Many-body Physics Homework 2

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September 18, 2022

Problem 4
Solution

(a) We do the Trotter decomposition again:

$$\langle \boldsymbol{k}_f | \mathrm{e}^{-\mathrm{i}Ht} | \boldsymbol{k}_i \rangle = \lim_{N\to\infty} \prod_{j=1}^{N-1} \int \frac{V}{(2\pi)^3} \, \mathrm{d}^3\boldsymbol{k}_j \cdot \prod_{j=1}^{N} \langle \boldsymbol{k}_j | \mathrm{e}^{-\mathrm{i}\Delta t H} | \boldsymbol{k}_{j-1} \rangle \,, \quad \boldsymbol{k}_0 = \boldsymbol{k}_i, \quad \boldsymbol{k}_N = \boldsymbol{k}_f.$$

Each time step is given by

$$\begin{aligned} & \langle \boldsymbol{k}_j | \mathrm{e}^{-\mathrm{i}\Delta t (H_0 + \hat{\boldsymbol{x}}^2/2\alpha - \boldsymbol{E}\cdot\hat{\boldsymbol{x}})} | \boldsymbol{k}_{j-1} \rangle \\ = {} & \langle \boldsymbol{k}_j | \mathrm{e}^{-\mathrm{i}\Delta t (\hat{\boldsymbol{x}}^2/2\alpha - \boldsymbol{E}\cdot\hat{\boldsymbol{x}})} | \boldsymbol{k}_{j-1} \rangle \, \mathrm{e}^{-\Delta t \epsilon_{\boldsymbol{k}_{j-1}}} \\ = {} & \mathrm{e}^{-\Delta t \epsilon_{\boldsymbol{k}_{j-1}}} \int \mathrm{d}^3\boldsymbol{r} \, u^*_{\boldsymbol{k}_j}(\boldsymbol{r}) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\Delta t (\boldsymbol{r}^2/2\alpha - \boldsymbol{E}\cdot\boldsymbol{r})} u_{\boldsymbol{k}_{j-1}}(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{j-1}\cdot\boldsymbol{r}} \\ = {} & \mathrm{e}^{-\Delta t \epsilon_{\boldsymbol{k}_{j-1}}} \int \mathrm{d}^3\boldsymbol{r} \, u^*_{\boldsymbol{k}_j}(\boldsymbol{r}) u_{\boldsymbol{k}_{j-1}}(\boldsymbol{r}) \mathrm{e}^{-\frac{1}{2}\frac{\mathrm{i}\Delta t}{\alpha}\boldsymbol{r}^2 + \mathrm{i}\boldsymbol{r}\cdot(\Delta t \boldsymbol{E} + \boldsymbol{k}_{j-1} - \boldsymbol{k}_j)}. \end{aligned}$$

The semi-classical dynamics only works when $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ is "concentrated" enough in the reciprocal space, which means $u_{\boldsymbol{k}}(\boldsymbol{r})$ should be very smooth compared with $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$ (or otherwise the picture of an electron with a certain momentum traveling in the material is simply wrong). Thus, we have

$$\begin{aligned} & \int \mathrm{d}^3\boldsymbol{r} \, u^*_{\boldsymbol{k}_j}(\boldsymbol{r}) u_{\boldsymbol{k}_{j-1}}(\boldsymbol{r}) \mathrm{e}^{-\frac{1}{2}\frac{\mathrm{i}\Delta t}{\alpha}\boldsymbol{r}^2 + \mathrm{i}\boldsymbol{r}\cdot(\Delta t \boldsymbol{E} + \boldsymbol{k}_{j-1} - \boldsymbol{k}_j)} \\ = {} & \frac{1}{V_{\text{u.c.}}} \int_{\text{u.c.}} \mathrm{d}^3\boldsymbol{r} \, u^*_{\boldsymbol{k}_j}(\boldsymbol{r}) u_{\boldsymbol{k}_{j-1}}(\boldsymbol{r}) \int \mathrm{d}^3\boldsymbol{r} \, \mathrm{e}^{-\frac{1}{2}\frac{\mathrm{i}\Delta t}{\alpha}\boldsymbol{r}^2 + \mathrm{i}\boldsymbol{r}\cdot(\Delta t \boldsymbol{E} + \boldsymbol{k}_{j-1} - \boldsymbol{k}_j)}, \end{aligned}$$

and the Gaussian integral on the RHS can be evaluated as

$$\begin{aligned} & \int \mathrm{d}^3\boldsymbol{r} \, \mathrm{e}^{-\frac{1}{2}\frac{\mathrm{i}\Delta t}{\alpha}\boldsymbol{r}^2 + \mathrm{i}\boldsymbol{r}\cdot(\Delta t \boldsymbol{E} + \boldsymbol{k}_{j-1} - \boldsymbol{k}_j)} \\ = {} & \sqrt{\frac{(2\pi)^3}{(\mathrm{i}\Delta t/\alpha)^3}} \mathrm{e}^{\frac{1}{2}\frac{\alpha}{\mathrm{i}\Delta t}(\mathrm{i}(\Delta t \boldsymbol{E} + \boldsymbol{k}_{j-1} - \boldsymbol{k}_j))^2} \\ = {} & \sqrt{\frac{(2\pi)^3}{(\mathrm{i}\Delta t/\alpha)^3}} \mathrm{e}^{\frac{\mathrm{i}\alpha}{2}(\boldsymbol{E} - \dot{\boldsymbol{k}})^2 \Delta t}. \end{aligned}$$

Thus

$$\langle \boldsymbol{k}_f | \mathrm{e}^{-\mathrm{i}Ht} | \boldsymbol{k}_i \rangle = \lim_{N\to\infty} \mathcal{N} \prod_{j=1}^{N-1} \int \mathrm{d}^3\boldsymbol{k}_j \, \frac{1}{V_{\text{u.c.}}} \int \mathrm{d}^3\boldsymbol{r} \, u^*$$

For Putting all normalization factors into the measure, we get

$$\langle \boldsymbol{k}_f | \mathrm{e}^{-\mathrm{i}Ht} | \boldsymbol{k}_i \rangle = \int \mathcal{D}\boldsymbol{k} \tag{1}$$