

# The Nature and Extent of Particles

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Motivation: Classical (quantum) mechanics: point particles with exact (uncertain) position. How about quantum field theory?

We deal with its covariant formalism, but how does it describe particles?

**Classical Hamilton mechanics:** point particles with  $x(t)$ ,  $p(t)$

**Canonical QM:** Hermitian operators  $\hat{x}$ ,  $\hat{p}$ ,  $[\hat{x}, \hat{p}] = i\hbar$ ,  $\Delta x \Delta p \geq \hbar/2$

Position smeared out to wave function  $\Psi(t, x) = \langle x | \psi(t) \rangle$ , point particle with uncertain position  $\rightarrow$  interference effects

**Field theory:** degrees of freedom: immobile fields, no particle coordinates, *e.g.* classical electrodynamics  $\vec{E}(t, \vec{x})$ ,  $\vec{B}(t, \vec{x})$ , or continuum mechanics with density  $\rho(t, \vec{x})$ . A wave covers some region, not point-like.

## Canonical quantum field theory:

Operator-valued fields, excitations  $\sim$  “particles”, *e.g.* photons in QED, or phonons in field theory of a vibrating crystal, fields fluctuate in quanta.

### Terminology (in this talk)

- **“Particle”**: QM, position usually uncertain, but point-like
- **“Wavicle”**: Quantized field excitation, relativistic and more fundamental. Features and localization are subtle, to be discussed in a toy model.

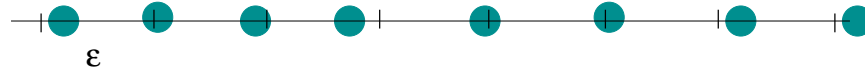
Term suggested by Wilczek, distinction unusual, but useful for this talk.

## Toy model: 1d chain of coupled ions

Ions described by particles in (non-relativistic) QM

“Crystal”: coupled harmonic oscillators, equilibrium distance  $\epsilon$

● ions



$$\begin{aligned}\hat{H} &= \sum_{n=1}^N \left[ \frac{1}{2M} \hat{p}_n^2 + \frac{1}{2} M \omega_0^2 (\hat{x}_{n+1} - \hat{x}_n - \epsilon)^2 \right] \\ &= \sum_{n=1}^N \left[ \frac{1}{2M} \hat{p}_n^2 + \frac{1}{2} M \omega_0^2 (\hat{y}_{n+1} - \hat{y}_n)^2 \right], \quad \hat{y}_n = \hat{x}_n - n\epsilon, \quad \hat{y}_{N+1} = \hat{y}_1\end{aligned}$$

$M$ : ion mass;  $\hat{y}_n$ : displacement; periodic b.c.:  $\hat{x}_{N+1} = \hat{x}_1 + \overbrace{N\epsilon}^L$   
Actually a ring, simplifies Fourier analysis, at the end  $N, L \rightarrow \infty$ .

Strictly speaking: model should be in space-time dimension  $> 2$  and  $L \rightarrow \infty$ , otherwise no crystalline order: requires spontaneous breaking of translation sym. [Mermin-Wagner Theorem], but 1d notation is instructive.

- $\mathbb{Z}(N)$  shift symmetry:  $\hat{y}_n \rightarrow \hat{y}_{n+1}$  ( $n < N$ ), and  $\hat{y}_N \rightarrow \hat{y}_1$

Fourier series:

$$\hat{y}(k) = \sum_{n=1}^N \hat{y}_n e^{-in\epsilon} = \hat{y}(-k)^\dagger = \hat{y}\left(k + \frac{2\pi}{\epsilon}\right), \quad \hat{y}_n = \frac{1}{N} \sum_k \hat{y}(k) e^{in\epsilon}$$

Bloch wave number  $k = \frac{2\pi m}{L} \in B = \left(-\frac{\pi}{\epsilon}, \frac{\pi}{\epsilon}\right]$   
(actually  $k_m$ , but this messes up the notation).

Periodicity over Brillouin zone  $B$  due to  $\epsilon > 0$ , and discrete if  $L > \infty$ .

For  $N$  even:  $m = -\frac{N}{2} + 1, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1, \frac{N}{2}$

- Sym. under continuous translation of all ions.

Noether: conservation of total momentum  $\hat{P} = \sum_n \hat{p}_n$

## Hamilton operator in Fourier space

$$\hat{T} = \frac{1}{2M} \sum_n \hat{p}_n^2 = \frac{1}{2MN} \sum_k \hat{p}(k)^\dagger \hat{p}(k) \quad (\text{Parseval})$$

$$\begin{aligned} \hat{V} &= \frac{M\omega_0^2}{2} \sum_n (\hat{y}_{n+1} - \hat{y}_n)^2 \\ &= \frac{M\omega_0^2}{2N^2} \sum_{k, k'} \hat{y}(k) \hat{y}(k') \left[ \sum_n \left( e^{-ik(n+1)\epsilon} - e^{-ikn\epsilon} \right) \left( e^{-ik'(n+1)\epsilon} - e^{-ik'n\epsilon} \right) \right] \\ &= \frac{M}{2N} \sum_k \hat{y}(k)^\dagger \hat{y}(k) \omega(k)^2, \quad \omega(k) = 2\omega_0 \left| \sin \frac{k\epsilon}{2} \right| \end{aligned}$$

where we used Poisson's formula:  $\frac{1}{N} \sum_n e^{i(k-k')n\epsilon} = \delta_{kk'}$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{P}^2}{2MN} + \frac{1}{N} \sum_{k \neq 0} \left[ \frac{\hat{p}(k)^\dagger \hat{p}(k)}{2M} + \frac{M\omega(k)^2}{2} \hat{y}(k)^\dagger \hat{y}(k) \right]$$

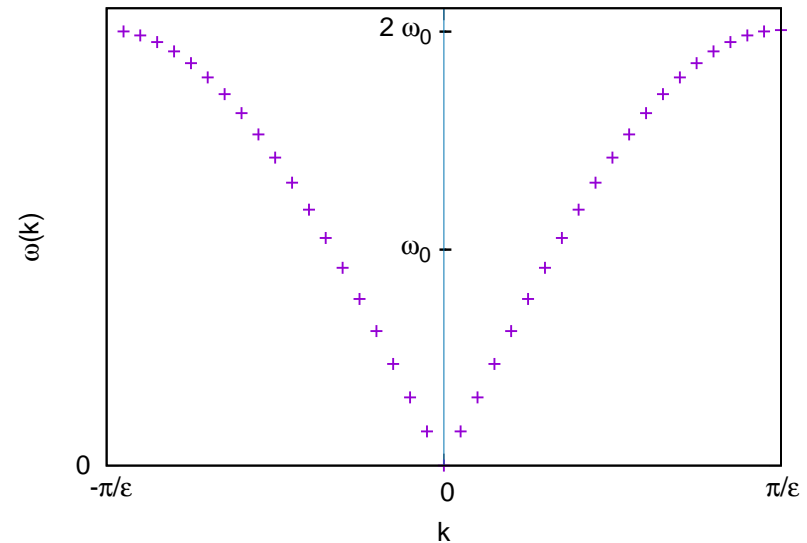
The  $k = 0$ -mode represents an overall motion, with  $\hat{P}$  and mass  $MN$ .

$k \neq 0$  (discrete, in  $B$ ) oscillations with  $\omega(k)$

$$\omega(k) = 2\omega_0 \left| \sin \frac{k\epsilon}{2} \right| \text{ for } N = 40 :$$

$$|k| \text{ small: } \omega \simeq \omega_0 |k| \epsilon,$$

$$|k| \lesssim \pi/\epsilon : \omega \lesssim 2\omega_0$$



## Phonons: quantized vibrations

Phonon annihilation and creation operator, analogous to harm. oscillator

$$\begin{aligned}\hat{a}(k) &= \frac{1}{\sqrt{2N}} \left( \alpha(k) \hat{y}(k) + \frac{i}{\hbar \alpha(k)} \hat{p}(k) \right) \\ \hat{a}(k)^\dagger &= \frac{1}{\sqrt{2N}} \left( \alpha(k) \hat{y}(k)^\dagger - \frac{i}{\hbar \alpha(k)} \hat{p}(k)^\dagger \right) \\ \alpha(k) &\doteq \sqrt{M \omega(k) / \hbar} \quad (\text{for } k \neq 0)\end{aligned}$$

Familiar commutation relations

$$[\hat{y}_n, \hat{p}_{n'}] = i\hbar \delta_{nn'} \quad , \quad [\hat{y}_n, \hat{y}_{n'}] = 0 = [\hat{p}_n, \hat{p}_{n'}]$$

imply in Fourier space

$$[\hat{y}(k), \hat{p}(k')^\dagger] = i\hbar N \delta_{kk'} , \quad [\hat{y}(k), \hat{y}(k')] = 0 = [\hat{p}(k), \hat{p}(k')]$$

and therefore

$$[\hat{a}(k), \hat{a}(k')^\dagger] = i\hbar N \delta_{kk'} , \quad [\hat{a}(k), \hat{a}(k')] = 0 = [\hat{a}(k)^\dagger, \hat{a}(k')^\dagger]$$

Computation of  $\hat{a}(k)^\dagger \hat{a}(k)$  leads to another familiar expression:

$$\hat{H} = \frac{\hat{P}^2}{2NM} + \sum_{k \neq 0} \hbar \omega(k) \left( \underbrace{\hat{a}(k)^\dagger \hat{a}(k)}_{\hat{\nu}(k)} + \frac{1}{2} \right)$$

$\hat{\nu}(k)$ : phonon number operator of the Bloch wave number  $k$



## Quantum states of a vibrating crystal

Energy eigenstates are given by:

- total momentum  $P$
- phonon occupation number  $\nu(k)$  to each Bloch wave number

Ground state  $|0\rangle$  :  $P = 0, \nu(k) = 0, \forall k$

$$\hat{P}|0\rangle = 0, \quad \hat{a}(k)|0\rangle = 0, \quad E_0 = \langle 0|\hat{H}|0\rangle = \frac{\hbar}{2} \sum_k \omega(k)$$

Thermodyn. limit  $N \rightarrow \infty$  :  $\sum_k \rightarrow \int_B dk$ , energy density

$$\frac{E_0}{L} = \frac{\hbar}{4\pi} \int_{-\pi/\epsilon}^{\pi/\epsilon} dk \, 2\omega_0 \left| \sin \frac{k\epsilon}{2} \right| = \frac{2\hbar\omega_0}{\pi\epsilon} \underbrace{\quad}_{\epsilon \rightarrow 0} \infty$$

**Cosmological Constant** (truncate  $\frac{\pi}{\epsilon} = M_{\text{Planck}}$ , requires TINY  $\omega_0 \dots$ ).

Consider only energy differences, but maintain  $N \rightarrow \infty$

$\frac{P^2}{2MN} = 0$  at any finite  $P$ , degenerate ground states

SSB of translation invariance, phonon as Nambu-Goldstone boson (in  $d > 2$ )

- 1-phonon state:  $|k\rangle = \hat{a}(k)^\dagger |0\rangle$

$$E(k) - E_0 = \hbar\omega(k) = 2\hbar\omega_0 \left| \sin \frac{k\epsilon}{2} \right|$$

▷ **small**  $|k|$  :  $E(k) \simeq \hbar|k| \omega_0\epsilon$

linear in  $\hbar k$ , *i.e.* “**relativistic**” with respect to  $c \doteq \omega_0\epsilon$  : **speed of sound**

▷  $|k| \rightarrow \frac{\pi}{\epsilon}$  : **group velocity**  $c(k) = \left| \frac{\partial E}{\partial(\hbar k)} \right| = \omega_0\epsilon \cos \frac{k\epsilon}{2} \rightarrow 0$

- 2-phonon state :  $|k_1, k_2\rangle = \hat{a}(k_1)^\dagger \hat{a}(k_2)^\dagger |0\rangle = |k_2, k_1\rangle$

**Bosons,  $\nu(k)$  unlimited**

# Wavicle localization

How extended are wavicle, in this case 1-phonon states?

QM position eigenstate

$$|n\rangle = \frac{\epsilon}{2\pi} \int_B dk |k\rangle e^{ikn\epsilon} = \hat{a}_n^\dagger |0\rangle \quad \text{with} \quad \hat{a}_n^\dagger = \frac{\epsilon}{2\pi} \int_B dk \hat{a}(k)^\dagger e^{ikn\epsilon}$$

$$\Rightarrow [\hat{a}_n, \hat{a}_{n'}^\dagger] = \delta_{nn'} , \quad [\hat{a}_n, \hat{a}_{n'}] = 0 = [\hat{a}_n^\dagger, \hat{a}_{n'}^\dagger]$$

QM picture:  $\hat{a}_n^\dagger$  creates a phonon, solely at position  $n$ .

Works for decoupled oscillators (no geometry!), but fails in field theory:

$$\hat{a}_n^\dagger = \frac{\epsilon}{2\pi} \int_B dk \frac{1}{\sqrt{2N}} \underbrace{\left( \alpha(k) \hat{y}(k)^\dagger - \frac{i}{\hbar \alpha(k)} \hat{p}(k)^\dagger e^{ikn\epsilon} \right)}_{\hat{a}(k)^\dagger}, \quad \alpha(k) \doteq \sqrt{\frac{M\omega(k)}{\hbar}}$$

Convolution in coordinate space:

$$\hat{a}_n^\dagger = \frac{1}{\sqrt{N}} \sum_{n'} \left( f_{n-n'} \hat{y}_n - g_{n-n'} \frac{i}{\hbar} \hat{p}_n \right)$$

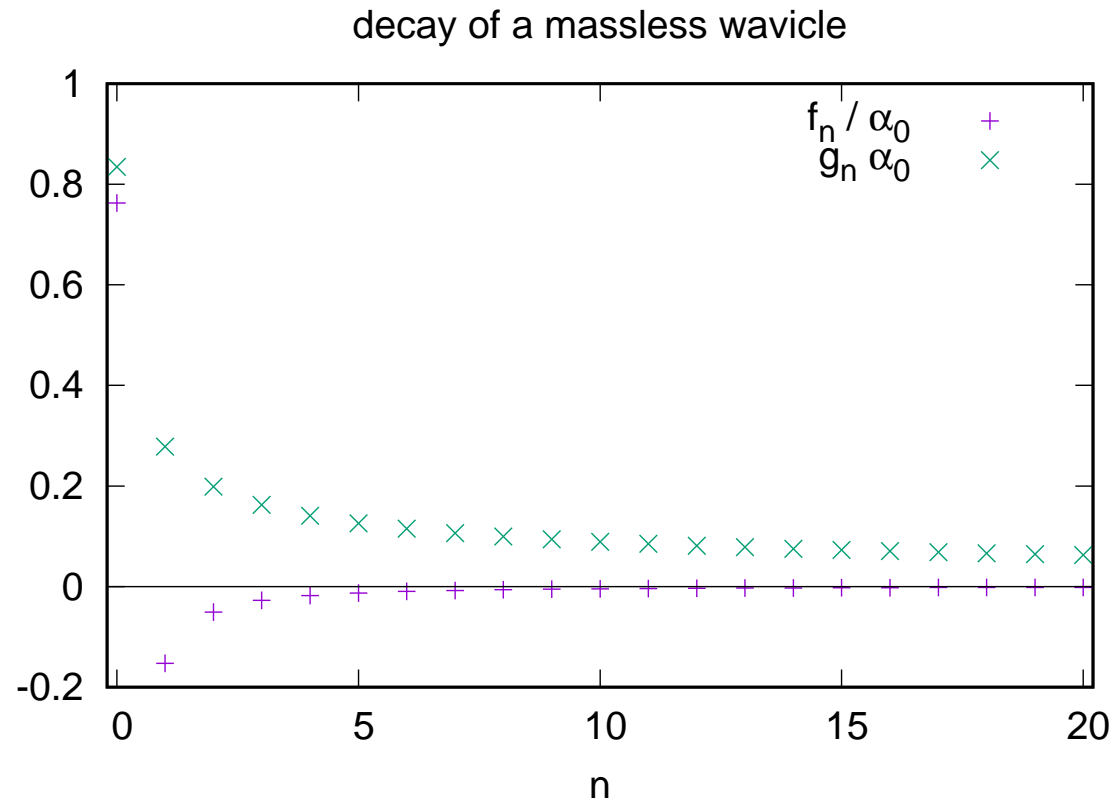
$$f_n = f_{-n} = \frac{\epsilon}{2\pi\sqrt{\hbar}} \int_B dk \left( M\omega_0 \left| \sin \frac{k\epsilon}{2} \right| \right)^{1/2} \cos(kn\epsilon)$$

$$g_n = g_{-n} = \frac{\epsilon\sqrt{\hbar}}{2\pi} \int_B dk \left( M\omega_0 \left| \sin \frac{k\epsilon}{2} \right| \right)^{-1/2} \cos(kn\epsilon)$$

At large  $|n|$  :

$$f_n \propto \frac{1}{|n|^{3/2}} , \quad g_n \propto \frac{1}{|n|^{1/2}}$$

**Power-law decays**  $\longrightarrow$  **non-local!** Creation of one phonon at position  $n$  requires exciting the entire crystal, in a coordinated manner.



Wavicle decay, in units of  $\alpha_0 \doteq \sqrt{M\omega_0/\hbar}$ . The convolution terms  $f_n$  and  $g_n$  describe excitations of ions, at distance  $n\epsilon$ , regarding **displacement** and **momentum**. Both are non-local;  $g_n$  decays very slowly.

## Massive wavicles

So far: phonon mass = 0 ( $\neq$  ion mass  $M$ ), NGBs in  $d > 2$

Add mass by explicit translation sym. breaking:

$$\hat{V}' = \frac{M\omega_0'^2}{2} \sum_n (\overbrace{\hat{x}_n - n\epsilon}^{\hat{y}_n})^2 = \frac{M\omega_0'^2}{2N} \sum_k \hat{y}(k)^\dagger \hat{y}(k)$$

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}' = \hbar \sum_k \left( \hat{v}(k) + \frac{1}{2} \right) \omega(k)$$

$$\omega(k) = \left[ \left( 2\omega_0 \sin \frac{k\epsilon}{2} \right)^2 + \omega_0'^2 \right]^{1/2}$$

At small  $|k|$ : “relativistic”

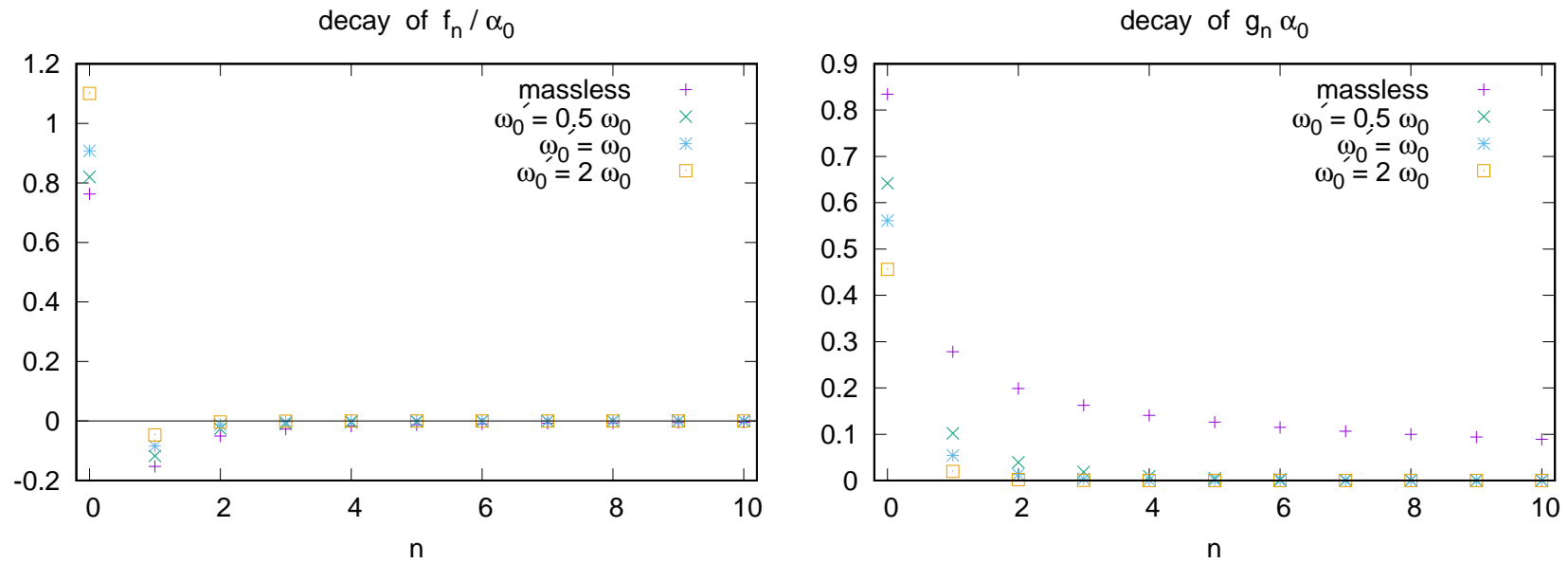
$$E_{\text{phonon}}(k) = \hbar\omega(k) \simeq \left[ (\hbar kc)^2 + \overbrace{(\hbar\omega'_0)^2}^{mc^2} \right]^{1/2}$$

Phonon mass  $m = \frac{\hbar\omega'_0}{c^2} = \frac{\hbar\omega'_0}{\omega_0^2\epsilon^2}$  (with  $c = \omega_0\epsilon$ )

Now  $f_n, g_n$  decay exponentially:

$$f_n, g_n \propto \exp\left(-\frac{mc \overbrace{|n|\epsilon}^{|x|}}{\hbar}\right) \doteq \exp\left(-\frac{|x|}{\lambda_{\text{phonon}}}\right), \quad \lambda_{\text{phonon}} = \frac{\hbar}{mc}$$

Compton wave length, localization scale of a massive phonon, local



Decay of  $f_n$  and  $g_n$  (in units of  $\alpha_0$ ), related to ion displacement and momentum, for wavicle mass  $m = \hbar\omega'_0/c^2$ , with  $\omega'_0 = 0, 0.5\omega_0, \omega_0, 2\omega_0$ .



## Transition to field theory, continuum limit

Debye: field theory of vibrating solid  $\sim$  lattice regularized quantum field theory

Scalar field and its conjugate:

$$\begin{aligned}\hat{\Phi}(x = n\epsilon) &= \sqrt{M\omega_0^2\epsilon} \hat{y}_n \\ \hat{\Pi}(x = n\epsilon) &= \frac{1}{\sqrt{M\omega_0^2\epsilon}} \hat{p}_n = -\frac{i\hbar}{\sqrt{M\omega_0^2\epsilon^3}} \frac{\partial}{\partial y_n} = -\frac{i\hbar}{\epsilon} \frac{\partial}{\partial \Phi}\end{aligned}$$

Constants arrange for right dimensions, and

$$[\hat{\Phi}(x), \hat{\Pi}(x')] = \frac{i\hbar}{\epsilon} \delta_{nn'} \xrightarrow{\epsilon \rightarrow 0} i\hbar \delta(x - x')$$

$$\begin{aligned}
\hat{H} &= \sum_n \left[ \frac{\hat{p}_n^2}{2M} + \frac{M\omega_0^2}{2} (\hat{y}_{n+1} - \hat{y}_n)^2 + \frac{M\omega_0'^2}{2} \hat{y}_n^2 \right] \\
&= \frac{\epsilon}{2} \sum_x \left[ c^2 \hat{\Pi}(x)^2 + \left( \frac{\hat{\Phi}(x+\epsilon) - \hat{\Phi}(x)}{\epsilon} \right)^2 + \left( \frac{mc}{\hbar} \right)^2 \hat{\Phi}(x)^2 \right] \\
&\xrightarrow{\epsilon \rightarrow 0} \frac{1}{2} \int_0^L dx \left[ c^2 \hat{\Pi}(x)^2 + \partial_x \hat{\Phi}(x) \partial_x \hat{\Phi}(x) + \left( \frac{mc}{\hbar} \right)^2 \hat{\Phi}(x)^2 \right]
\end{aligned}$$

Continuum limit: renormalize  $\omega_0$  such that  $c = \omega_0 \epsilon$  is kept finite,  
can be turned into the speed of light  $\rightarrow$  covariant field theory

Then  $\lambda_{\Phi}^{-1} = \frac{mc}{\hbar} = \frac{\omega_0'}{c}$  is finite as well, no need to renormalize  $\omega_0'$

## Reduction of a wavicle to a QM particle

In many setting, QM works to a good approximation;  
then wavicle reduction should be possible.

Recipe:

Construct  $\hat{H}_{\text{QM}}$  with spectrum of wavicle energies  $E(k) = \hbar\omega(k)$ .

Valid at low  $|k|$ , such that

$$\frac{2\pi}{|k|} \gg \lambda_{\Phi} = \frac{\hbar}{mc} \quad \Rightarrow \quad \hbar|k| \ll mc$$

Matches exactly non-relativistic limit for de Broglie momentum  $\hbar|k|$ ,  
if transition to quantum field theory converts  $c$  into speed of light.

Then QM is not that wrong:  $\approx$  non-relativistic point particles

Example: H-atom, characteristic scale  $r_{\text{Bohr}} = \frac{\hbar^2}{e^2 m_e} \simeq 0.53 \text{ \AA}$

QM for electron works quite well, because

$$\lambda_e = \frac{\hbar}{m_e c} = \alpha r_{\text{Bohr}} \quad \text{with} \quad \alpha = \frac{e^2}{\hbar c} = \frac{1}{137.036 \dots}$$

$\lambda_e$  does not know about the electric charge.  $\alpha$  relates it to the H-atom, at a larger scale, since the coupling is rather weak.

Still, high energy reveals corrections, in particular the Lamb shift.

**Conclusion: Quantized field excitations (“wavicles”, *i.e.* particles in a fundamental and covariant sense) are not point-like.**

They decay exponentially over the range of the Compton wave length  $\hbar/mc$ ; in the massless case (photons), they are non-local.

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