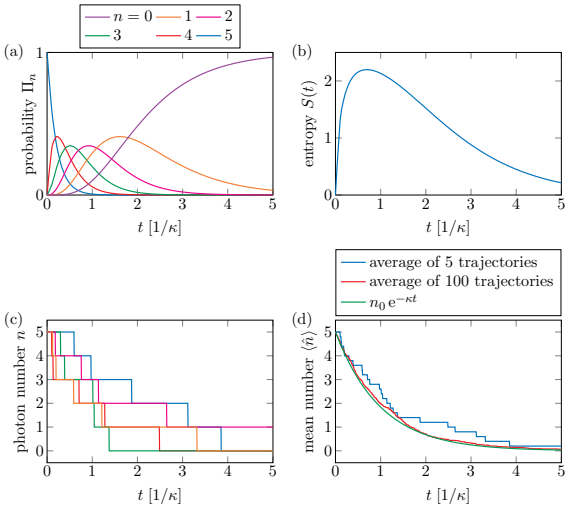
Exactly: $\langle\hat{n}\rangle(t) = \langle\hat{n}\rangle(0)\mathrm{e}^{-\kappa t}$, κ: photon loss rate (cavity linewidth).

Fock state $|n_0\rangle$: $\hat{\rho}_S$ stays diagonal,

$$\Pi_n(t) = \binom{n_0}{n}\mathrm{e}^{-n\kappa t}\left(1-\mathrm{e}^{-\kappa t}\right)^{n_0-n}.$$

Mixed at intermediate times (entropy > 0), then $\hat{\rho}_S \to |0\rangle\langle 0|$.

Finite temperature: second channel $\hat{L}' = \sqrt{\kappa\bar{n}_{\mathrm{th}}}\,\hat{a}^\dagger$; negligible for optical photons at room temperature.



$n_0 = 5$. (a) $\Pi_n(t)$. (b) von Neumann entropy. (c) 5 quantum trajectories. (d) Mean photon number from trajectory averages.

Cavity decay: trajectories, Fock and coherent states

Fock state. Jumps $|n\rangle \to |n-1\rangle$ at rate $\langle n|\hat{L}^\dagger \hat{L}|n\rangle = \kappa n$. Between jumps,

$$\hat{H}_{\text{eff}} = \hbar\left(\omega - \frac{\mathrm{i}\kappa}{2}\right)\hat{n}$$

only reduces the norm of $|n\rangle$ (by $\mathrm{e}^{-n\kappa t/2}$): a trajectory stays in a Fock state, a staircase of jumps at random times. $\mathbb{E}_{\text{traj}}[n(t)] \to \langle\hat{n}\rangle(0)\mathrm{e}^{-\kappa t}$ (figure c, d).

Coherent state $|\alpha_0\rangle$, with $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$:

- a jump leaves it unchanged: $\hat{L}|\alpha\rangle/\|\hat{L}|\alpha\rangle\| = \mathrm{e}^{\mathrm{i}\arg\alpha}|\alpha\rangle$;
- no-jump evolution: $\mathrm{e}^{-\mathrm{i}\hat{H}_{\text{eff}}t/\hbar}|\alpha\rangle \propto |\alpha\,\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{-\kappa t/2}\rangle$.

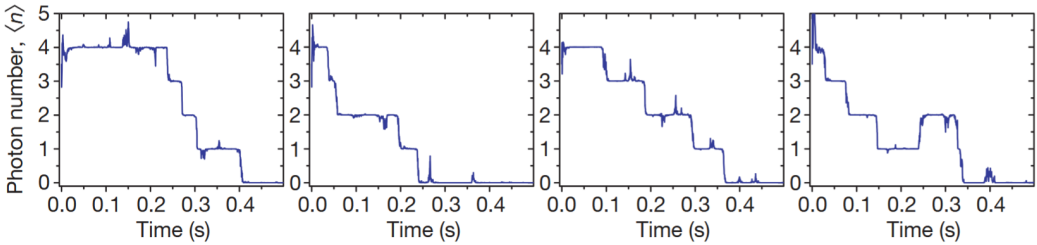
Whatever the jump record, the same state:

$$\hat{\rho}_S(t) = |\alpha(t)\rangle\langle\alpha(t)|, \qquad \alpha(t) = \alpha_0\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{-\kappa t/2}: \quad \text{stays pure.}$$

Jumps still occur (rate $\kappa|\alpha(t)|^2$), but carry no information. Coherent states are the pointer states of the damped oscillator; superpositions of them decohere.

Check: $\mathrm{d}\langle\hat{a}\rangle/\mathrm{d}t = (-\mathrm{i}\omega - \kappa/2)\langle\hat{a}\rangle$; the field decays at $\kappa/2$, half the photon-number rate.

Observing quantum jumps of light



Initial coherent state (~ 4 photons), projected onto a Fock state, then staircase of jumps $|n\rangle \to |n-1\rangle$. Rightmost: an upward step, a thermal photon ($\hat{L}' \propto \hat{a}^\dagger$). From [21].

- Microwave photons in a superconducting cavity, $Q \simeq 4 \times 10^{10}$, $1/\kappa \simeq 0.13\,\mathrm{s}$ [22, 21].
- Circular Rydberg atoms, far detuned: a phase shift $\propto n$, read interferometrically. Quantum non-demolition (QND) measurement of $\hat{n}$.
- Monitoring does not perturb the decay: $[\hat{n}, \hat{H}_S] = 0$, the atoms exchange no energy, and $\hat{H}_{\mathrm{eff}} \propto \hat{n}$ leaves Fock states unchanged. No Zeno effect: $\tau_E \ll$ time between atoms.
- Reading the environment unravels the Lindblad evolution into trajectories. Nobel Prize 2012 [23, 24].

Summary – Chapter 1

- **Effective Hamiltonians**: projecting onto a subspace A gives an energy-dependent $\hat{H}_{\text{eff}}(E)$; at second order, virtual couplings to B. Two-photon (Raman) couplings and light shifts; projection onto the lowest Landau level and Hall drift.
- **Berry phase**: adiabatic following of an internal state gives a gauge field, the Berry connection $\mathbf{A}$, of curvature $\mathbf{\Omega}$; for a spin, a monopole in parameter space and a geometric phase $\propto$ solid angle.
- **Coupling to a continuum**: Fermi's golden rule at short times; the resolvent gives a complex pole, i.e. a level shift and an exponential decay at rate Γ. Deviations near band edges (dressed bound states). Purcell effect, inhibited emission.
- **Open quantum systems**: tracing out the environment gives the Lindblad equation, with jump operators and a non-Hermitian effective Hamiltonian; equivalently, quantum trajectories. Example: quantum jumps of light in a cavity.

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