

Statistical-physics derivation of Fermi's golden rule

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“Fermi's golden rule” refers to first-order time-dependent perturbation theory (Dirac 1927)
 or first Born approximation in scattering theory (Born 1926).

1 . The issue in Schrödinger's quantum dynamics

Complex-valued $\psi(\mathbf{r}, t)$ such that $\int_{\Omega} |\psi|^2 d^3\mathbf{r} = 1$, ruled by $\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} [H_0 + v(\mathbf{r})]\psi$

$\therefore \Omega = \text{box volume}; H_0 \equiv \frac{(-i\hbar\nabla)^2}{2m}; v(\mathbf{r}) = \text{perturbing potential energy.}$

Stationary states of H_0 are $|\mathbf{p}\rangle \equiv \frac{1}{\sqrt{\Omega}} \exp(i\frac{\mathbf{p}\cdot\mathbf{r}}{\hbar}) \therefore \mathbf{p} \in \text{BZ}$ (discretized reciprocal space $\times \hbar$).

Perturbation $v(\mathbf{r})$ entails a transition probability per unit time $\mathbf{p} \rightarrow \mathbf{p}'$,

$$W_{\mathbf{p},\mathbf{p}'} \equiv \frac{2\pi}{\hbar} |(\mathbf{p}'|v|\mathbf{p})|^2 \delta\left(\frac{p'^2}{2m} - \frac{p^2}{2m}\right) \quad \text{“golden rule”} \rightarrow \text{lifetime } \tau(\mathbf{p}) = 1/\int_{\text{BZ}} W_{\mathbf{p},\mathbf{p}'} \frac{\Omega d^3\mathbf{p}'}{h^3}$$

- to the lowest order in $v(\mathbf{r})$;

- conditional upon *small energy uncertainty* $\frac{\hbar}{\tau(\mathbf{p})}$; otherwise $\delta \rightarrow \text{Lorentzian}$.

Textbook derivations : Schiff, Messiah, Cohen-Tannoudji *et al.*, Merzbacher, Ridley, Le Bellac...

2 . The issue in Wigner's **phase space** quantum dynamics

Real-valued $f_W(\mathbf{r}, \mathbf{p}, t)$ such that $\int_{\Omega} \int_{\text{BZ}} f_W(\mathbf{r}, \mathbf{p}, t) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3} = 1$, ruled by

$$\frac{\partial f_W}{\partial t} = -\frac{\mathbf{p}}{m} \cdot \nabla f_W + \frac{1}{i\hbar} \int_{\text{BZ}} f_W(\mathbf{r}, \mathbf{p}', t) v_W(\mathbf{r}, \mathbf{p} - \mathbf{p}') \frac{\Omega d^3\mathbf{p}'}{h^3} \therefore v_W(\mathbf{r}, \mathbf{q}) \equiv \int_{\Omega} [v(\mathbf{r} + \frac{\mathbf{s}}{2}) - v(\mathbf{r} - \frac{\mathbf{s}}{2})] \exp(-\frac{i\mathbf{q} \cdot \mathbf{s}}{\hbar}) \frac{d^3\mathbf{s}}{\Omega}.$$

Population $f(\mathbf{p}, t)$ of state $|\mathbf{p}\rangle = \textit{marginal distribution} \int_{\Omega} f_W(\mathbf{r}, \mathbf{p}, t) \frac{d^3\mathbf{r}}{\Omega}.$

Question: Can one derive a “Pauli master equation” ruling $f(\mathbf{p}, t)$,

i. e.
$$\frac{\partial f}{\partial t} = \int_{\text{BZ}} [W_{\mathbf{p}', \mathbf{p}} f(\mathbf{p}', t) - W_{\mathbf{p}, \mathbf{p}'} f(\mathbf{p}, t)] \frac{\Omega d^3\mathbf{p}'}{h^3} \quad ???$$

Answer:

Simplify Wigner's dynamical equation

taking advantage of the **weakness** and **small range** of $v(\mathbf{r})$

$$v(\mathbf{r}) = v_O(\mathbf{r} - \mathbf{R}) \therefore \mathbf{R} = \textit{centre of force}; \text{ for example, } v_O(\rho) = \mathbf{v}_0 \left(\frac{\rho_0}{\rho} \right) \exp\left(-\frac{\rho}{\rho_0}\right).$$

A given centre \mathbf{R} entails a specific $f_{W, \mathbf{R}}$. Take $\mathbf{R} = \textit{random variable}$ uniformly distributed in Ω . Distinct values $\mathbf{R}_1 \neq \mathbf{R}_2$ yield distinct realisations of random function $f_{W, \mathbf{R}}$ which differ by a term $O(v_0)$, whence

$$f_{\mathbf{W},\mathbf{R}} = \langle f_{\mathbf{W},\mathbf{R}} \rangle + O(v_0)$$

\therefore ensemble average $\langle \dots \rangle \equiv \int_{\Omega} (\dots) \frac{d^3\mathbf{R}}{\Omega}$ does not depend on the choice of \mathbf{R} i.e. the realisation of $v(\mathbf{r})$.

Expand $f_{\mathbf{W},\mathbf{R}}$ in powers of the scaled perturbation strength,

$$f_{\mathbf{W},\mathbf{R}} = f_0 + \eta f_1 + \eta^2 f_2 + O(\eta^3)$$

where

$$\eta \equiv \frac{v_0}{E_{\text{typ}}}, \quad f_0 \equiv \langle f_{\mathbf{W},\mathbf{R}} \rangle \quad \text{and} \quad f_1, f_2 \dots \text{ depend on the choice of } \mathbf{R}.$$

Goal: from the Wigner equation on $f_{\mathbf{W},\mathbf{R}}$, get a *closed-form equation* on f_0 .

Method: multiple-scale expansion based upon $\rho_0 \ll \Omega^{-1/3}$,

$$f_{\mathbf{W}}(\mathbf{r}, \mathbf{r}') = f_0(\mathbf{r}, \mathbf{r}') + \eta f_1(\mathbf{r}, \mathbf{r}') + \eta^2 f_2(\mathbf{r}, \mathbf{r}') + O(\eta^3)$$

where

- $\mathbf{r}' = \varepsilon \mathbf{r}$ = “fast spatial variable” varying on the small scale ρ_0
- \mathbf{r} = formally independent “slow” spatial variable.

One may choose $\varepsilon = \eta^2$ (*). The expansion yields a linear Boltzmann equation ruling $f_0(\mathbf{r}, \mathbf{p})$:

$$\frac{\partial f_0}{\partial t} = -\frac{\mathbf{p}}{m} \cdot \nabla f_0 + \int_{\text{BZ}} W_{\mathbf{p},\mathbf{p}'} [f_0(\mathbf{r}, \mathbf{p}', t) - f_0(\mathbf{r}, \mathbf{p}, t)] \frac{\Omega d^3\mathbf{p}'}{h^3}$$

where $W_{\mathbf{p},\mathbf{p}'}$ is given by the **golden-rule formula**.

- Upon integration over \mathbf{r} ,
- the **Pauli master equation** on populations $f(\mathbf{p})$ ensues, **QED**;
 - **no Lorentzian lifetime broadening** in $W_{\mathbf{p},\mathbf{p}'}$ (the δ function is exact).

(*) E. Bringuier, Disorder-induced quantum-to-classical transition, submitted to *Eur. Phys. J. Web Conf.*