Quantum dynamics of many interacting particles:
Feynman and Schwinger approaches

Nobel prize winners 1965

for fundamental work in quantum electrodynamics, with deep-ploughing consequences for the physics of elementary particles

together with

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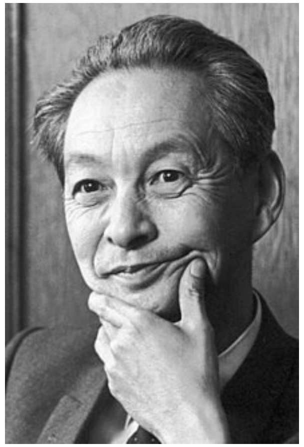

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Layout

- Classical mechanics:
  - A. Equations of motion & conservation laws
  - B. Least action principle
- Quantum mechanics:
  - A. Particle wave duality
  - B. Wave equation & path integral
- Quantum many-body systems:
  - A. Indistinguishable particles — Second quantization & many-body Green functions
  - B. Green functions approach — fundamental Schwinger functional equation0
  - C. Generating functional approach — renormalized perturbation theory via Feynman diagrams

Classical mechanics

Nature's laws are independent of spatial and temporal scaling

Newton's law of particle dynamics

Dynamics of elementary measurable objects

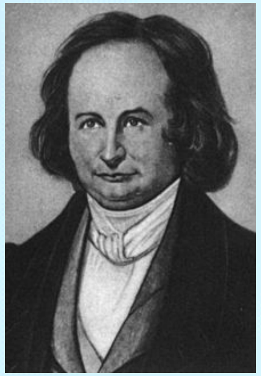
- Extreme downsizing of observables to elementary objects
  - mass point (volume differential — particle) described by a single coordinate vector $\vec{x}$
- Extreme downscaling of time differences — time differential dt (microscopic evolution)
- Acting force $\vec{F}$ determines the dynamics of the mass point

$$m\frac{d^2\vec{x}}{dt^2} = \vec{F}(\vec{x})$$

- Initial conditions at $t = 0$: $\vec{x}, \dot{\vec{x}}$
- Many mass points — superposition principle

$$\sum_{i=1}^{N} m_i \frac{d^2\vec{x}_i}{dt^2} = \vec{F}(\vec{x}_1, \ldots \vec{x}_N)$$

Hamilton & Hamilton-Jacobi equations



- Conserving systems: $\vec{F}(\vec{x}) = -\nabla V(\vec{x})$
- Energy is conserved during dynamics: $\frac{d}{dt}E(\vec{x}(t)) = \frac{d}{dt}\left[\frac{m}{2}\dot{\vec{x}}(t)^2 + V\left(\vec{x}(t)\right)\right] = 0$
- Momentum: $\vec{p} = m\dot{\vec{x}}$ & Hamiltonian: $H(\vec{p},\vec{x}) = \frac{1}{2m}\vec{p}^2 + V(\vec{x})$
- Hamilton equations: First-order differential equations

$$\dot{x}_l(t) = \frac{\partial H}{\partial p_l}\ , \dot{p}_l(t) = -\frac{\partial H}{\partial x_l}$$

- Conserving quantities: α_k (time independent) to replace momentum variables, $p_l = \frac{\partial S(q_k,\alpha_k)}{\partial q_l}$
- Hamilton-Jacobi equations for $S(q_k,\alpha_k;t)$:

$$H\left(\frac{\partial S}{\partial q_k}, q_k; t\right) + \frac{\partial S}{\partial t} = 0$$

Least action (Hamilton) principle — generating functional

- Functional of action on the space of trajectories parametrized by time:

$$\mathscr{A} = \int dt \left[\sum_k p_k(t)\dot{q}_k(t) - H(p_k(t), q_k(t)) \right] = \int dt \mathscr{L}(q_k(t), \dot{q}_k(t))$$

where $\mathscr{L}(q_k, \dot{q}_k)$ is the Lagrangian

- Hamilton (least action) principle

$$\delta\mathscr{A} = \int dt \sum_k \left[\left(\dot{q}_k - \frac{\partial H}{\partial p_k} \right) \delta p_k - \left(\dot{p}_k + \frac{\partial H}{\partial q_k} \right) \delta q_k \right] = 0$$

- Two ways to determine the dynamics of complicated system with many variables
  - ★ Solving the set of Hamilton local differential equations for $q_k(t)$ and $p_k(t)$
  - ★ Minimizing the global functional of action $\mathscr{A}(p_k, q_k)$ in the space of admissible trajectories

The two approaches may differ in approximate solutions

Quantum mechanics

Spatial scaling breaks down at microscopic lengths – discretization

Uncertainty principle - particle-wave dualism

- To solve the Hamilton equations — precise values for coordinates and velocities (momenta) needed
- Heisenberg uncertainty principle: $\Delta q \times \Delta p \geq \frac{\hbar}{2}$
- Localized elementary object (particle) $\Delta q = 0$
- Delocalized elementary object (wave) $\Delta p = 0$
- Particle description — using measurable quantities

Localized objects do not have deterministic evolution

- Wave description — allows for a deterministic evolution

Delocalized waves do not have direct interpretation

Schrödinger equation and Feynman path integral

- Wave function $\psi(\vec{x}, t)$ obeys local Schrödinger differential equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x}, t) = -\left[\frac{\hbar^2}{2m}\nabla^2 - V(\vec{x})\right]\psi(\vec{x}, t)$$

- Coordinates and momenta represented by operators: canonical commutation relations

$$[\hat{x}, \hat{p}] = i\hbar \Rightarrow \hat{p} = -i\hbar\frac{d}{dx}$$

- Action & amplitude for particle trajectories: $K(q, \dot{q}, t) = e^{\frac{i}{\hbar}\int^t dt \mathscr{L}(q(t), \dot{q}(t))}$; each trajectory equally probable
- Quantum interference — amplitude for a transition of a particle between two measurements

$$K(x_0, t_0; x_N, t_N) = \int_{-\infty}^{\infty} dx_1 \ldots \int_{-\infty}^{\infty} dx_{N-1} \exp\left\{\frac{i}{\hbar}\sum_{i=1}^{N}\mathscr{L}\left(x_i, \frac{x_i - x_{i-1}}{\Delta t}\right)\Delta t\right\}, \Delta t = \frac{t_N - t_0}{N}, N \to \infty$$

- Probability of particle transitions: $P(x_0, t_0; x_N, t_N) = |K(x_0, t_0; x_N, t_N)|^2$
- Classical trajectory (most probable) in $\hbar \to 0$ leading to $\delta\mathscr{A} = 0$ (Hamilton-Jacobi)

Many interacting quantum particles

Indistinguishability of identical particles

Second quantization

- Quantum particles are independent ($\mathscr{H}_2 = \mathscr{H}_1 \otimes \mathscr{H}_1$) objects but indistinguishable:

$$|\psi_1, \psi_2 > = \frac{1}{\sqrt{2}} \left[|\psi_1 > |\psi_2 > \pm |\psi_2 > |\psi_1 > \right]$$

- Completeness of the energy spectrum of 1P Hamiltonian: $\hat{1} = \sum_l |\phi_l > < \phi_l|$
- Ordering of energy eigenenergies bounded from below: $0 = E_0 < E_1 < E_2 < \ldots$
- Occupation number representation: $|\phi_i >$ occupied by n_i particles: $|N; n_1, \ldots, n_l, \ldots >$, $N = \sum_i n_i$
- Second quantization: transformation $\mathscr{H}_1 \to \mathscr{H}_{Fock} = \sum_{n=0}^{\infty} \oplus S_\pm \mathscr{H}_1^n$, $\mathscr{H}_0$ – Fock vacuum (cyclic vector with E_0)
- Wave vectors to operators: $|\psi > = \sum_l c_l |\Phi_l > \to \sum_l c_l \hat{a}_l^\dagger$ and $< \psi| = \sum_l c_l^* < \Phi_l| \to \sum_l c_l^* \hat{a}_l$
- Canonical commutation relations: $\left[\hat{a}_l, \hat{a}_k^\dagger\right]_\pm = \hat{a}_l \hat{a}_k^\dagger \pm \hat{a}_k^\dagger \hat{a}_l = \delta_{l,k} \hat{1}$

Many-body Hamiltonian & operator Schödinger equation

- Interacting fermions

$$\hat{H}^{el-el} = \mathscr{V}\int \frac{d^3p}{(2\pi\hbar)^3}\frac{\vec{p}^2}{2m}\hat{a}^\dagger_{\vec{p}}a_{\vec{p}} + \frac{\mathscr{V}}{2}\int \frac{d^3q}{(2\pi\hbar)^3}u(\vec{q}) : \hat{\rho}(\vec{q})\rho(-\vec{q}) :$$

The operator of particle density $\hat{\rho}(\vec{q}) = \int \frac{d^3p}{(2\pi\hbar)^3}\hat{a}^\dagger_{\vec{p}+\vec{q}}\hat{a}_{\vec{p}}$ and interaction strength $u(\vec{q}) = \int d^3r e^{\frac{i}{\hbar}\vec{q}\cdot\vec{r}}U(r)$

- Thermodynamic (grand) potential $\Omega(T,V,\mu) = -k_BT\log\left[\mathrm{Tr}_{Fock}\exp\{-\beta(\hat{H}^{el-el} - \mu\hat{N})\}\right]$
- Grand potential can be understood as an evolution functional in imaginary time $\beta \to \frac{i}{\hbar}t$
- Schrödinger equation for wave operator: $-\hbar\frac{\partial}{\partial\tau}\hat{\psi}(\tau) = \left[\hat{H}_0 + \hat{H}_I\right]\hat{\psi}(\tau)$
- Eigenvectors are known only for $\hat{H}_0$, but not for the full Hamiltonian $\hat{H}_0 + \hat{H}_I$
- Interaction-induced quantum fluctuations due to non-commutativity $\left[\hat{H}_0, \hat{H}_I\right] \neq 0$

Many-body Green functions

- Elementary objects of quantum many-body here are creation and annihilation operators $\hat{a}^\dagger_\lambda$ and $\hat{a}_\lambda$
- These operators are not hermitian, hence non-measurable
- Imaginary-time evolution (Heisenberg): $\hat{a}_\lambda(\tau) = e^{\tau\hat{H}}\hat{a}_\lambda e^{-\tau\hat{H}}$, $\tau \in (0,\beta)$
- Quantum amplitudes for transitions between two "asymptotic" states λ, λ'
- Thermal average of time-ordered product — 1P Green function

$$\mathcal{G}(\lambda, \lambda'; \tau - \tau') = -\frac{1}{\mathcal{Z}}\mathrm{Tr}\left\{ T_\tau \left[\hat{a}_\lambda(\tau)\hat{a}^\dagger_{\lambda'}(\tau')\right] e^{-\beta\left(\hat{H}_0 + \hat{H}_I - \mu\hat{N}\right)}\right\}$$

with partition sum $\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta\left(\hat{H}_0 + \hat{H}_I - \mu\hat{N}\right)}\right]$

- 2P Green function: $\mathcal{G}(\lambda_1, \tau_1\lambda_2, \tau_2, \lambda_3, \tau_3, \lambda_4, \tau_4) = \frac{1}{\mathcal{Z}}\mathrm{Tr}\left\{ T_\tau \left[\hat{a}_{\lambda_1}(\tau_1)\hat{a}_{\lambda_3}(\tau_3)\hat{a}^\dagger_{\lambda_4}(\tau_4)\hat{a}^\dagger_{\lambda_2}(\tau_2)\right] e^{-\beta\left(\hat{H}_0 + \hat{H}_I - \mu\hat{N}\right)}\right\}$

Schwinger approach – equation based

Equations for Green functions

- Schwinger equation matches 1P & 2P Green functions

$$G(1,\bar{1}) = G^{(0)}(1,\bar{1}) + \int d\bar{2}d2G^{(0)}(1,\bar{2})U(\bar{2}-2)G_{(2)}(\bar{1}\bar{2},22)$$

- Dyson equation — 1P self-energy Σ replaces 2P GF in Schwinger equation

$$G(1,\bar{1}) = G^{(0)}(1-\bar{1}) + \int d3d\bar{3}G^{(0)}(1-\bar{3})\Sigma(\bar{3},3)G(3,\bar{1})$$

- 2P Dyson equation — 2P vertex

$$G_{(2)}(1\bar{1},3\bar{3}) = G(1,\bar{1})G(3,\bar{3}) + \int d1'd\bar{1}'d3'd\bar{3}'G(1,\bar{1}')G(1'\bar{1})\Gamma(1'\bar{1}',3'\bar{3}')G(3,\bar{3}')G(3'\bar{3})$$

- Schwinger-Dyson equation

$$\Sigma(\bar{1}-1) = \int d2U(1-2)G(2,2^{+})\delta(1-\bar{1}) - U(1-\bar{1})G(\bar{1}-1)$$

$$-\int d2d\bar{4}d4d3U(1-2)G(4-1)G(2-\bar{4})G(3-2)\Gamma(4,\bar{4},3,\bar{1})$$

Ward identity & Schwinger field theory

- Bethe-Salpeter equations — 2P irreducible vertex Λ (2P self-energy)

$$\Gamma(1,\bar{2},2,\bar{1}) = \Lambda(1,\bar{2},2,\bar{1}) + \int d\bar{3}d3d\bar{4}d4\Lambda(1,\bar{2},3,\bar{3})G(3-\bar{4})G(4-\bar{3})\Gamma(4,\bar{4},2,\bar{1})$$

where $1 = (\vec{p}, \tau, \sigma)$ are particle degrees of freedom when annihilated and $\bar{1}$ when created

- Generalized Ward identity connecting 1P & 2P irreducible vertices (conserving theory)

$$\Lambda(\bar{1},2,\bar{3},3) = \frac{\delta\Sigma(\bar{3},3)}{\delta G(2,\bar{1})}$$

- Putting all exact equations together —> Schwinger field theory

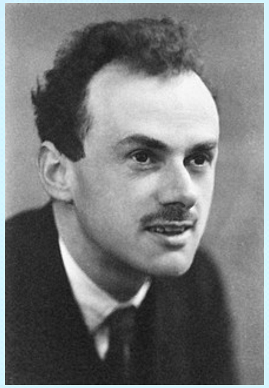
$$\Sigma = UG - UGG\star\left[1 + \frac{\delta\Sigma}{\delta G}GG\star\right]^{-1}\frac{\delta\Sigma}{\delta G}$$

Closed formulation — no perturbative (diagrammatic) input & Wick's contractions

- A solution only perturbative via expansion in interaction U

Feynman approach – functional based

Dirac picture – full perturbative solution



- Eigenstates and eigenenergies of $\hat{H}_0$ are known
- Evolution of operators (Dirac) interactive picture: $\hat{A}(\tau) = e^{\tau \hat{H}_0} \hat{A} e^{-\tau \hat{H}_0}$
- Thermodynamic S-matrix: $\hat{S}_\mu(\beta,0) = T_\tau exp\left\{ -\int_0^\beta d\tau \hat{H}_I(\tau) \right\}$, only perturbative definition
- Thermal averaging $\langle \hat{X} \rangle = \dfrac{1}{\mathcal{Z}_0} \mathrm{Tr}\left[\hat{X} e^{-\beta(\hat{H}_0) - \mu \hat{N})} \right]$
- 1P Green function (diagonal in momentum representation)

$$\mathcal{G}(\vec{p}, \tau - \tau') = -\frac{1}{\left\langle \hat{S}_\mu(\beta,0) \right\rangle} \left\langle T_\tau \left[\hat{a}_{\vec{p}}(\tau) \hat{a}^\dagger_{\vec{p}}(\tau') \hat{S}_\mu(\beta,0) \right] \right\rangle$$

- Unperturbed Green function ($\hat{H}_I = 0$)

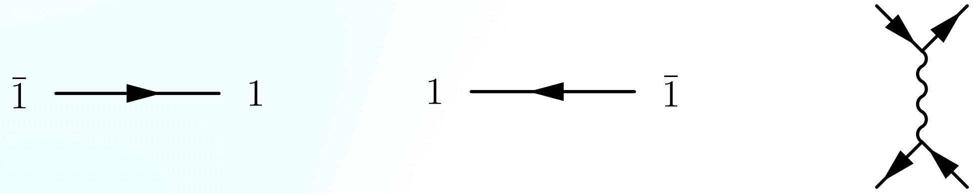
$$\mathcal{G}_0(\vec{p}, \tau - \tau') = -\left\langle T_\tau \left[\hat{a}_{\vec{p}}(\tau) \hat{a}^\dagger_{\vec{p}}(\tau') \right] \right\rangle$$

Perturbation expansion — Feynman diagrams

- Solution is perturbative due to time-ordering product defined only on polynomials
- Thermodynamic S-matrix

$$\hat{S}_\mu(\beta,0) = 1 + \sum_{n=1}^{\infty} (-1)^n \int_0^\beta dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n \left\langle \hat{H}_I(t_1)\hat{H}_I(t_2)\ldots\hat{H}_I(t_n)\right\rangle$$

- Expressions $\left\langle \hat{a}^\dagger_{i_1}\ldots\hat{a}^\dagger_{i_n}\hat{a}_{i_n}\ldots\hat{a}_{i_+}\right\rangle$ are explicitly known and $\left[\hat{a}^\dagger_\alpha, \left[\hat{a}_\beta, \hat{H}_0\right]\right] = c_{\alpha\beta}\hat{1}$
- Perturbation expansion is a sum of products of Wick's contractions $\left\langle T_\tau\left[\hat{a}_{\vec{p}}(\tau)\hat{a}^\dagger_{\vec{p}}(\tau')\right]\right\rangle$ (bare Green functions)
- Feynman diagrams — graphical representation of unlabelled Wick's contractions



Thermodynamic potential — Luttinger-Ward functional

- Solution of Schwinger theory: $\Sigma[U,G]$; How to get the thermodynamic potential?
- Luttinger-Ward functional Φ such that $\Sigma[U,G] = \dfrac{\delta\Phi[U,G]}{\delta G}$
- Generating thermodynamic functional (analogue to Hamilton classical action $q \to G$ and $p \to \Sigma$)

$$\frac{1}{N}\bar{\Omega}[G,\Sigma] = -\frac{1}{\beta N}\sum_{\sigma,\omega_n,\mathbf{k}} e^{i\omega_n 0^+}\left\{\ln\left[i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - \Sigma_\sigma(\mathbf{k},i\omega_n)\right] + G_\sigma(\mathbf{k},i\omega_n)\Sigma_\sigma(\mathbf{k},i\omega_n)\right\} + \Phi[G,U]$$

- Equilibrium state from $\delta\bar{\Omega} = \dfrac{\delta\bar{\Omega}}{\delta\Sigma}\delta\Sigma + \dfrac{\delta\bar{\Omega}}{\delta G}\delta G = \left[\left(G^{(0)-1} - \Sigma\right)^{-1} - G\right]\delta\Sigma - \left[\Sigma - \dfrac{\delta\Phi}{\delta G}\right]\delta G = 0$
- Feynman field theory — Feynman diagrams determine the thermodynamic potential (Hamilton-Jacobi-like)

$$\Omega\left[G^{(0)-1},U\right] = -k_BT\ln\left[\mathscr{Z}_0\left\langle \hat{S}_\mu(\beta,0)\right\rangle\right] = N\Phi[G,U] - \mathrm{Tr}\left[\ln\left(G^{(0)-1} - \frac{\delta\Phi}{\delta G}\right) + G\frac{\delta\Phi}{\delta G}\right]$$

Input to the Feynman approach is a renormalized perturbation theory

Response functions & conserving approximations

- Φ-derivable approximations — analytic form of $\Phi[G,U]$ for given $\Sigma[G,U]$ (not always possible)
- Thermodynamic potential does not contain 2P functions — conserving form not guaranteed
- Schwinger-Dyson equation representing the self-energy $\Sigma[G,U]$ via 2PI vertex $\Lambda[G,U]$

$$\Sigma[G,U] = UG\left[1 - G\left(1 + \Lambda[G,U]GG\star\right)^{-1}\Lambda[G,U]\right]$$

- Conserving approximations $\Lambda[G,U] = \dfrac{\delta\Sigma}{\delta G}$ results in Schwinger theory (unreachable)
- Conserving response function $\chi = \dfrac{dG}{dh} = \left[1 + \dfrac{\delta\Sigma[G,U]}{\delta G}GG\star\right]^{-1} GG$
- Inconsistency in determining critical behavior (diverging response function)

$$1 + \Lambda[G,U]GG \neq 1 + \frac{\delta\Sigma[G,U]}{\delta G}GG$$

Conclusions — Thermodynamics of correlated electrons

- Perturbation theory needed — Feynman diagrams representing virtual physical processes
- Non-perturbative approximations — infinite series of diagrams
- Approximation generators — Schwinger-Dyson equation determining the self-energy from 2PIR vertex
- Conserving approximations — only fully renormalized Green functions in Feynman diagrams
- Luttinger-Ward functional (thermodynamic potential) connects thermal & mechanical parts
- Conserving 2P vertex — via Ward identity from self-energy
- Thermodynamic consistency — only a single divergent 2P vertex; the task to solve

Matching the vertex from Schwinger-Dyson equation
with the conserving one from Ward identity