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0.1 Some books on Quantum Field Theory

- 1. L H Ryder, Quantum Field Theory, 2nd Ed. (1996).
- 2. K Huang, Quantum Field Theory: From Operators to Path Integrals, 2nd Ed. (2010).
- 3. K Huang, Statistical mechanics 2nd Ed. (2008), [Appendix A].
- 4. P Ramond, Field Theory: A Modern Primer (1981).
- 5. C Itzykson and J-B Zuber, Quantum Field Theory (1980).
- 6. A Zee, Quantum Field Theory in a Nutshell, 2nd Ed. (2010).
- 7. V P Nair, Quantum Field Theory: A Modern Perspective (2006).
- 8. A Lahiri and P Pal, A First Book of Quantum Field Theory, 2nd Ed. (2005).
- 9. S Weinberg, Quantum Theory of Fields, Vol I and II (2005).
- 10. J D Bjorken and S Drell, Relativistic Quantum Fields (1965).
- 11. M D Schwartz, Quantum Field Theory and the Standard Model (2014).
- 12. M E Peskin and D V Schroeder, An Introduction to Quantum Field Theory (1995).
- 13. A Das, Lectures on Quantum Field Theory (2008).
- 14. M Srednicki, Quantum Field Theory (2006).

15. F Mandl and G Shaw, Quantum Field Theory, 2nd Ed. (2010).

16. R D Klauber, Student Friendly Quantum Field Theory, 2nd Ed. (2013).

0.2 Classical fields model systems with infinitely many degrees of freedom

• The number of degrees of freedom is the number of real coordinates needed to specify the instantaneous location of all parts of the system under consideration.

• A point particle moving in a room has three degrees of freedom: the cartesian coordinates of its position.

• A rigid rock has six degrees of freedom: 3 to locate its center of mass (or other marked point) and three angles to orient it holding the CM fixed.

• The solar system with the Sun and nine planets, all treated as point particles has $10 \times 3 = 30$ degrees of freedom.

• The $\approx 10^{24}$ gas molecules in a football have about 5×10^{24} degrees of freedom, when treated as rigid rotors (diatomic molecules O_2 , N_2).

• For practical and conceptual purposes, it is fruitful to treat a stretched string, gas, liquid or deformable solid as a system with a continuously infinite number of degrees of freedom. These could be the displacement of the string at each point along its length, the density, pressure and components of the velocity of the fluid at each point in the container, etc. Pressure p(r,t) is an example of a scalar field while velocity v(r,t) is a vector field. Fields are dynamical variables (quantities that evolve in time) that depend on position, so they have infinitely many degrees of freedom.

• A system with finitely many degrees of freedom is sometimes called a mechanical system. The name continuum mechanics is used for the study of systems whose variables are fields.

• The electric and magnetic vectors $E(\mathbf{r}, t)$ and $B(\mathbf{r}, t)$ and the gravitational potential $V(\mathbf{r}, t)$ are other examples of fields. In particle physics, we have fields associated with various particles: the electron Dirac field $\psi^{\alpha}(x)$, the photon vector potential field $A_{\mu}(x)$, the Higgs scalar field $\phi(x)$, gluon gauge fields $A_{\mu}^{a}(x)$ and so forth.

0.3 Examples of field equations

• In classical mechanics, the dynamics of a system of N particles moving in 3d space and labeled by a = 1, 2, 3, ..., N, is governed by Newton's equations of motion $m_a \ddot{r}_a = f_a$. Here r_a is the position of particle a while m_a is its mass and f_a the force acting on it. These are a (generally nonlinear) system of second order ordinary differential equations (ODEs) for the position coordinates of the particles. There are as many equations (3N) as there are degrees of freedom.

• Fields have infinitely many degrees of freedom. So we might expect to model their dynamics by an infinite collection of ODEs. This is essentially true, except that these infinite systems of ODEs can often be arranged as a single or finite system of partial differential equations (PDEs). Thus, the classical dynamics of fields is governed by field equations, which are typically PDEs: they involve both spatial and time derivatives of the fields.

• Here are a few representative examples of field equations. Some are linear (usually

due to some approximation) while others are nonlinear. Some are nonrelativistic while others are relativistic.

• d'Alembert's wave equation for the height u(x,t) of a stretched string executing small transverse oscillations is

$$\rho \frac{\partial^2 u}{\partial t^2} = \tau \frac{\partial^2 u}{\partial x^2} \quad \text{or} \quad \rho u_{tt} = \tau u_{xx}. \tag{1}$$

We call u(x, t) a 1 + 1 dimensional field since there is one space and one time coordinate. ρ is the uniform mass per unit length of the string while τ is the constant tension in the string. The quantity $c = \sqrt{\tau/\rho}$ turns out to be the speed at which disturbances propagate along the string. d'Alembert's equation is linear in the height u because we restricted to small oscillations. Although it describes nonrelativistic phenomena, this approximate equation is invariant under Lorentz transformations if u is considered as a scalar and c a constant speed, analogous to that of light.

• According to Maxwell theory, the electric field vector E(r,t) in vacuum and in the absence of electric charges and currents satisfies a linear vector wave equation in three dimensional space

$$\frac{1}{c^2}\frac{\partial^2 \boldsymbol{E}}{\partial t^2} - \boldsymbol{\nabla}^2 \boldsymbol{E} = 0.$$
⁽²⁾

Here, $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ is the Laplace operator. Evidently, each component of the electric field satisfies a 3 + 1 dimensional d'Alembert wave equation. Disturbances in the electric field propagate at a speed *c*, the speed of light. The magnetic field B(x, y, z, t) also obeys the same equation and both fields must be solenoidal in the absence of sources: $\nabla \cdot E = 0$ and $\nabla \cdot B = 0$. These are the equations of a 3+1 dimensional relativistic field theory. In the presence of sources (electric charges and currents), Maxwell's equations in rationalized Heaviside-Lorentz units are

$$\nabla \cdot \boldsymbol{B} = 0, \quad \nabla \times \boldsymbol{E} = -\frac{1}{c} \frac{\partial B}{\partial t}, \quad \nabla \cdot \boldsymbol{E} = \rho, \quad \nabla \times \boldsymbol{B} = \frac{\boldsymbol{j}}{c} + \frac{1}{c} \frac{\partial E}{\partial t}.$$
 (3)

They can be written in a manifestly Lorentz covariant form. The homogeneous Maxwell equations $(\nabla \cdot B = 0 \text{ and } \nabla \times E = -(1/c)\frac{\partial B}{\partial t})$ are automatically satisfied if we introduce the scalar and vector potentials (ϕ, A) via $E = -\nabla \phi - c^{-1}\frac{\partial A}{\partial t}$ and $B = \nabla \times A$. They are combined in the 4-vector potential $A^{\mu} = (\phi, A)$. The components of E and B then arise as the components of the antisymmetric field strength tensor $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$. The remaining two inhomogeneous Maxwell equations then become $\partial_{\mu}F^{\mu\nu} = j^{\nu}/c$, where $j^{\nu} = (c\rho, j)$ is the 4-vector current density, composed of the charge density and electric current density.

• Fourier's heat conduction equation for the absolute temperature T on a plate in the x-y plane is

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right). \tag{4}$$

Here α is the thermal diffusivity, it controls the rate at which heat diffuses. This is an example of a 2 + 1 dimensional nonrelativistic field equation. It is linear in the temperature T. This linearity is an approximation, which is justified when Fourier's

empirical law on the proportionality of the heat flux vector to the temperature gradient holds.

• The **Euler equations** for a nonrelativistic incompressible inviscid fluid flowing in three dimensional space are a system of PDEs for the velocity v density ρ and pressure p:

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} \boldsymbol{v} = -\frac{1}{\rho} \boldsymbol{\nabla} p, \quad \frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0 \quad \text{and} \quad \boldsymbol{\nabla} \cdot \boldsymbol{v} = 0.$$
(5)

These equations are nonlinear in v due to the 'advection' term $v \cdot \nabla v$.

• **The Klein-Gordon field equation** is a relativistic wave equation that is obtained from d'Alembert's wave equation in 3+1 dimensions by adding a wavelength term (more commonly called a 'mass' term):

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} - \boldsymbol{\nabla}^2\phi + \frac{1}{\lambda^2}\phi = 0.$$
(6)

Here, λ is a parameter with dimensions of length. It is sometimes called the Compton wavelength and controls the distance over which influences decay. The reason for the name 'mass term' becomes clearer when one studies the corresponding quantum theory where the quantity $m = h/\lambda c$ may be interpreted as the mass of a particle, with h denoting Planck's constant. The Klein-Gordon equation was originally introduced in an attempt at a relativistic treatment of a quantum mechanical particle. However, there are physical difficulties with such a relativistic quantum mechanical interpretation. Thus, it is better to view the Klein-Gordon field equation as a classical field equation. It is Lorentz invariant if ϕ is treated as a scalar under Lorentz transformations. It is sometimes written as $(\Box + 1/\lambda^2)\phi = 0$ where $\Box = (1/c^2)\partial_t^2 - \nabla^2$ is called the d'Alembertian or wave operator.

• The Dirac equation is another classical field equation. It is a relativistic linear wave equation for a 4-component Dirac field $\psi^{\alpha}(\mathbf{r},t)$ where $\alpha = 1, 2, 3, 4$:

$$\left(i\gamma^{0}\frac{1}{c}\frac{\partial\psi}{\partial t} + i\gamma^{1}\frac{\partial}{\partial x} + i\gamma^{2}\frac{\partial}{\partial y} + i\gamma^{3}\frac{\partial}{\partial z} - \frac{1}{\lambda}\right)\psi = 0.$$
(7)

As with the Klein-Gordon equation, λ is a parameter with dimensions of length. $\gamma^0, \gamma^1, \gamma^2$ and γ^3 are four constant 4×4 matrices called Dirac matrices. The Dirac equation was originally introduced as a relativistic quantum mechanical wave equation for an electron. However, such a relativistic quantum mechanical treatment is physically problematic and valid at best as an approximation. In view of this, it is better to regard the Dirac equation as a classical field equation. Despite the use of the symbol ψ , we do not regard ψ as a quantum mechanical probability amplitude. Instead, ψ is a field like the electric field.

• Self-interacting scalar field. The Klein-Gordon and Dirac equations are linear relativistic field equations. Physically, this means they describe noninteracting systems. An important example of a relativistic system with interactions is the self-interacting scalar field with a cubically nonlinear field equation:

$$\frac{1}{c^2}\partial_t^2\phi - \boldsymbol{\nabla}^2\phi + \frac{1}{\lambda^2}\phi + g\phi^3 = 0.$$
(8)

The reason to consider a cubic (rather than quadratic) interaction is to ensure that the $\phi \rightarrow -\phi$ symmetry of the Klein-Gordon equation is retained.

• Yang-Mills equations are a matrix or 'nonabelian' generalization of Maxwell's equations. The vector potential $A_{\mu}(x) = A^a_{\mu}T^a$ is now an $N \times N$ matrix in the Lie algebra of a so-called gauge group (e.g., SU(2) or SU(3)) with structure constants f^{abc} and generators T^a satisfying $[T^a, T^b] = if^{abc}T^c$ and $\operatorname{tr} T^aT^b = (1/2)\delta^{ab}$. The field strength is $F^a_{\mu\nu} = \partial_{\mu}A^a_{\nu} - \partial_{\nu}A^a_{\mu} + gf^{abc}A^b_{\mu}A^c_{\nu}$. In the absence of sources, the field equations are a system of nonlinear PDEs for the gauge potentials A^{μ} :

$$\partial^{\mu}F^{a}_{\mu\nu} + gf^{abc}A^{\mu b}F^{\mu\nu c} = 0 \tag{9}$$

Here, g is a coupling constant like the electric charge or fine-structure constant. In fact, when the gauge group is the abelian group U(1), the Yang-Mills equations reduce to Maxwell's equations.

• Einstein equations of general relativity. Einstein's field equations are PDEs for the metric tensor $g_{\mu\nu}$ of space-time:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu}.$$
 (10)

Here $R_{\mu\nu}$ is the Ricci curvature tensor and $R = g^{\mu\nu}R_{\mu\nu}$ the Ricci scalar curvature. The Ricci curvature $R_{\mu\nu}$ is the trace $R^{\lambda}_{\ \mu\lambda\nu}$ of the Riemann curvature tensor $R^{\lambda}_{\ \mu\rho\nu}$, which is constructed from the metric. $T_{\mu\nu}$ is the energy-momentum or stress tensor of the matter present. G, c and Λ are Newton's gravitational constant, the speed of light and the cosmological constant.

• It is important to recognize that the Schrödinger wave equation $i\hbar \frac{\partial \psi}{\partial t} = H\psi$, say for a particle in a potential [where $H = -(\hbar^2/2m)\nabla^2 + V(\mathbf{r})$] is not a classical field equation, although it is a PDE. It is an equation for the quantum mechanical probability amplitude or wavefunction ψ . In this case, ψ is not a classical field and the equation describes just one particle.

0.4 Approaches to the quantum theory

• The passage from a classical theory to a corresponding quantum theory is called quantization. Quantization does not necessarily imply any notion of discreteness.

• The quantization of systems with finitely many degrees of freedom (mechanical systems) is sometimes called first quantization.

• The quantization of fields (systems with infinitely many degrees of freedom) is called second quantization. The name second quantization should not give the impression that quantization is performed twice. The name comes from some historical confusions.

• There are several approaches to the quantum theory. In particle mechanics (e.g., atomic physics), one usually uses one of three methods:

1. The Schrödinger approach via the Schrödinger equation for the wavefunction describing the system's state. This is the quantum analogue of the Hamilton-Jacobi equation of classical mechanics.

- 2. The Heisenberg approach via the Heisenberg equations of motion for operator observables and their commutation relations. This is the quantum analogue of the Poisson bracket-Hamiltonian formulation of classical mechanics.
- 3. Feynman's approach via path integrals, which is the quantum analogue of the principal of extremal action.

• Notably, in all three approaches, the process of quantization does not start directly from Newton's equation of motion but uses either the Hamiltonian or Lagrangian formulation of the classical theory. Direct quantization starting with the classical equations of motion can be done using the method of stochastic quantization, but is used less frequently.

• The quantization of fields is usually carried out using the 'canonical' Heisenberg operator approach or the path integral approach or occasionally in terms of the Schrödinger wave functional. Each of these uses either a Hamiltonian or a Lagrangian.

• For these reasons, it is useful to have a Lagrangian or Hamiltonian formulation of the field equations.

0.5 Action, Lagrangian and Euler-Lagrange equations for fields

• Not all field equations admit Lagrangian or Hamiltonian formulations. As a rule of thumb, dissipative systems (such as the heat equation or equations of viscous hydrodynamics) do not while conservative systems often do.

• There is no general recipe for finding a Lagrangian for a given set of equations of motion. However, in many cases, the difference between kinetic and potential energies does the job.

• Let us illustrate the Lagrangian and Hamiltonian formulations with the example of d'Alembert's wave equation $\rho u_{tt} = \tau u_{xx}$ for small transverse oscillations of a stretched string. For definiteness, we assume the string is clamped at x = 0 and $x = \ell$ (Dirichlet boundary conditions) or is free to move at the ends without any resistance: $u_x = 0$ at x = 0 and $x = \ell$ (Neumann boundary conditions).

• To begin with, we derive a conserved energy by using an integrating factor. Multiplying the wave equation by the velocity u_t and summing over the degrees of freedom (integrating in x), we get

$$\int_0^\ell \frac{1}{2} \rho(u_t^2)_t \, dx = \int_0^\ell \tau u_t u_{xx} \, dx. \tag{11}$$

Integrating by parts on the RHS, the boundary term $[\tau u_t u_x]_0^{\ell}$ vanishes with either Dirichlet or Neumann BCs. We get

$$\frac{d}{dt} \int_0^\ell \left(\frac{1}{2}\rho u_t^2 + \frac{1}{2}\tau u_x^2\right) dx = 0.$$
 (12)

Thus, we have found a conserved energy

$$E = T + V = \int_0^\ell \mathcal{E} \, dx \quad \text{where} \quad \mathcal{E} = \frac{1}{2}\rho u_t^2 + \frac{1}{2}\tau u_x^2. \tag{13}$$

The energy density $\mathcal{E} = \mathcal{T} + \mathcal{V}$ is a sum of kinetic and potential energy densities:

$$\mathcal{T} = \frac{1}{2}\rho u_t^2 \quad \text{and} \quad \mathcal{V} = \frac{1}{2}\tau u_x^2.$$
 (14)

• This suggests a Lagrangian

$$L = T - V = \int \mathcal{L} \, dx \quad \text{where} \quad \mathcal{L} = \mathcal{T} - \mathcal{V} = \frac{1}{2}\rho u_t^2 - \frac{1}{2}\tau u_x^2 \tag{15}$$

is called the Lagrangian density. In this case, \mathcal{L} is a quadratic polynomial in the time and space derivatives u_t and u_x of the field.

• The corresponding action is

$$S = \int_{t_1}^{t_2} L \, dt = \int_{t_1}^{t_2} \int_0^\ell \mathcal{L} \, dx \, dt.$$
 (16)

• The principle of extremal action says that if the Lagrangian is chosen suitably, the conditions for the action to be stationary with respect to small variations in u are equivalent to the equations of motion. Let us derive the Euler-Lagrange equations for extremization of S and verify that they are equivalent to d'Alembert's wave equation. Keeping only the first order terms in the variation,

$$\delta S = S[u + \delta u] - S[u] \approx \iint \left(\frac{\partial \mathcal{L}}{\partial u} \delta u + \frac{\partial \mathcal{L}}{\partial u_t} \delta u_t + \frac{\partial \mathcal{L}}{\partial u_x} \delta u_x + \frac{\partial \mathcal{L}}{\partial u_{xx}} \delta u_{xx} \right) dx dt$$
$$= \iint \left[\frac{\partial \mathcal{L}}{\partial u} - \partial_t \left(\frac{\partial \mathcal{L}}{\partial u_t} \right) - \partial_x \left(\frac{\partial \mathcal{L}}{\partial u_x} \right) + \partial_{xx} \left(\frac{\partial \mathcal{L}}{\partial u_x} \right) \right] \delta u \, dx \, dt.$$
(17)

Here, we assumed that the variations are such that $\partial_t \delta u = \delta \partial_t u$ and $\partial_x \delta u = \delta \partial_x u$. This allowed us to integrate by parts twice. Boundary terms vanish assuming the variations vanish at the initial and final times: $\delta u(x, t_1) = \delta u(x, t_2) = 0$. The condition for the first variation in the action to vanish for any sufficiently small δu is the EL equation

$$\partial_t \left(\frac{\partial \mathcal{L}}{\partial u_t} \right) = \frac{\partial \mathcal{L}}{\partial u} - \partial_x \left(\frac{\partial \mathcal{L}}{\partial u_x} \right) + \partial_{xx} \left(\frac{\partial \mathcal{L}}{\partial u_{xx}} \right).$$
(18)

For the case at hand,

$$\frac{\partial \mathcal{L}}{\partial u_t} = \rho u_t, \quad \frac{\partial \mathcal{L}}{\partial u} = 0, \quad \frac{\partial \mathcal{L}}{\partial u_x} = -\tau u_x, \quad \text{and}$$
(19)

Consequently, the EL equation is

$$\partial_t(\rho u_t) = \partial_x(\tau u_x) \quad \text{or} \quad \rho u_{tt} = \tau u_{xx},$$
(20)

which is the desired d'Alembert wave equation. Thus, we have found a Lagrangian formulation for the 1d wave equation.

• For the 3d wave equation $\rho u_{tt} = \tau \nabla^2 u$, verify that a suitable Lagrangian density is given by

$$\mathcal{L} = \frac{\rho}{2}u_t^2 - \frac{\tau}{2}|\boldsymbol{\nabla} u|^2.$$
(21)

• For the Klein-Gordon equation $(1/c^2)\phi_{tt} = \nabla^2 \phi - (1/\lambda^2)\phi$ (6), the EL equations (18) allow us to identify a Lagrangian density:

$$\mathcal{L} = \frac{1}{2c^2} (\partial_t \phi)^2 - \frac{1}{2} |\nabla \phi|^2 - \frac{\phi^2}{2\lambda^2}.$$
 (22)

• Similarly, show that a Lagrangian density for the self-interacting scalar field equation (8) is given by

$$\mathcal{L} = \frac{1}{2c^2} (\partial_t \phi)^2 - \frac{1}{2} |\nabla \phi|^2 - \frac{\phi^2}{2\lambda^2} - \frac{g}{4} \phi^4.$$
(23)

0.6 Hamiltonian and canonical Poisson bracket formulation for fields

The above field equations can also be given canonical Hamiltonian-Poisson bracket formulations. The Hamiltonian is obtained via a Legendre transform from the Lagrangian. Let us illustrate this with the example of the 1d wave equation. First, we view the Lagrangian as a function of coordinates u(x, t) and velocities $u_t(x, t)$. From (15), the momentum conjugate to the field u is given by

$$\pi(x,t) = \frac{\delta L}{\delta u_t(x,t)} = \rho u_t.$$
(24)

This allows us to express the velocity $u_t = \pi/\rho$ in terms of the conjugate momentum. The Hamiltonian is

$$H[u,\pi] = \int_0^\ell \pi u_t \, dx - L[u,u_t]$$
(25)

where u_t is to be eliminated in favor of u and π . We get

$$H[u,\pi] = \int_0^\ell \left(\frac{1}{\rho}\pi^2 - \frac{1}{2}\rho\frac{\pi^2}{\rho^2} + \frac{1}{2}\tau u_x^2\right)dx = \int_0^\ell \left(\frac{\pi^2}{2\rho} + \frac{\tau}{2}u_x^2\right)dx.$$
 (26)

The quantity in parentheses is the Hamiltonian density $\mathcal{H} = \frac{\pi^2}{2\rho} + \frac{\tau}{2}u_x^2$.

• Since $\pi(x)$ is the momentum conjugate to u(x) we propose the canonical equal-time Poisson brackets

$$\{u(x,t),\pi(x',t)\} = \delta(x-x'), \quad \{u(x,t),u(x',t)\} = \{\pi(x,t),\pi(x',t)\} = 0.$$
(27)

• We verify that Hamilton's equations $u_t = \{u, H\}$ and $\pi_t = \{\pi, H\}$ following from the Hamiltonian (26) along with these PBs, gives the desired wave equation.

• Since the Poisson brackets are canonical, Hamilton's equations can also be written in a canonical form. Recall that in classical mechanics with generalized coordinates q^i and conjugate momenta p_i , Hamilton's equations take the form

$$\dot{q}^i = \frac{\partial H}{\partial p_i}$$
 and $\dot{p}_i = -\frac{\partial H}{\partial q^i}$. (28)

In passing to field theory, these partial derivatives are replaced by functional derivatives. The corresponding Hamilton equations for a field u(x) and its conjugate momentum $\pi(x)$ are

$$\partial_t u(x) = \frac{\delta H}{\delta \pi(x)}$$
 and $\partial_t \pi(x) = -\frac{\delta H}{\delta u(x)}$. (29)

How do we compute functional derivatives? Recall the basic partial derivatives from multivariable calculus

$$\frac{\partial x}{\partial x} = 1, \quad \frac{\partial x}{\partial y} = 0 \quad \text{and more generally} \quad \frac{\partial x^i}{\partial x^j} = \delta^i_j$$
 (30)

where δ_j^i is the Kronecker symbol. This basic partial derivative coupled with the Leibniz product rule and chain rule allow us to compute derivatives of functions. The basic functional derivative is

$$\frac{\delta u(y)}{\delta u(x)} = \delta(x - y) \tag{31}$$

where the Dirac delta function plays the role of the Kronecker delta. Let us use this to evaluate Hamilton's equations. The first one is

$$\dot{u}(x) = \frac{\delta}{\delta\pi(x)} \int \left[\frac{1}{2\rho}\pi^2(y) + \frac{\tau}{2}u_y^2\right] dy = \int \frac{2}{2\rho}\pi(y)\frac{\delta\pi(y)}{\delta\pi(x)}dy = \int \frac{\pi(y)}{\rho}\delta(x-y)dy = \frac{\pi(x)}{\rho}$$
(32)

The second of Hamilton's equations is

$$\begin{aligned} \dot{\pi}(x) &= -\frac{\delta}{\delta u(x)} \int \left[\frac{1}{2\rho} \pi^2(y) + \frac{\tau}{2} u_y^2 \right] dy = -\int \left[\frac{\tau}{2} 2u_y \frac{\delta u_y(y)}{\delta u(x)} \right] dy \\ &= -\int \left[\tau u_y \partial_y \frac{\delta u(y)}{\delta u(x)} \right] dy = -\int \left[\tau u_y \partial_y \delta(x-y) \right] dy \\ &= \int \tau u_{yy} \delta(x-y) dy = \tau u_{xx}. \end{aligned}$$
(33)

Combining the two first order Hamilton equations $\dot{u} = \pi/\rho$ and $\dot{\pi} = \tau u_{xx}$, we recover the second order wave equation $\rho u_{tt} = \tau u_{xx}$.

0.7 Which classical fields are to be quantized?

It is physically justified to quantize some of the field theories mentioned above. Although quantum effects are not significant in the vibrations of a macroscopic stretched string, the quantum version of the wave equation arises in studying massless scalar particles. The quantum theory of the Maxwell field is a part of quantum electrodynamics. The quantized Klein-Gordon and self-interacting scalar fields arise as ingredients in the physics of pions and the Higgs particle. The quantized Dirac field is used to model electrons. Quantum Yang-Mills theory is at the heart of our description of the strong and weak forces. On the other hand, it is not quite appropriate to quantize the Euler equations of fluid mechanics or the heat equation to study quantum fluids or quantum effects in heat transport. The fluid and heat equations deal with some effective approximate classical degrees of freedom. A quantum fluid like a Bose condensate or superfluid Helium require a different treatment that takes into account the atomic structure of these fluids. General relativity (GR) describes classical gravity. Although quantum effects in gravity have not yet been found in nature, there is much effort to develop a quantum theory of gravity. However, a quantization of GR along the lines adopted for the Maxwell, Klein-Gordon, Dirac and Yang-Mills fields runs into some conceptual problems that have not yet been overcome. In fact, it is unclear what degrees of freedom are relevant to a description of quantum gravity.

0.8 Nonlinear Schrödinger field in 1 + 1 dimensions

• The nonlinear Schrödinger field is a complex scalar field $\psi(x, t)$. Although the twoand three-dimensional versions are also of interest, it is often studied in one spatial dimension, where it finds application to light propagation in nonlinear optical fibers and Bose-Einstein condensates in cigar-shaped traps in a mean field approximation. We will use the one-dimensional nonlinear Schrödinger field to illustrate many features of classical and quantum field theory.

0.8.1 Classical nonlinear Schrödinger equation & conserved quantities

• Classically, the nonlinear Schrödinger field evolves according to the cubically nonlinear Schrödinger field equation (NLSE)

$$i\partial_t \psi = -\alpha\beta\partial_x^2 \psi + \alpha\kappa |\psi|^2 \psi. \tag{34}$$

Here, α, β and κ are constant real parameters¹. Comparing the linear terms, we infer that $\alpha\beta$ has dimensions of areal speed, L^2/T . We will fix the other dimensions shortly. The coupling constant κ controls nonlinearities.

• We will work with decaying boundary conditions, i.e., $|\psi(x,t)| \to 0$ sufficiently fast as $x \to \pm \infty$ at all times t.

• Using the NLSE and its complex conjugate, we verify that the real (and nonnegative) quantity

$$N = \int \psi^* \psi \, dx \tag{35}$$

is independent of time. Indeed,

$$\dot{N} = \int \left[(-i\alpha\beta\psi^{*\prime\prime} + i\alpha\kappa|\psi|^2\psi^*)\psi + \psi^*(i\alpha\beta\psi^{\prime\prime} - i\alpha\kappa|\psi|^2\psi) \right] dx$$

= $i\alpha\beta\int \left[-\psi^*\psi^{\prime\prime} + \psi^*\psi^{\prime\prime} \right] dx = 0.$ (36)

We integrated by parts twice. Boundary terms do not contribute with decaying BCs. We will postulate that N is dimensionless. The quantum version of N will be an

¹Although it is only the products $\alpha\beta$ and $\alpha\kappa$ that appear in the NLSE, the three will appear separately in the Hamiltonian and Poisson brackets to be introduced shortly. The constant α is introduced so that the conserved quantity N is dimensionless.

operator whose measured values give the number of particles. Using this, we infer the dimensions

$$[\psi] = [\psi^*] = L^{-1/2}, \quad [\alpha\beta] = L^2/T, \quad [\beta/\kappa] = L \text{ and } [\alpha\kappa] = L/T.$$
 (37)

These relations still do not allow us to fix the dimensions of α , β and κ since it is only the products $\alpha\beta$ and $\alpha\kappa$ that appeared in the NLSE.

• It can be shown that the structure of the NLSE (first order in time and second order in space derivatives) allows it to be viewed as a 1 + 1 dimensional nonrelativistic field theory. In fact, the quantum theory will describe a fixed number of particles. By contrast, in interacting relativistic field theories, processes like pair-production and annihilation allow the number of particles to change with time.

• The NLSE admits a second conserved quantity. We verify that

$$H = \int \left(\beta |\partial_x \psi|^2 + \frac{1}{2}\kappa |\psi(x)|^4\right) dx = \int \left(-\beta \psi^* \partial_x^2 \psi + \frac{1}{2}\kappa |\psi(x)|^4\right) dx \quad (38)$$

is independent of time. We will interpret the manifestly real quantity H as the total energy of the system, a sum of kinetic and potential contributions. Combining with (37), this implies the following dimensions for the parameters:

$$[\beta] = \text{energy} \cdot L^2 = \frac{ML^4}{T^2}, \quad [\kappa] = \text{energy} \cdot L = \frac{ML^3}{T^2}, \quad [\alpha] = 1/\text{action} = \frac{T}{ML^2}.$$
(39)

• One checks that α, β and κ have independent dimensions. In other words, there is no nontrivial dimensionless combination that can be formed from them. In fact, requiring that $[\alpha]^a [\beta]^b [\kappa]^c = 1$, leads to the homogeneous system $A(a \ b \ c)^t = 0$, with coefficient matrix $A = \begin{pmatrix} 1 & -2 & -2 \\ 1 & -1 & -1 \\ 2 & -4 & -3 \end{pmatrix}$ having unit determinant.

• Thus, the nonlinear Schrödinger field theory does not have any dimensionless free parameters. One is free to work in units where α , β and κ take specific numerical values. Without loss of generality, α and β may both be taken positive: a change in sign of either of them can be compensated for by exchanging the roles of ψ and ψ^* and reversing the sign of κ . Once the signs of α and β have been fixed, the sign of κ acquires a physical meaning.

• Assuming $\alpha > 0$ and $\beta > 0$ (in fact, one often works in units where $\alpha = 1$ and $\beta = \frac{1}{2}$), the equation is called repulsive or defocusing if $\kappa > 0$ and attractive or focusing if $\kappa < 0$. If $\kappa > 0$, then the energy $H \ge 0$. By a choice of units, κ can be taken equal to ± 1 in these two cases. When $\kappa = 0$, (34) reduces to the free particle linear Schrödinger equation of quantum mechanics $[i\hbar\partial_t\psi = -(\hbar^2/2m)\psi'']$, which explains the name. However, the name can be misleading, as ψ here is a classical field, not a quantum wavefunction.

• The classical NLSE admits a third conserved quantity

$$P = i\alpha\beta \int \psi^* \psi' \, dx. \tag{40}$$

Integrating by parts, we check that $P = P^*$ is real. As defined, P has dimensions of speed. We may interpret it as the total field velocity. We check that it is independent

of time:

$$\dot{P} = i\alpha\beta \int (\dot{\psi}^{*}\psi' + \psi^{*}\dot{\psi}') dx$$

$$= i\alpha\beta \int [(-i\alpha\beta\psi^{*''} + i\alpha\kappa|\psi|^{2}\psi^{*})\psi' + \psi^{*}(i\alpha\beta\psi'' - i\alpha\kappa|\psi|^{2}\psi)'] dx$$

$$= -\alpha^{2}\beta \int [-\beta\psi^{*''}\psi' + \kappa|\psi|^{2}\psi^{*}\psi' - \psi^{*'}(\beta\psi'' - \kappa|\psi|^{2}\psi)] dx$$

$$= -\alpha^{2}\beta^{2} \int [\psi^{*'}\psi'' - \psi^{*'}\psi''] dx - \alpha^{2}\beta\kappa \int |\psi|^{2}(\psi^{*}\psi' + \psi^{*'}\psi) dx$$

$$= -\alpha^{2}\beta\kappa \int |\psi|^{2}(|\psi|^{2})' dx = -\frac{\alpha^{2}\beta\kappa}{2} \int (|\psi|^{4})' dx = 0.$$
(41)

We integrated by parts thrice and omitted boundary terms which vanish for decaying BCs.

0.8.2 Hamiltonian-Poisson bracket and Lagrangian formulations of NLSE

• The cubic NLSE admits a Hamiltonian-Poisson bracket formulation if we take the energy (38) as the Hamiltonian and postulate the 'canonical' PBs

$$\{\psi(x),\psi^*(x')\} = -i\alpha\delta(x-x'), \quad \{\psi(x),\psi(x')\} = \{\psi^*(x),\psi^*(x')\} = 0.$$
(42)

Recall that the operation of taking Poisson brackets introduces a factor of 1/action: in particle mechanics, this comes from the derivatives with respect to coordinates and momenta:

$$\{f,g\} = \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}.$$
(43)

The factor of α on the RHS of (42) ensures that the PBs have consistent dimensions. We may interpret the PBs as saying that $i\psi^*/\alpha$ is the field conjugate to ψ .

• Using the linearity and Leibniz rule properties of PBs, Hamilton's equation for ψ is

$$\partial_{t}\psi(x) = \{\psi(x), H\}$$

$$= \int dy \left[\beta\partial_{y}\psi(y)\partial_{y}\{\psi(x), \psi^{*}(y)\} + \kappa\psi(y)^{2}2\psi^{*}(y)\{\psi(x), \psi^{*}(y)\}\right]$$

$$= \int dy \left[i\alpha\beta\partial_{y}^{2}\psi(y) - 2i\alpha\kappa\psi(y)^{2}\psi^{*}(y)\right]\delta(x-y)$$

$$= i\alpha\beta\partial_{x}^{2}\psi - i\alpha\kappa|\psi(x)|^{2}\psi(x). \qquad (44)$$

We integrated by parts and used decaying BCs to ignore the boundary term. Hamilton's equation agrees with (34) upon multiplying by *i*. Hamilton's equation for ψ^* gives the complex conjugate of the NLSE:

$$\dot{\psi}^* = -i\alpha\beta\psi^{*\prime\prime} + i\alpha\kappa|\psi|^2\psi^*. \tag{45}$$

- Verify that $\{N, H\} = 0$, which is expected from the conservation of N.
- Verify that $\{P, H\} = 0$, which is expected from the conservation of P.

Lagrangian for the NLSE. Recall from (42) that $\pi = i\psi^*/\alpha$ is the field conjugate to ψ . As in mechanics, we define the Lagrangian via an (inverse) Legendre transform:

$$L = \int \pi \dot{\psi} \, dx - H \quad \text{where} \quad \pi = i\psi^*/\alpha \tag{46}$$

is used to eliminate π . From the Hamiltonian in (38), we get

$$L = \int \left[\frac{i}{\alpha}\psi^*\dot{\psi} + \beta\psi^*\partial_x^2\psi - \frac{1}{2}\kappa\psi^*\psi^*\psi\psi\right] dx.$$
 (47)

The integrand is the Lagrangian density \mathcal{L} . It is a polynomial in ψ, ψ^* and their space and time derivatives.

• To be sure, let us check whether the Euler-Lagrange equations that follow from this Lagrangian reproduce the nonlinear Schrödinger equation. Since \mathcal{L} does not depend on derivatives of ψ^* , the corresponding EL equation is simply $\frac{\partial \mathcal{L}}{\partial \psi^*} = 0$, i.e.,

$$(i/\alpha)\dot{\psi} + \beta\partial_x^2\psi - \kappa\psi^*\psi\psi = 0, \tag{48}$$

which agrees with (34). On the other hand, proceeding as in (18), the EL equation for ψ is

$$\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial \psi_x} + \frac{\partial^2}{\partial x^2}\frac{\partial \mathcal{L}}{\partial \psi_{xx}}.$$
(49)

This leads to

$$\partial_t (i\psi^*/\alpha) = -\kappa\psi^*\psi^*\psi + \partial_x^2(\beta\psi^*)$$

or $i\partial_t\psi^* = \alpha\beta\partial_x^2\psi^* - \alpha\kappa|\psi|^2\psi^*,$ (50)

which agrees with the complex conjugate NLSE (45).

• Thus, we have furnished Hamiltonian-Poisson bracket and Lagrangian formulations for the NLSE.

0.8.3 Noether's Theorem and conserved quantities

• In classical mechanics, Noether's theorem constructs a conserved quantity associated to each infinitesimal symmetry of the Lagrangian. If $q^i \rightarrow q^i + \delta q^i$ is an infinitesimal symmetry of the Lagrangian (and therefore of the equations of motion), then the corresponding conserved quantity is the Noether charge $Q = p_i \delta q^i$. Here, a sum over degrees of freedom labeled by *i* is implied and p_i are the momenta conjugate to the generalized coordinates q^i . In a field theory with field $\phi(x)$ and conjugate momentum field $\pi(x)$, the conserved quantity associated to the infinitesimal symmetry $\phi \rightarrow \phi + \delta \phi$ is given by $\int \pi(x) \delta \phi(x) dx$. The integral over *x* plays the role of the sum over degrees of freedom.

• The conservation of N (35) and P (40) in the nonlinear Schrödinger field theory could have been arrived at by an application of Noether's theorem.

• Global U(1) symmetry and conservation of N. We begin by noting that a change in phase

$$\psi \to e^{i\theta}\psi$$
 and $\psi^* \to e^{-i\theta}\psi^*$ (51)

leaves the NLSE (34), the Hamiltonian (38) and the Lagrangian (47) unchanged. This is called the global U(1) symmetry of the NLSE. The qualifier *global* is used to imply that θ is constant, independent of x and t. Taking θ small, we get the infinitesimal symmetry

 $\psi \to \psi + i\theta\psi$ so that $\delta\psi = i\theta\psi$. (52)

Recalling that the momentum conjugate to ψ is $i\psi^*/\alpha$, Noether's theorem then guarantees the conservation of

$$\int (i\psi^*/\alpha)(i\theta\psi)\,dx = -\frac{\theta}{\alpha}\int |\psi|^2\,dx.$$
(53)

Up to constant factors, this is equal to N (35).

• Translation invariance and conservation of P. The NLSE is translation-invariant: x does not appear explicitly, it enters only through derivatives and in the arguments of fields. Thus, a constant shift $x \rightarrow x + a$ leaves the NLSE (34), the Hamiltonian (38) and the Lagrangian (47) unaltered. Taking a small, the corresponding infinitesimal symmetry transformation is

$$\psi(x) \to \psi(x) + a\psi'(x)$$
 so that $\delta\psi = a\psi'$. (54)

The resulting conserved Noether charge is

$$\int (i\psi^*/\alpha)(a\psi')\,dx = \frac{ia}{\alpha}\int \psi^*(x)\psi'(x)\,dx,\tag{55}$$

which we notice is proportional to P.

0.8.4 Canonical commutation relations

• In passing from the classical mechanics of a particle to the corresponding quantum theory, we replace the dynamical variables q, p by operators (often matrices or differential operators) acting on a suitable quantum state space. The latter is a linear vector space with inner product, i.e., a Hilbert space. The operators are required to obey commutation relations that replace classical Poisson brackets. For position and momentum:

$$\{q^i, p_j\} = \delta^i_j \quad \rightsquigarrow \quad [q^i, p_j] = i\hbar \delta^i_j I \tag{56}$$

where [A, B] = AB - BA is the commutator of operators, I is the identity and δ_j^i is the Kronecker symbol.

• The reduced Planck's constant $\hbar = h/2\pi$, with dimensions of action is a new parameter that is present in the quantum theory. As a consequence, unlike the classical theory, the quantum theory appears to possesses a dimensionless parameter, namely $\hbar\alpha$. However, we will see that it can be absorbed into a redefinition of the fields. Thus, the quantum theory can be formulated in terms of three dimensionful parameters. They will be physically interpreted as Planck's constant, the mass and interaction strength of a collection of identical particles.

• In a similar manner, to quantize the nonlinear Schrödinger field, we replace the classical field $\psi(x)$ and its complex conjugate $\psi^*(x)$ with the field operator $\psi(x)$ and

its hermitian adjoint $\psi^{\dagger}(x)$. By analogy with (56) and based on (42), they are required to satisfy the commutation relations

$$\begin{bmatrix} \psi(x), \psi^{\dagger}(y) \end{bmatrix} = -i\alpha \, i\hbar \, \delta(x-y) = \alpha \hbar \delta(x-y) \quad \text{and} \\ \begin{bmatrix} \psi(x), \psi(y) \end{bmatrix} = \begin{bmatrix} \psi^{\dagger}(x), \psi^{\dagger}(y) \end{bmatrix} = 0.$$
 (57)

These commutation relations are not quite 'canonical' due to the $\alpha\hbar$ factor on the right. Getting rid of this factor will make things easier to interpret. However, $\alpha\hbar$ is a dimensionless free parameter, so we are not free, for instance, to put it equal to one [Although we are free to work in units where $\alpha = 1$, in those units \hbar cannot also, in general, be taken equal to 1]. To make the commutation relations take a canonical form, we will define rescaled field operators

$$\phi(x) = \psi(x)/\sqrt{\hbar\alpha}$$
 and $\phi^{\dagger}(x) = \psi^{\dagger}(x)/\sqrt{\hbar\alpha}$. (58)

These rescaled operators satisfy so-called canonical commutation relations

$$[\phi(x), \phi^{\dagger}(y)] = \delta(x - y), \quad [\phi(x), \phi(y)] = [\phi^{\dagger}(x), \phi^{\dagger}(y)] = 0.$$
(59)

The fields ϕ and ϕ^{\dagger} continue to have dimensions of $1/\sqrt{L}$ as in the classical theory.

0.8.5 Number and Hamiltonian operators

• Next, we define a dimensionless 'number operator'

$$\mathbf{N} = \frac{N}{\hbar\alpha} = \int \boldsymbol{\phi}^{\dagger}(x)\boldsymbol{\phi}(x) \, dx. \tag{60}$$

The name will be justified shortly. This operator is hermitian and positive definite by construction. Thus, its eigenvalues must be nonnegative.

• The Hamiltonian operator (with dimensions of energy) is similarly defined:

$$\boldsymbol{H} = \frac{H}{\hbar\alpha} = \beta \int \partial_x \boldsymbol{\phi}^{\dagger}(x) \partial_x \boldsymbol{\phi}(x) dx + \frac{\kappa \hbar \alpha}{2} \int \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}(x) \boldsymbol{\phi}(x) dx.$$
(61)

It too is a hermitian operator. Notice that we have ordered the operators with ϕ^{\dagger} to the left of ϕ . Although the order did not matter classically, it can have an effect in the quantum theory since the field operators generally do not commute. This choice is part of the definition of the quantum theory and is called *normal ordering*.

• We will assume that the fields (and states they act on) are such that integration by parts with decaying BCs is permitted, so that we may write

$$\boldsymbol{H} = -\beta \int \boldsymbol{\phi}^{\dagger}(x) \partial_x^2 \boldsymbol{\phi}(x) \, dx + \frac{\kappa \hbar \alpha}{2} \int \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}(x) \boldsymbol{\phi}(x) \, dx. \tag{62}$$

• We then verify that [H, N] = 0. It follows that the hermitian operators N and H are simultaneously diagonalizable. They have a common set of eigenvectors which can be chosen to form an orthonormal basis for the Hilbert space. We will denote these common eigenvectors $|E, N\rangle$ where E and N are the corresponding eigenvalues:

$$\langle E, N | E', N' \rangle = \delta_{EE'} \delta_{NN'}, \quad \boldsymbol{H} | E, N \rangle = E | E, N \rangle \quad \text{and} \quad \boldsymbol{N} | E, N \rangle = N | E, N \rangle.$$

(63)

0.8.6 Raising and lowering operators, vacuum state

• Raising and lowering property. From the canonical commutation relations (59) and definition of N, we show that

$$[\mathbf{N}, \boldsymbol{\phi}(x)] = -\boldsymbol{\phi}(x) \quad \text{and} \quad [\mathbf{N}, \boldsymbol{\phi}^{\dagger}(x)] = \boldsymbol{\phi}^{\dagger}(x). \tag{64}$$

In anticipation of its interpretation, we will say that the state $|E, N\rangle$ has N particles. Using these commutators, we show that

$$N(\phi(x)|E,N\rangle) = (N-1)\phi(x)|E,N\rangle \text{ and}
 N(\phi^{\dagger}(x)|E,N\rangle) = (N+1)\phi^{\dagger}(x)|E,N\rangle.$$
(65)

What this means is that if $|E, N\rangle$ is an eigenstate of N with eigenvalue N, then $\phi^{\dagger}|E, N\rangle$ is also an eigenstate but with eigenvalue N + 1. Similarly, $\phi|E, N\rangle$ is an eigenstate of N with eigenvalue N - 1. In other words, $\phi(x)$ lowers N by one while $\phi^{\dagger}(x)$ raises N by one. ϕ and ϕ^{\dagger} are called lowering and raising operators or annihilation and creation operators.

• Vacuum state. Recall that N (60) is a positive definite operator, so its eigenvalues must be ≥ 0 . For this to be consistent with the lowering property of ϕ , there must be a state $|E_0, 0\rangle$ (called a vacuum state) which is annihilated by $\phi(x)$, i.e.,

$$\phi|E_0,0\rangle = 0|E_0,0\rangle = 0.$$
 (66)

If this were not the case, then by repeated application of ϕ , we could produce eigenstates of N with negative eigenvalues. We will say that the vacuum state has no particles.

• What is more, since H is normal ordered with ϕ to the right, it must annihilate a vacuum state:

$$\boldsymbol{H}|E_0,0\rangle = 0. \tag{67}$$

Thus, we infer that the energy of the vacuum state vanishes: $E_0 = 0$. Although we will not attempt to prove it here, it turns out there is only one such vacuum state, which we denote $|0,0\rangle$ or $|0\rangle$ for short. Furthermore, if $\kappa > 0$ (repulsive or defocusing NLSE), then H is a positive definite operator and the vacuum must be the ground state.

• Since $\phi^{\dagger}(x)$ is a raising operator, by successively applying it to the vacuum state, we obtain eigenstates of N

$$\phi^{\dagger}(x_1)|0\rangle, \quad \phi^{\dagger}(x_2)\phi^{\dagger}(x_1)|0\rangle, \dots$$
 (68)

with eigenvalues N = 1, 2, 3, ... These are states with 1, 2, 3, ... particles. Although these states are generally not eigenstates of H, since [N, H] = 0, eigenstates of H can be obtained by taking suitable linear combinations of states with the same number of particles.

0.8.7 N-particle wave function and its normalization

• An N-particle wavefunction. Suppose $|E, N\rangle$ is an N-particle state with energy E. Then applying N lowering operators, we arrive at a state

$$\phi(x_1)\phi(x_2)\cdots\phi(x_N)|E,N\rangle \tag{69}$$

with zero particles. So it must be proportional to the vacuum state and must be orthogonal to all other basis states $|E', N'\rangle$:

$$\langle E', N' | \boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N) | E, N \rangle = 0 \quad \text{if} \quad N' \neq 0.$$
 (70)

This leads us to define a complex function of N positions:

$$\Psi_{EN}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \langle 0 | \boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N) | E, N \rangle.$$
(71)

Since the field operators ϕ commute, Ψ is a symmetric function of the N position coordinates. Recall that the wavefunction of a system of identical bosons must be symmetric under exchange of the coordinates of any pair of bosons. Thus, we should view Ψ as a candidate for an N-boson wavefunction in many-body quantum mechanics. We will establish its properties in the sequel.

 \bullet The numerical prefactor $1/\sqrt{N!}$ in (71) ensures that this wavefunction has unit L^2 norm-squared. We will show that

$$\mathcal{I} = \int dx_1 \cdots dx_N \Psi_{EN}^*(x_1, \cdots, x_N) \Psi(x_1, \cdots, x_N) = 1.$$
(72)

To begin with, Eq. (71) allows us to write

$$\mathcal{I} = \frac{1}{N!} \int d^N x \, \langle E, N | \boldsymbol{\phi}^{\dagger}(x_N) \cdots \boldsymbol{\phi}^{\dagger}(x_1) | 0 \rangle \langle 0 | \boldsymbol{\phi}(x_1) \cdots \boldsymbol{\phi}(x_N) | E, N \rangle. \tag{73}$$

Using the orthogonality (70), we introduce a sum over all the basis states:

$$\mathcal{I} = \frac{1}{N!} \int d^N x \sum_{E',N'} \langle E, N | \phi^{\dagger}(x_N) \cdots \phi^{\dagger}(x_1) | E'N' \rangle \langle E'N' | \phi(x_1) \cdots \phi(x_N) | E, N \rangle.$$
(74)

The completeness relation or resolution of the identity

$$\sum_{E',N'} |E'N'\rangle\langle E'N'| = I \tag{75}$$

then allows us to write

$$\mathcal{I} = \frac{1}{N!} \int d^N x \, \langle E, N | \boldsymbol{\phi}^{\dagger}(x_N) \cdots \boldsymbol{\phi}^{\dagger}(x_1) \boldsymbol{\phi}(x_1) \cdots \boldsymbol{\phi}(x_N) | E, N \rangle. \tag{76}$$

The integral over x_1 gives us the number operator $N = \int dx_1 \phi^{\dagger}(x_1) \phi(x_1)$. • We will show that the subsequent integral over x_2 is

$$\nu_2 = \int dx_2 \boldsymbol{\phi}^{\dagger}(x_2) \boldsymbol{N} \boldsymbol{\phi}(x_2) = \boldsymbol{N}(\boldsymbol{N} - I)$$
(77)

and that

$$\int dx_3 \psi^{\dagger}(x_3) \mathbf{N}(\mathbf{N}-1) \psi(x_3) = \mathbf{N}(\mathbf{N}-I)(\mathbf{N}-2I).$$
(78)

It is then plausible (and possible to show by induction) that

$$\int d^N x \, \boldsymbol{\phi}^{\dagger}(x_N) \cdots \boldsymbol{\phi}^{\dagger}(x_1) \boldsymbol{\phi}(x_1) \cdots \boldsymbol{\phi}(x_N) = \boldsymbol{N}(\boldsymbol{N} - I)(\boldsymbol{N} - 2I) \cdots (\boldsymbol{N} - (N - 1)I)I.$$
(79)

Taking the expectation value in the state $|E, N\rangle$, it then follows that $\mathcal{I} = N!/N! = 1$, which implies that the N-body wavefunction Ψ_{EN} (71) has unit norm.

• We now sketch the proof of these claims. It is convenient to define the number density operator

$$\boldsymbol{n}(x) = \boldsymbol{\phi}^{\dagger}(x)\boldsymbol{\phi}(x)$$
 so that $\boldsymbol{N} = \int \boldsymbol{n}(x) \, dx.$ (80)

Then the canonical commutation relation (59)

$$\phi^{\dagger}(x_2)\phi(x_1) - \phi(x_1)\phi^{\dagger}(x_2) = -[\phi(x_1),\phi^{\dagger}(x_2)] = -\delta(x_1 - x_2), \quad (81)$$

upon multiplying on the left by $\phi^{\dagger}(x_1)$ leads to the commutator identity

$$\phi^{\dagger}(x_2)\boldsymbol{n}(x_1) = \boldsymbol{n}(x_1)\phi^{\dagger}(x_2) - \phi^{\dagger}(x_1)\delta(x_1 - x_2).$$
(82)

We note in passing that the delta function is an even function of its argument. Using this identity, the integral over x_1 and x_2 is

$$\int dx_1 dx_2 \boldsymbol{\phi}^{\dagger}(x_2) \boldsymbol{n}(x_1) \boldsymbol{\phi}(x_2) = \int dx_1 dx_2 \, \boldsymbol{n}(x_1) \boldsymbol{\phi}^{\dagger}(x_2) \boldsymbol{\psi}(x_2) - \int dx_1 dx_2 \, \delta(x_2 - x_1) \boldsymbol{\phi}^{\dagger}(x_1) \boldsymbol{\phi}(x_2) = \boldsymbol{N}^2 - \boldsymbol{N} = \boldsymbol{N}(\boldsymbol{N} - \boldsymbol{I}).$$
(83)

Using this, the integral over x_3 is

$$\int dx_3 \boldsymbol{\phi}^{\dagger}(x_3) \boldsymbol{N}(\boldsymbol{N}-I) \boldsymbol{\phi}(x_3) = \int dx_3 \boldsymbol{\phi}^{\dagger}(x_3) \boldsymbol{N}^2 \boldsymbol{\phi}(x_3) - (\boldsymbol{N}^2 - \boldsymbol{N}).$$
(84)

We will show that the first term is

$$\nu_3 = \int dx_3 \boldsymbol{\phi}^{\dagger}(x_3) \boldsymbol{N}^2 \boldsymbol{\phi}(x_3) = \boldsymbol{N}(\boldsymbol{N} - I)^2.$$
(85)

It then follows that

$$\int dx_3 \phi^{\dagger}(x_3) \mathbf{N}(\mathbf{N} - I) \phi(x_3) = \mathbf{N}(\mathbf{N} - I)(\mathbf{N} - 2I).$$
(86)

To find ν_3 , we use (82) to write

$$\begin{aligned} \phi^{\dagger}(3) \boldsymbol{n}(1) \boldsymbol{n}(2) &= \boldsymbol{n}(x_1) \phi^{\dagger}(x_3) \boldsymbol{n}(x_2) - \phi^{\dagger}(x_1) \boldsymbol{n}(x_2) \delta(x_1 - x_3) \\ &= \boldsymbol{n}(1) [\boldsymbol{n}(2) \phi^{\dagger}(3) - \phi^{\dagger}(2) \delta(x_2 - x_3)] - \phi^{\dagger}(1) \boldsymbol{n}(2) \delta(x_1 - x_3) \\ &= \boldsymbol{n}(1) \boldsymbol{n}(2) \phi^{\dagger}(3) - \boldsymbol{n}(1) \phi^{\dagger}(2) \delta(x_2 - x_3) \\ &- [\boldsymbol{n}(2) \phi^{\dagger}(1) - \phi^{\dagger}(2) \delta(x_1 - x_2)] \delta(x_1 - x_3) \end{aligned}$$

$$= n(1)n(2)\phi^{\dagger}(3) - \delta(x_2 - x_3)n(1)\phi^{\dagger}(2) -\delta(x_1 - x_3)n(2)\phi^{\dagger}(1) + \delta(x_1 - x_3)\delta(x_1 - x_2)\phi^{\dagger}(2).$$
(87)

We have abbreviated $\phi(x_1) = \phi(1)$ etc. Multiplying on the right by $\phi(3)$,

$$\phi^{\dagger}(3)\boldsymbol{n}(1)\boldsymbol{n}(2)\phi(3) = \boldsymbol{n}(1)\boldsymbol{n}(2)\boldsymbol{n}(3) - \delta(x_2 - x_3)\boldsymbol{n}(1)\boldsymbol{n}(2) \\ -\delta(x_1 - x_3)\boldsymbol{n}(2)\boldsymbol{n}(3) + \delta(x_1 - x_3)\delta(x_1 - x_2)\boldsymbol{n}(2).$$
(88)

Integrating over x_1, x_2 and x_3 , we get formula (85) for ν_3 :

$$\nu_3 = N^3 - N^2 - N^2 + N = N(N-1)^2.$$
 (89)

The proof of the general case by induction is left as an exercise.

0.8.8 Interpretation: system of N bosons with contact interactions

• We now return to the Hamiltonian operator (62) of the quantum Schrödinger field:

$$\boldsymbol{H} = \boldsymbol{T} + \boldsymbol{V} = -\beta \int \boldsymbol{\phi}^{\dagger}(x) \partial_x^2 \boldsymbol{\phi}(x) \, dx + \frac{\kappa \hbar \alpha}{2} \int \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}(x) \boldsymbol{\phi}(x) \, dx. \tag{90}$$

• We will now interpret this quantum field theory in terms of a (first quantized) quantum mechanical system of N identical bosons. Let x_1, \dots, x_N denote the positions of the N point particles. We associate to the field Hamiltonian (90) an N-body quantum mechanical Hamiltonian

$$H_N = -\beta \left(\partial_{x_1}^2 + \dots + \partial_{x_N}^2\right) + \sum_{1 \le i < j \le N} \kappa \hbar \alpha \,\delta(x_i - x_j). \tag{91}$$

Each pair of particles interacts via a contact (delta function) potential with strength $\kappa\hbar\alpha$. It is attractive/repulsive according as $\kappa < 0$ or $\kappa > 0$.

• The coefficients in (91) can be related to the ones familiar from quantum mechanics. Indeed, putting

$$\beta = \frac{\hbar^2}{2m}$$
 and $\kappa \hbar \alpha = g,$ (92)

where m is the mass of the particles, the many body Hamiltonian becomes

$$H_N = -\frac{\hbar^2}{2m} \left(\partial_{x_1}^2 + \dots + \partial_{x_N}^2 \right) + \sum_{1 \le i < j \le N} g \,\delta(x_i - x_j). \tag{93}$$

The dimensions are verified to be consistent. The dimension of g is the same as that of κ (energy $\times L$) with $\hbar \alpha$ dimensionless. On the other hand, $\hbar^2/2m$ has dimensions of energy $\times L^2$ which is the same as that of β (39).

• Interestingly, the formulation of this many body quantum system as a QFT allows us to write an expression for the position space energy eigenfunctions in terms of matrix elements of the field operators. Indeed, if Ψ_{EN} is defined as in (71):

$$\Psi_{EN}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \langle 0 | \boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N) | E, N \rangle, \qquad (94)$$

then

$$H_N \Psi_{EN}(x_1, x_2, \dots, x_N) = E \,\Psi_{EN}(x_1, x_2, \dots, x_N).$$
(95)

The dimension of the N-body wave function Ψ_{EN} is $L^{-N/2}$, which is consistent with that of the field $[\psi] = L^{-1/2}$, with the bra and ket vectors $\langle 0 |$ and $|EN \rangle$ being dimensionless.

• Let us sketch the proof of (95). To begin with, we recall from (63) that

$$\boldsymbol{H}|E,N\rangle = E|E,N\rangle$$
 and that $\boldsymbol{H}|0\rangle = 0 \Rightarrow \langle 0|\boldsymbol{H}=0.$ (96)

We exploit this to write $E\Psi_{EN}$ as the matrix element of a commutator:

$$E\Psi_{EN}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \left\{ \langle 0 | \boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N) \boldsymbol{H} | \boldsymbol{E}, N \rangle - \langle 0 | \boldsymbol{H} \boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N) | \boldsymbol{E}, N \rangle \right\}$$
$$= \frac{1}{\sqrt{N!}} \left\{ \langle 0 | [\boldsymbol{\phi}(x_1) \boldsymbol{\phi}(x_2) \cdots \boldsymbol{\phi}(x_N), \boldsymbol{H}] | \boldsymbol{E}, N \rangle.$$
(97)

Next, by repeated use of the Leibniz rule $[A_1A_2, H] = [A_1, H]A_2 + A_1[A_2, H]$, we write the commutator as a sum

$$[\phi_1\phi_2\cdots\phi_N,\boldsymbol{H}] = \sum_{j=1}^N \phi_1\cdots\phi_{j-1}[\phi_j,\boldsymbol{H}]\phi_{j+1}\cdots\phi_N.$$
(98)

For instance, when N = 3, we have

$$\begin{bmatrix} \phi_1 \phi_2 \phi_3, H \end{bmatrix} = \begin{bmatrix} \phi_1, H \end{bmatrix} \phi_2 \phi_3 + \phi_1 \begin{bmatrix} \phi_2 \phi_3, H \end{bmatrix} = \begin{bmatrix} \phi_1, H \end{bmatrix} \phi_2 \phi_3 + \phi_1 \begin{bmatrix} \phi_2, H \end{bmatrix} \phi_3 + \phi_1 \phi_2 \begin{bmatrix} \phi_3, H \end{bmatrix}.$$
(99)

The general case can be established by induction.

• Next, we show that the commutator

$$\begin{bmatrix} \boldsymbol{\phi}(x_j), \boldsymbol{H} \end{bmatrix} = -\beta \partial_{x_j}^2 \boldsymbol{\phi}(x_j) + \hbar \alpha \kappa \boldsymbol{\phi}^{\dagger}(x_j) \boldsymbol{\phi}(x_j) \boldsymbol{\phi}(x_j) \\ = \left(-\beta \partial_{x_j}^2 + \hbar \alpha \kappa \boldsymbol{n}(x_j) \right) \boldsymbol{\phi}(x_j).$$
(100)

To see this, we deal with the kinetic and potential operators separately. First,

$$\begin{aligned} [\phi(x_j), \mathbf{T}] &= -\beta [\phi(x_j), \int \phi^{\dagger}(x) \partial_x^2 \phi(x) dx] \\ &= -\beta \int [\phi(x_j), \phi^{\dagger}(x)] \partial_x^2 \phi(x) dx \\ &= -\beta \int \delta(x_j - x) \partial_x^2 \phi(x) dx = -\beta \partial_{x_j}^2 \phi(x). \end{aligned}$$
(101)

And next,

$$[\boldsymbol{\phi}(x_j), \boldsymbol{V}] = \frac{1}{2} \hbar \alpha \kappa \int [\boldsymbol{\phi}(x_j), \boldsymbol{\phi}^{\dagger}(x) \boldsymbol{\phi}^{\dagger}(x)] \boldsymbol{\phi}(x) \boldsymbol{\phi}(x)$$

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$$= \frac{1}{2}\hbar\alpha\kappa \int \left(\phi^{\dagger}(x)[\phi(x_{j}),\phi^{\dagger}(x)] + [\phi(x_{j}),\phi^{\dagger}(x)]\phi^{\dagger}(x)\right)\phi(x)\phi(x)\,dx$$

$$= \hbar\alpha\kappa \int \delta(x_{j}-x)\phi^{\dagger}(x)\phi(x)\phi(x)\,dx$$

$$= \hbar\alpha\kappa \mathbf{n}(x_{j})\phi(x_{j}), \qquad (102)$$

implying (100). Putting this in (98), we get

$$[\boldsymbol{\phi}_{1}\cdots\boldsymbol{\phi}_{N},\boldsymbol{H}] = -\beta \sum_{j=1}^{N} \partial_{x_{j}}^{2} \boldsymbol{\phi}_{1}\cdots\boldsymbol{\phi}_{N} + \hbar\alpha\kappa \sum_{j=1}^{N} \boldsymbol{\phi}_{1}\cdots\boldsymbol{\phi}_{j-1}\boldsymbol{n}(x_{j})\boldsymbol{\phi}_{j}\boldsymbol{\phi}_{j+1}.$$
(103)

Consequently, (97) becomes

$$E\Psi_{EN}(x_1,\ldots,x_N) = -\beta \sum_{j=1}^N \partial_{x_j}^2 \Psi_{EN}(x_1,\ldots,x_N) + \frac{\hbar\kappa\alpha}{\sqrt{N!}} \sum_{j=1}^N \langle 0|\phi_1\cdots\phi_{j-1}\boldsymbol{n}(x_j)\phi_j\cdots\phi_N|EN\rangle.$$
(104)

To simplify the potential term, we use $\langle 0 | \phi^{\dagger} = 0$. To exploit this, we move $n(x_i)$ all the way to the left using the commutator relation (show this!)

$$[\boldsymbol{\phi}(x), \boldsymbol{n}(y)] = \delta(x - y)\boldsymbol{\phi}(y). \tag{105}$$

• For instance, for N = 2, the sum over j has two terms:

$$\frac{\langle 0|\boldsymbol{n}(x_1)\boldsymbol{\phi}_1\boldsymbol{\phi}_2|E2\rangle + \langle 0|\boldsymbol{\phi}_1\boldsymbol{n}(x_2)\boldsymbol{\phi}_2|E2\rangle}{= \delta(x_1 - x_2)\langle 0|\boldsymbol{\phi}(x_1)\boldsymbol{\phi}(x_2)|E2\rangle} = \delta(x_1 - x_2)\langle 0|\boldsymbol{\phi}(x_1)\boldsymbol{\phi}(x_2)|E2\rangle.$$
(106)

So for N = 2 we get

$$E\Psi_{E,2}(x_1, x_2) = \left[-\beta(\partial_{x_1}^2 + \partial_{x_2}^2) + \hbar\alpha\kappa\delta(x_1 - x_2)\right]\Psi_{E,2}(x_1, x_2).$$
(107)

This shows that $\Psi_{E,2}$ is an eigenstate of the 2-body Hamiltonian with energy E. rally we write

$$\phi_{1}\cdots\phi_{j-1}\boldsymbol{n}(x_{j})\phi_{j}\cdots\phi_{N} = \phi_{1}\cdots\phi_{j-2}\boldsymbol{n}(x_{j})\phi_{j-1}\cdots\phi_{N} \\ +\delta(x_{j}-x_{j-1})\phi_{1}\cdots\phi_{N} \\ = \phi_{1}\cdots\phi_{j-3}\boldsymbol{n}(x_{j})\phi_{j-2}\cdots\phi_{N} \\ +[\delta(x_{j}-x_{j-1})+\delta(x_{j}-x_{j-2})]\phi_{1}\cdots\phi_{N} \\ = \cdots \\ = \boldsymbol{n}(x_{j})\phi_{1}\cdots\phi_{N} + \sum_{i=1}^{j-1}\delta(x_{i}-x_{j})\phi_{1}\cdots\phi_{N}$$
(108)

Returning to (104), n annihilates $\langle 0 |$. Performing the sum over j, we get

$$E\Psi_{EN}(x_1,\ldots,x_N) = -\beta \sum_{j=1}^N \partial_{x_j}^2 \Psi_{EN}(x_1,\ldots,x_N)$$

$$+\frac{\hbar\kappa\alpha}{\sqrt{N!}}\sum_{1\leq i< j\leq N}\delta(x_i-x_j)\langle 0|\phi_1\cdots\phi_N|EN\rangle$$
$$= \left[-\beta\sum_{j=1}^N\partial_{x_j}^2 + \hbar\kappa\alpha\sum_{i< j}\delta(x_i-x_j)\right]\Psi_{EN}(x_1,\ldots,x_N)$$
$$= H_N\Psi_{EN}(x_1,\ldots,x_N).$$
(109)

Thus, we have shown that $\Psi_{EN}(x_1, \ldots, x_N)$ is an eigenstate of the *N*-body quantum mechanical Hamiltonian (91) with eigenvalue *E*.

• To summarize, we have established that the quantum nonlinear Schrödinger field theory describes a system of N identical nonrelativistic bosons moving on a line and interacting via contact (delta function) potentials (either attractive or repulsive) for each N = 0, 1, 2, ... Such a system models dilute atomic Bose gases (such as Rubidium-87) at low temperatures in cigar-shaped traps. Since the atoms are neutral, they do not interact via long-range electrostatic Coulomb forces, but rather via shortrange residual forces which we have treated as as arising from delta function potentials. What is more, one learns in quantum scattering theory that (in three dimensions) it is the s-wave part of the interparticle wavefunction that is most significant as the interatomic spacing $r \rightarrow 0$, since the wavefunction has a factor r^l , which reduces the amplitude of higher angular momentum (l = 1, 2, 3, ...) partial waves as $r \rightarrow 0$. Thus, when we take the interparticle interaction to be very short-ranged, it is the swave scattering that may be expected to dominate. Moreover, the sign of the s-wave scattering length (positive/negative) is roughly correlated with whether the interaction is repulsive or attractive ($\kappa > 0$ or $\kappa < 0$).

• For any fixed N, this N-body system has only a finite number of degrees of freedom (N). The field theory acquires an infinite number of degrees of freedom by virtue of including all possible values of N. Of course, since N is conserved, the number of particles cannot change during the course of time evolution and is fixed by initial conditions.

• We note that although our classical nonlinear Schrödinger field theory had three dimensionful parameters (β , α , κ), after rescaling the fields and Hamiltonian in the quantum theory, we were left with only two combinations $\beta = \hbar^2/2m$ and $g = \hbar\kappa\alpha$ aside from the (reduced) Planck constant \hbar .