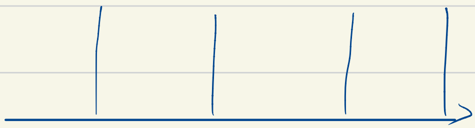
Reading Material.

Landau 力学 27-29节

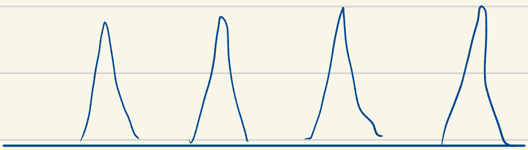
P89，注释①

$$V(x) = \sum_n \frac{A}{(x-na)^2 + P^2}$$

$P \to 0$



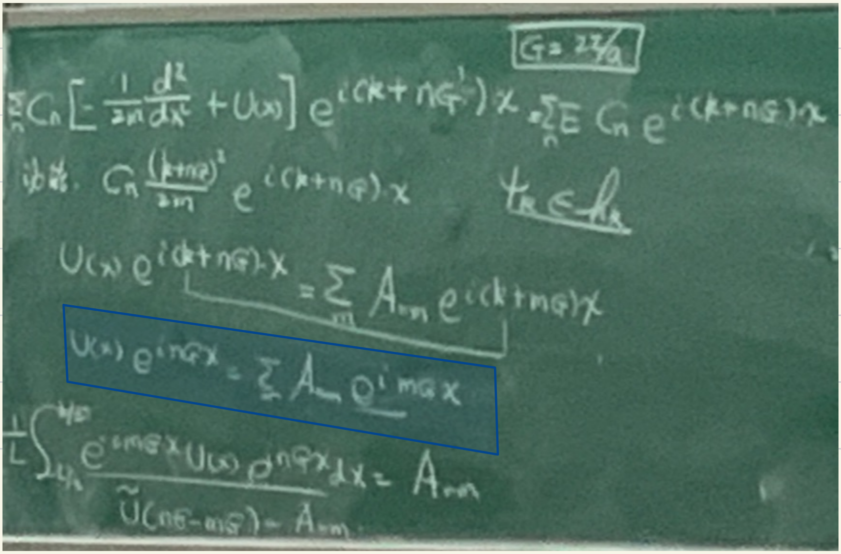
P较大



或 $V(x) = \sum_n A e^{-\frac{(x-na)^2}{2\sigma^2}}$

如何求解 $\left(-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right)\varphi_k(x) = E_k \varphi_k(x)$

$$\varphi_k(x) = \sum_n C_n e^{i(k+Gn)x}, \quad G = \frac{2\pi}{a}$$



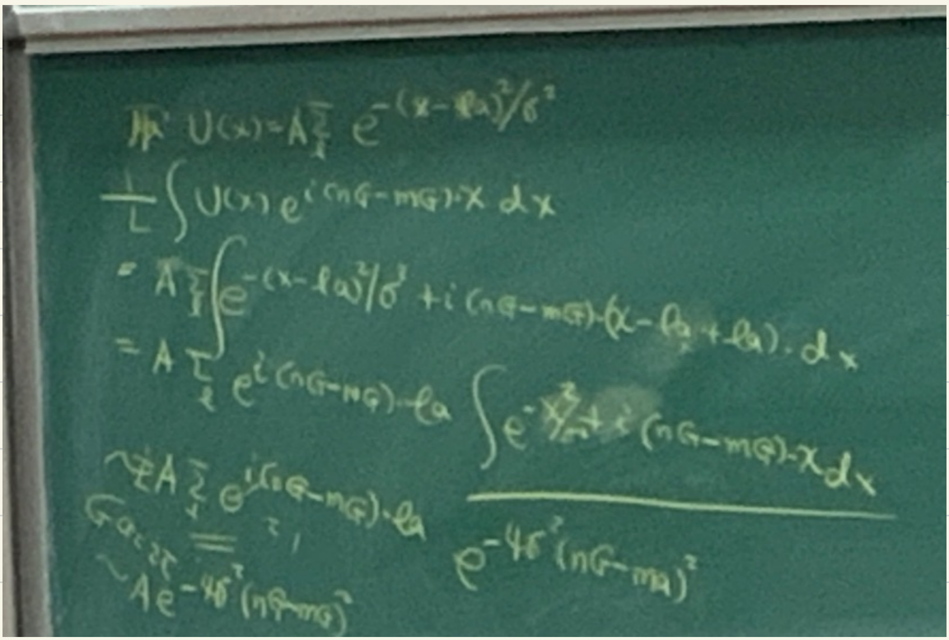
$$\Rightarrow \sum_n \frac{1}{2}(k+nG)^2 e^{i(k+nG)x} + \sum_{nm} A_{nm} C_n e^{i(k+mG)x} = \sum_n E C_n e^{i(k+nG)x}$$

取 $e^{i(k+lG)}$ 分量

$$\frac{(k+lG)^2}{2} C_l + \sum_n A_{nl} C_n = E C_l$$

$$A_{nl} = \tilde{U}(nG-lG)$$

计算 A_{nl}



无法进行解析计算时，我们也可以进行数值计算。

一个常用的计算 A_{nl} 的技巧是快速Fourier变换。

BZ、倒格点

2D、3D怎么取 $\vec{G}$

$$\vec{R} = n\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$e^{i(\vec{k}+\vec{G})\cdot(\vec{x}+\vec{R})}$$

$$= e^{i(\vec{k}+\vec{G})\vec{x}} e^{i\vec{k}\cdot\vec{R}}$$

$$\Rightarrow \vec{G}\cdot\vec{R} = 2\pi m \Rightarrow \begin{cases} \vec{a}_1 = \dfrac{2\pi\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \\ \vec{a}_2 = \dfrac{2\pi\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \\ \vec{a}_3 = 2\pi\vec{a}_3/V \end{cases}$$

二次量子化

(正则量子化)

$$H = \sum_{ij} h_{ij} C_i^\dagger C_j \qquad HC = EC \qquad \sum_j h_{ij} C_j = E C_i$$

Ref: ① Joy. Schondan, second quantization.

② Simons. Chap 2

量子化条件 $[q_i, p_i] = i\hbar\delta_{ij}$.

$$a^\pm = \frac{1}{\sqrt{\hbar\omega}}\left(\sqrt{\tfrac{1}{2}m\omega^2}\,x \pm i\frac{p}{\sqrt{2m}}\right)$$

$$\Downarrow$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega(a^\dagger a + 1/2)$$

$$\int |p\rangle\langle p| dp = \int |x\rangle\langle x| dx = 1 \qquad \sum_n |n\rangle\langle n| = 1$$

P.S. 哈密顿力学

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \{p_i, H\}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \{q_i, H\}$$

$$\{q_i, q_j\} = 0$$

泊松括号

$$\{p_i, p_j\} = 0$$

$$\{p_i, q_j\} = \delta_{ij}$$

为什么要使用产生湮灭算符表示

二次量子化 解决的问题 ① 算子.

② 推广到任意的维度.

③ 利于在全同粒子中使用

$$[x, p] = i\hbar \underset{\text{等价于}}{\Longleftrightarrow} [a, a^+] = 1.$$

$\Downarrow$ 推广到多自由度.

$$\begin{cases} [a_i, a_j^+] = \delta_{ij} \\ [a_i, a_j] = 0 \\ [a_i^+, a_j^+] = 0 \end{cases}$$

$\Leftarrow$ 和泊松括号类似.

则作用于态上有

$$\begin{cases} a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle = \sqrt{n}\,|n-1\rangle \\ a^+a|n\rangle = n|n\rangle \end{cases}$$

一个应用.

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \lambda x^4 \\ &= \hbar\omega(a^+a + \tfrac{1}{2}) + \lambda \left(\sqrt{\frac{\hbar}{2m\omega}}\right)^4 (a+a^+)^4 \\ &= \hbar\omega(a^+a + \tfrac{1}{2}) + \lambda'(a+a^+)^4 \end{aligned}$$

可以直接利用其作用在态上的规则来进行求解.

$$\langle n|(a+a^\dagger)^4|m\rangle = \langle n|\, a^{s_1} a^{s_2} a^{s_3} a^{s_4} |m\rangle . \qquad s = \underset{a}{\underset{\downarrow}{-1}}\, ,\ \underset{a^\dagger}{\underset{\downarrow}{1}}$$

$$a^s|n\rangle = \sqrt{n+\frac{1+s}{2}}\,|n+s\rangle$$ 我们可以不用求解积分。

全同粒子的表示。$\begin{cases} \text{对易、反对易} \\ \text{简洁的表示} \end{cases}$