I.3 From one to many: Many-body quantum systems

Our goal is to apply phase space methods to develop approximate descriptions of interacting many-body systems which allow for efficient numerical simulations. It is clear that this will only work in limited cases but for those phase-space methods can be useful.

1-particle quantum mechanics $\longrightarrow$ N-particle quantum mechanics

$$\psi(\vec{r},t) \qquad\qquad \psi(\vec{r}_1,\vec{r}_2,\dots \vec{r}_N,t)$$

Hilbert space:

$$\mathcal{H} \longrightarrow \bigotimes_{i=1}^{N} \mathcal{H}_i$$

but identical quantum particles are indistinguishable!

$\Rightarrow$ 2 types of particles

$\boxed{\text{Bosons}}$

wavefunction totally symmetric under particle exchange

[$\boxed{\text{Fermions}}$

wavefunction totally antisymmetric under particle exchange]

no simple phase space formalism

(A) Efficient way to guarantee exchange symmetries: Second quantization

complete basis in $\bigotimes_{i=1}^{N} \mathcal{H}_i$

(26) $$\phi_{n_1}(\vec{r}_1)\,\phi_{n_2}(\vec{r}_2)\cdots\phi_{n_N}(\vec{r}_N)$$

where

$\phi_n(\vec{r})$ orthonormal single-particle wavefunction

e.g. particle in harmonic trap

$$\phi_1(x) \sim H_1\left(\frac{x}{\ell_0}\right) e^{-x^2/\ell_0^2}$$

$$\phi_0(x) \sim e^{-x^2/\ell_0^2}$$

due to symmetry requirement: many body state fully determined by numbers of particles in different states, e.g.

(27) $$|\Psi_N\rangle \Longleftrightarrow |n_1, n_2, \ldots\rangle \qquad \sum_{i=0}^{\infty} n_i = N$$

$\Rightarrow$ Fock space

$$\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$$

no particle one particle ... etc

vacuum $|0\rangle$

Bosons | Fermions

$n_i = 0, 1, 2, 3, \ldots$ | $n_i = 0, 1$

introduce Fock-space operators to "walk" around in Fock space in analogy to non-hermitian ladder operators (angular momentum, harmonic oscillator...)

(28)
$$|n+1\rangle \equiv \frac{1}{\sqrt{n+1}} b^+ |n\rangle$$
$$|n\rangle \equiv \frac{1}{\sqrt{n}} b |n+1\rangle$$

then a^+a is a number operator (see H.-Osc.)

Many-body state with n_1 particle in $\phi_1(\vec{r})$; n_2 particle in $\phi_2(\vec{r})$, etc.

(29) $$|\psi\rangle \sim b_1^{+\,n_1} \, b_2^{+\,n_2} \cdots |0\rangle \qquad \sum_{i=0}^{\infty} n_i = N$$

N-body wavefunction

(30) $$\psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) = \langle \vec{r}_1, \vec{r}_2 \ldots \vec{r}_N | \psi \rangle$$

How can we ensure that wavefunction is totally symmetric or totally antisymmetric?

simple solution!

(31) $$\boxed{[b_i, b_j^+] = \delta_{ij}}$$ $\Rightarrow$ symmetric

notation: $b_i \rightarrow a_i$ $[a,b] = ab - ba$

(32) $$\boxed{\underset{\text{anti-commutator}}{\{b_i, b_j^+\}} = \delta_{ij}}$$ $\Rightarrow$ antisymmetric

notation: $b_i \rightarrow c_i$ $\{a,b\} = ab + ba$

Pauli principle

(33) $$c_i^{+2} = 0$$

field operator (Schrödinger field)

(34) $$\hat{\psi}(\vec{r}) = \sum_{j=0}^{\infty} \phi_j(\vec{r})\,\hat{a}_j$$ boson

$$[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = \sum_{j,l=0}^{\infty} \phi_j(\vec{r})\phi_l^*(\vec{r}\,')\underbrace{[\hat{a}_j, \hat{a}_l^+]}_{\delta_{jl}}$$

$$= \sum_{j=0}^{\infty} \phi_j(\vec{r})\phi_j^*(\vec{r}\,')$$

$$= \delta^{(3)}(\vec{r} - \vec{r}\,')$$

(35) $$\boxed{[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = \delta^{(3)}(\vec{r} - \vec{r}\,')}$$ boson

similarly for fermion

(36) $$\hat{\Psi}(\vec{r}) = \sum_{j=0}^{\infty} \phi_j(\vec{r})\hat{c}_j$$

(37) $$\boxed{\{\hat{\Psi}(\vec{r}), \hat{\Psi}^+(\vec{r}\,')\} = \delta^{(3)}(\vec{r}-\vec{r}\,')}$$ fermion

1-body wavefunction

(38) $$\phi(\vec{r}) = \langle 0|\hat{\Psi}(\vec{r})|\Psi\rangle$$

say $|\Psi\rangle = \sum_j \alpha_j \hat{a}_j^+|0\rangle$ $\qquad \sum_j |\alpha_j|^2 = 1$

$$\phi(\vec{r}) = \langle 0|\sum_e \phi_e(\vec{r})\hat{a}_e \sum_j \alpha_j \hat{a}_j^+|0\rangle$$

$$= \sum_{e,j} \alpha_j \phi_e(\vec{r}) \underbrace{\langle 0|\hat{a}_e \hat{a}_j^+|0\rangle}_{=\delta_{ej}}$$

$$\phi(\vec{r}) = \sum_j \alpha_j \phi_j(\vec{r})$$ as expected ✓

N-body wavefunction

(39) $$\boxed{\phi(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N) = \langle 0|\hat{\Psi}(\vec{r}_1)\hat{\Psi}(\vec{r}_2)\ldots\hat{\Psi}(\vec{r}_N)|\Psi\rangle}$$

In this form one easily sees the totally symmetric or totally anti-symmetric form

$$\phi(\vec{r}_1, \ldots \vec{r}_j \ldots \vec{r}_e \ldots \vec{r}_N) \hat{=} \langle 0| \ldots \hat{\vec{\Psi}}(\vec{r}_j) \ldots \hat{\vec{\Psi}}(\vec{r}_e) \ldots |\Psi\rangle$$

exchange   exchange

Single- and n-particle Hamiltonian

Schrödinger eq. for single-particle wavefunction

(40) $$i\hbar \frac{d}{dt} \phi(\vec{r},t) = h\, \phi(\vec{r},t)$$

(41) with $$\phi(\vec{r},t) = \langle 0|\, \hat{\vec{\Psi}}(\vec{r},t)\, |\Psi\rangle$$

Heisenberg picture

$$i\hbar \frac{d}{dt} \hat{\vec{\Psi}}(\vec{r},t) = \left[\hat{\vec{\Psi}}(\vec{r},t), \hat{H}\right]$$

where

(42) $$\boxed{\hat{H} = \int d^3r\ \hat{\vec{\Psi}}^{\dagger}(\vec{r})\, h(\vec{r})\, \hat{\vec{\Psi}}(\vec{r})}$$

single-particle Hamiltonian

$$\Rightarrow i\hbar \frac{d}{dt} \hat{\vec{\Psi}} = \int d^3r' \left[\underbrace{\hat{\vec{\Psi}}(\vec{r}), \hat{\Psi}^{\dagger}}_{\delta^{(3)}(r-r')}(\vec{r}')\, h\, \hat{\vec{\Psi}}(\vec{r}')\right]$$

$$= h\, \hat{\vec{\Psi}}$$

substituting into (41)

$$i\hbar \frac{d}{dt} \phi = h \langle 0|\, \hat{\vec{\Psi}}(r,t)\, |\Psi\rangle = h\phi \quad \checkmark$$

For interacting systems we have to consider many-particle wavefunctions. For the typical two-body interactions we have to look at the two-particle wavefunction at the least:

$$i\hbar \frac{d}{dt} \phi(\vec{r}_1, \vec{r}_2, t) = h(\vec{r}_1, \vec{r}_2)\, \phi(\vec{r}_1, \vec{r}_2, t)$$

in second quantization this can be reproduced by

$$\boxed{\hat{H} = \int d^3r \int d^3r' \, \hat{\Psi}^+(\vec{r})\, \hat{\Psi}^+(\vec{r}')\, h(\vec{r}, \vec{r}')\, \hat{\Psi}(\vec{r}')\, \hat{\Psi}(\vec{r})}$$

(43) two-particle Hamiltonian (interaction)

(B) Ultra cold atoms with contact interaction

Systems of ultra-cold, neutral atoms are described in second quantization by a complex (non-hermitian) Schrödinger field $\hat{\Psi}(\vec{r}, t) \neq \hat{\Psi}^+(\vec{r}, t)$ with point interaction

(44)
$$\hat{H} = \int d^3r \, \hat{\Psi}^+(\vec{r}) \left[-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) \right] \hat{\Psi}(\vec{r}) + \int d^3r \int d^3r' \, \hat{\Psi}^+(\vec{r})\, \hat{\Psi}^+(\vec{r}')\, V(\vec{r} - \vec{r}')\, \hat{\Psi}(\vec{r})\, \hat{\Psi}(\vec{r}')$$

and

(45) $$\boxed{V(\vec{r}-\vec{r}') \simeq g\,\delta^{(3)}(\vec{r}-\vec{r}')}$$ pseudo-potential approximation

Here the microscopic atom-atom interaction is replaced by an effective pseudo-potential which has the same scattering properties at low temperatura (kinetic energies)

(46) $$\boxed{\begin{aligned}\hat{H} = &\int d^3\vec{r}\ \hat{\psi}^+(\vec{r})\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right]\hat{\psi}(\vec{r}) \\ &+ g\int d^3r\ \hat{\psi}^+(\vec{r})\,\hat{\psi}^+(\vec{r})\,\hat{\psi}(\vec{r})\,\hat{\psi}(\vec{r})\end{aligned}}$$

many-body Hamiltonian of ultra-cold gases

(C) Quantized electromagnetic field

A second field in which we are interested in quantum effects is

quantum nonlinear optics

Here the electromagnetic field $\vec{E}$ (and $\vec{B}$) is considered as a quantum field

Maxwell equations (SI units)

$$\boxed{\begin{aligned}&\vec{\nabla}\cdot\vec{B} = 0\\ &\vec{\nabla}\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = 0\end{aligned}} \quad (47) \qquad \text{homogeneous MWE}$$

$$\boxed{\begin{aligned}&\vec{\nabla}\cdot\vec{E} = \frac{\rho}{\varepsilon_0}\\ &\vec{\nabla}\times\vec{B} - \frac{1}{c^2}\frac{\partial}{\partial t}\vec{E} = \mu_0\vec{j}\end{aligned}} \quad (48) \qquad \text{inhomogeneous MWE}$$

$$c^2 = \frac{1}{\mu_0\varepsilon_0}$$

only consistent if

$$\boxed{\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{j} = 0} \quad (49) \qquad \text{continuity equation}$$

Homogeneous equations can be solved introducing potentials

$$\vec{B} = \vec{\nabla}\times\vec{A} \qquad \vec{E} = -\vec{\nabla}\phi - \frac{\partial}{\partial t}\vec{A} \quad (50)$$

$\vec{A}$: vector potential ; ϕ : scalar potential

radiation (Coulomb) gauge $\quad (\vec{j} = 0, \rho = 0)$ source free case

$$\vec{\nabla}\cdot\vec{A} = 0 \qquad \phi = 0 \quad (51)$$

Then one finds a wave equation for $\vec{A}$

$$(52) \qquad \boxed{\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta\right)\vec{A}(\vec{r},t) = 0}$$

The solutions of this equation are plane waves which are transversal

$$(53) \qquad \vec{A}(\vec{r},t) \sim \vec{e}(\vec{k})\, e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

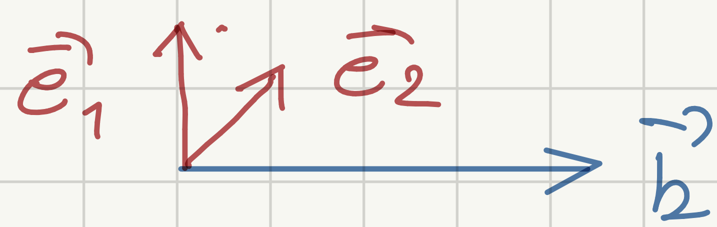
with

$$(54) \qquad \boxed{\omega = |\vec{k}|c} \qquad \boxed{\vec{e}(\vec{k})\cdot\vec{k} = 0}$$

transversality $\vec{\nabla}\cdot\vec{A} = 0$

For a given wave-vector $\vec{k}$ there are only two independent polarizations

$$\vec{e}_1(\vec{k})\cdot\vec{e}_2(\vec{k}) = 0 \qquad \vec{e}_i(\vec{k})\cdot\vec{k} = 0$$



e.g. linear polarizations

General Fourier-representation of $\vec{A}(\vec{r},t)$

$$(55) \qquad \vec{A}(\vec{r},t) = \frac{1}{\sqrt{2\varepsilon_0 L^3}} \sum_{\vec{k}_n} \sum_{\lambda=1,2} \vec{e}_\lambda(\vec{k})\, q_\lambda(\vec{k},t)\, e^{i\vec{k}\cdot\vec{r}}$$

$\Rightarrow \cdots \Rightarrow$ $q_\lambda(\vec{k},t)$ fulfill harmonic oscillator equations but are complex

(56) $$\ddot{q}_\lambda(\vec{k},t) + \omega_{\vec{k}}^2 \, q_\lambda(\vec{k},t) = 0$$

$$\vec{A} = \vec{A}^* \qquad q_\lambda^*(-\vec{k}) = q_\lambda(\vec{k})$$

classical harmonic oscillators

$\downarrow$

quantum harmonic oscillators

<u>canonical momenta</u> (mass = 1)

$$p_\lambda(\vec{k}) = \dot{q}_\lambda(\vec{k})$$

$$q_\lambda \to \hat{q}_\lambda \qquad p_\lambda \to \hat{p}_\lambda$$

(57) $$\left[\hat{q}_\lambda(\vec{k}), \hat{p}_{\lambda'}(\vec{k}')\right] = i\hbar\, \delta_{\lambda\lambda'} \delta_{\vec{k}\vec{k}'}$$

introduce ladder operators

(58) $$\hat{a}_\lambda(\vec{k}) = \sqrt{\frac{\omega_k}{2\hbar}} \left[\hat{q}_\lambda + i\hat{p}_\lambda\right]$$

(59) $$\boxed{\left[\hat{a}_\lambda(\vec{k}), \hat{a}^\dagger_{\lambda'}(\vec{k}')\right] = \delta_{\lambda\lambda'} \delta_{\vec{k}\vec{k}'}}$$

with this we eventually arrive at (Heisenberg pict.)

(60)
$$\boxed{\begin{aligned}\hat{\vec{A}}(\vec{r},t) = \sqrt{\frac{\hbar}{4\pi\varepsilon_0 L^3}} \sum_{\vec{k},\lambda} \frac{1}{\sqrt{\omega_k}} \vec{e}_\lambda(\vec{k}) \cdot \\ \cdot \left[\hat{a}_\lambda(\vec{k},t) e^{i\vec{k}\cdot\vec{r}} + \hat{a}^+_\lambda(\vec{k},t) e^{-i\vec{k}\cdot\vec{r}}\right]\end{aligned}}$$

(free Hamiltonian)

(61)
$$\boxed{\hat{H} = \sum_{\vec{k},\lambda} \hbar\omega_{\vec{k}} \left[\underbrace{\hat{a}^+_\lambda(\vec{k})\, \hat{a}_\lambda(\vec{k})}_{\text{number operator of photons in mode } (\vec{k},\lambda)} + \frac{1}{2}\right]}$$

number operator of photons in mode $(\vec{k},\lambda)$

divergent vacuum term $\to$ ignored

solution of time evolution $\hat{a}_\lambda(\vec{k},t) = \hat{a}_\lambda(\vec{k}) e^{-i\omega_k t}$

$\Rightarrow$

(62)
$$\boxed{\begin{aligned}\hat{\vec{E}}(\vec{r},t) = -\frac{\partial\hat{\vec{A}}(\vec{r},t)}{\partial t} = \\ = \sqrt{\frac{\hbar}{4\pi\varepsilon_0 L^3}} \sum_{\vec{k},\lambda} i\sqrt{\omega_{\vec{k}}}\, \vec{e}_\lambda(\vec{k}) \left[\hat{a}_\lambda(\vec{k}) e^{i\vec{k}\cdot\vec{r}} - \hat{a}^+_\lambda(\vec{k}) e^{-i\vec{k}\cdot\vec{r}}\right]\end{aligned}}$$

negative frequency part

positive frequency part