Homework 10

Jiinyuan Wu

November 15, 2022

Problem 1
Solution

(a) From

$$w\left(\boldsymbol{r}-\boldsymbol{r}_n\right)=N^{-1/2}\sum_{\boldsymbol{k}}\exp\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_n\right)\psi_{\boldsymbol{k}}(\boldsymbol{r}) \tag{1}$$

we have

$$\begin{aligned}\int \mathrm{d}^3\boldsymbol{r}\, w(\boldsymbol{r}-\boldsymbol{r}_n)w^*(\boldsymbol{r}-\boldsymbol{r}_m)&=\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_n}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_m}\int \mathrm{d}^3\boldsymbol{r}\,\psi_{\boldsymbol{k}}(\boldsymbol{r})\psi^*_{\boldsymbol{k}'}(\boldsymbol{r})\\ &=\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\boldsymbol{k}\boldsymbol{k}'}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_n}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_m}\\ &=\frac{1}{N}\sum_{\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_m-\boldsymbol{r}_n)}\\ &=\delta_{mn}.\end{aligned}$$

So when $m\neq n$, we have

$$\int \mathrm{d}^3\boldsymbol{r}\, w(\boldsymbol{r}-\boldsymbol{r}_n)w^*(\boldsymbol{r}-\boldsymbol{r}_m)=0. \tag{2}$$

(b) We have

$$\begin{aligned}w(x-x_n)&=\frac{1}{\sqrt{N}}\sum_k \mathrm{e}^{-\mathrm{i}kx_n}\underbrace{\frac{1}{\sqrt{N}}\mathrm{e}^{\mathrm{i}kx}u_0(x)}_{\psi_k(x)}\\ &=\frac{1}{N}u_0(x)\sum_k \mathrm{e}^{\mathrm{i}k(x-x_n)}\\ &=\frac{1}{N}u_0(x)\sum_{i=1}^{N}\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi i/L}\\ &=\frac{1}{N}u_0(x)\frac{\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi/L}\left(1-\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi N/L}\right)}{1-\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi/L}}\\ &=\frac{1}{N}u_0(x)\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi/L}\frac{\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi N/L}}{\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi/L}}\frac{\mathrm{e}^{-\mathrm{i}(x-x_n)\cdot\pi N/L}-\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi N/L}}{\mathrm{e}^{-\mathrm{i}(x-x_n)\cdot\pi/L}-\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi/L}}\\ &=\frac{1}{N}u_0(x)\mathrm{e}^{\mathrm{i}(x-x_n)\cdot 2\pi/L}\frac{\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi N/L}}{\mathrm{e}^{\mathrm{i}(x-x_n)\cdot\pi/L}}\frac{\sin\pi(x-x_n)N/L}{\sin\pi(x-x_n)/L}.\end{aligned}$$

Note that $L=Na$, and therefore

$$\frac{\sin\pi(x-x_n)N/L}{\sin\pi(x-x_n)/L}=\frac{\sin\pi(x-x_n)/a}{\sin\pi(x-x_n)/Na}\approx\frac{\sin\pi(x-x_n)/a}{\pi(x-x_n)/Na},$$

and therefore

$$w(x-x_n)=\mathrm{e}^{\mathrm{i}\cdot\text{some number}}\cdot u_0(x)\frac{\sin\pi(x-x_n)/a}{\pi(x-x_n)/a}, \tag{3}$$

and we can just throw away the unitary prefactor and therefore

$$w(x-x_n)=u_0(x)\frac{\sin\pi(x-x_n)/a}{\pi(x-x_n)/a}. \tag{4}$$

Problem 2

Solution

(a) Following the standard procedure to find the band structure, we have

$$\begin{aligned} E_{\boldsymbol{k}} &= A + \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} h(\boldsymbol{R}) \\ &= A - t\mathrm{e}^{\mathrm{i}ka} - t\mathrm{e}^{-\mathrm{i}ka} = A - 2t\cos(ka). \end{aligned} \tag{5}$$

(b) The smallest energy is taken when $k = 0$, and here we have

$$m^* = \frac{1}{\hbar^2}\frac{\partial^2 E_k}{\partial k^2} = 2t\frac{a^2}{\hbar^2}\cos ka|_{k=0} = 2t\frac{a^2}{\hbar^2}. \tag{6}$$

The largest energy is taken when $k = \pm\pi/a$, and

$$m^* = \frac{1}{\hbar^2}\frac{\partial^2 E_k}{\partial k^2} = 2t\frac{a^2}{\hbar^2}\cos ka|_{k=\pi/a} = -2t\frac{a^2}{\hbar^2}. \tag{7}$$