UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

Wednesday 26 April 2023, 10.30 to 12.30

THEORETICAL PHYSICS 2

*Answer **all four** questions.*

The approximate number of marks allotted to each part of a question is indicated in the right margin where appropriate.

The paper contains **five** *sides, including this one, and is accompanied by a booklet giving values of constants and containing mathematical formulae which you may quote without proof. (The booklet is available for separate download.)*

1 Consider a dimerized chain with two sites a, b in N unit cells described by the Hamiltonian

$$H = \sum_{j=1}^{N} (t + \delta t) c^\dagger_{a,j} c_{b,j} + (t - \delta t) c^\dagger_{a,j+1} c_{b,j} + h.c.,$$

where $h.c.$ refers to the Hermitian conjugate, and t and δt are hopping parameters that we leave implicit.

(a) Using a Fourier transform $c_{j,\alpha} = \frac{1}{\sqrt{N}} \sum_k c_{k,\alpha} e^{ikj}$, show that the above Hamiltonian can be rewritten as

$$H(k) = \sum_{k,\alpha,\beta} H_{\alpha,\beta}(k) c^\dagger_{\alpha,k} c_{\beta,k},$$

where $\alpha, \beta \in a, b$ and $H_{\alpha,\beta}(k) = \mathbf{d}(k) \cdot \boldsymbol{\sigma}$ in terms of the Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and vector $\mathbf{d}(k) = ((t + \delta t) + (t - \delta t)\cos(k), (t - \delta t)\sin(k), 0)$. [3]

(b) Show that the spectrum consists of two energy bands,

$$E(k) = \pm\sqrt{((t + \delta t) + (t - \delta t)\cos(k))^2 + ((t - \delta t)\sin(k))^2}.$$

[2]

(c) Assuming now that $\delta t = -t$, show that the eigenstates $|u_k, \pm\rangle$ read

$$|u_k, \pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-ik} \\ 1 \end{pmatrix}$$

and that evaluating the Berry potential $\mathbf{A}_\pm = -i\langle u_k, \pm|\nabla|u, \pm\rangle$ over the closed path $k \to k + 2\pi$ renders $\oint A_\pm \mathrm{d}k = -\pi$. (Note that $A_\pm$ is just a scalar in our one-dimensional case.) [5]

(d) Assuming that $\delta t = t$, show that the eigenstates $|u_k, \pm\rangle$ are

$$|u_k, \pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$$

and that evaluating the Berry potential $A_\pm = -i\langle u_k, \pm|\nabla|u, \pm\rangle$ over the closed path $k \to k + 2\pi$ renders $\oint A_\pm \mathrm{d}k = 0$. [5]

(e) Show that for general δt, the eigenstates are given as

$$|u_k, \pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{i\phi_k} \\ 1 \end{pmatrix},$$

where $\phi_k = \tan^{-1} \frac{v \sin k}{v + w \cos k}$, for $v = (t + \delta t)$ and $w = (t - \delta t)$. Why is $\oint A_\pm \mathrm{d}k = 0$ over the closed path $k \to k + 2\pi$ undefined when $v = w$? What does it evaluate to for $v > w$ and $v < w$ and how does this compare to the above answers? Finally, how does $\oint A_\pm \mathrm{d}k = 0$ over the closed path $k \to k + 2\pi$ change when we assign a different gauge to the eigenstates $|u_k, \pm\rangle \to e^{i\varphi_k}|u_k, \pm\rangle$? [10]

2 Consider an electron with mass m and charge e moving in three dimensions under a uniform electric field $\mathbf{E}$ where the Hamiltonian is given by,

$$H = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}\cdot\mathbf{r}\,.$$

Starting from $\mathbf{r}_i$ at $t_i = 0$, the probability amplitude for finding the electron at $\mathbf{r}_f$ at $t_f = t$ is given by the propagator

$$K(\mathbf{r}_f, t|\mathbf{r}_i, 0) = \theta(t)\langle\mathbf{r}_f|U(t,0)|\mathbf{r}_i\rangle\,,$$

for the time-evolution operator $U(t,0)$.

(a) Calculate how $K(\mathbf{r}_i, t|\mathbf{r}_f, 0)$ is related to $K(\mathbf{r}_f, t|\mathbf{r}_i, 0)$ and comment on your answer. [3]

(b) Consider the parity operator $\mathcal{P}|\mathbf{r}\rangle = |-\mathbf{r}\rangle$. Calculate whether the propagator satisfies reflection symmetry $K(\mathbf{r}_f, t|\mathbf{r}_i, 0) \stackrel{?}{=} K(-\mathbf{r}_f, t|-\mathbf{r}_i, 0)$. Compare this with the result for the free particle propagator $K_0(\mathbf{r}_f, t|\mathbf{r}_i, 0)$ for $H_0 = \mathbf{p}^2/2m$. [5]

(c) For the propagator in momentum space $\tilde{K}(\mathbf{p}_f, t|\mathbf{p}_i, 0)$, show that the probability of finding the electron with momentum $\mathbf{p}_f$ after time t vanishes unless $\mathbf{p}_f = \mathbf{p}_i + e\mathbf{E}t$. [6]

Now consider the electric field to be along the y-axis, $\mathbf{E} = E\hat{y}$.

(d) Write down the classical action and calculate the propagator for this electric field. [6]

[*Hint: The free particle propagator is* $K_0(\mathbf{r}_f, t|\mathbf{r}_i, 0) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \exp\left\{i\frac{m}{2\hbar t}(\mathbf{r}_f - \mathbf{r}_i)^2\right\}$.]

(e) Consider a wave packet of electrons with the same energy moving in the $(x-y)$-plane starting from point A at the origin as shown in the figure. The wave packet splits into two that travel along two different paths, ABC (path 1) and ADC (path 2), to finally meet at C with coordinates (d_x, d_y). Assuming that the size of the wave packet is much smaller than all other length scales, calculate the phase difference between the two paths and comment on it.

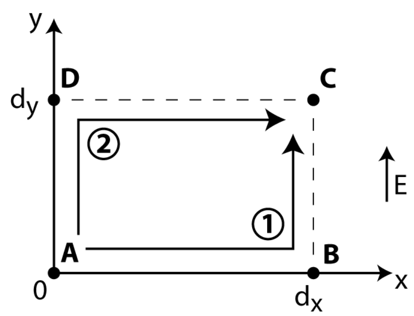

Figure 1:

[5]

V7.1

3 We consider a model for electron-phonon coupling given as $H = H_0 + H_1$, where

$$H_0 = \sum_{\mathbf{q},\mathbf{k}} \hbar\omega_{\mathbf{q}} \hat{b}^\dagger_{\mathbf{q}} \hat{b}_{\mathbf{q}} + \epsilon_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}}$$

$$H_1 = \sum_{\mathbf{q},\mathbf{k}} M_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}} (\hat{b}_{\mathbf{q}} + \hat{b}^\dagger_{-\mathbf{q}}).$$

Here the operators $\hat{b}^\dagger_{\mathbf{q}}$ describe the bosonic creation operator for phonons, that is lattice vibrations, with momentum $\mathbf{q}$ and frequency $\omega_{\mathbf{q}}$; and $\hat{a}^\dagger_{\mathbf{k}}$ denote creation operators for electrons with energy $\epsilon_{\mathbf{k}}$ and wave vector $\mathbf{k}$. We assume that H_1 is a weak coupling term that we can treat perturbatively in this problem.

(a) Give the fundamental algebraic relations that the phonon operators $\hat{b}^\dagger_{\mathbf{q}}$ and $\hat{b}_{\mathbf{q}}$, and electron operators $\hat{a}^\dagger_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ must obey due to their particle nature. [3]

(b) We may perform a similarity transformation $\tilde{H} = e^{-S} H e^{S}$. Assume S is of the same order as H_1 and remember that H_1 is treated perturbatively. Show that if S satisfies

$$H_1 + [H_0, S] = 0,$$

the first order term of $\tilde{H}$ when written as perturbative series vanishes, rendering only H_0 plus higher order terms. What is the second order term in the expansion in this case?

[*Hint: Recall that* $e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + ...$]

[8]

(c) We assume that S has the form,

$$S = \sum_{\mathbf{q},\mathbf{k}} (\alpha \hat{b}^\dagger_{-\mathbf{q}} + \beta \hat{b}_{\mathbf{q}}) M_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}}.$$

Compute α and β such that the condition in part (*b*) is fulfilled. Write down the explicit form of S and give an interpretation for the denominator of α and β. [11]

[*Hint: Note that* $[AB, CD] = A[B, C]D + [A, C]BD + CA[B, D] + C[A, D]B$ *and that a similar (but not the same!) relation for* $[AB, CD]$ *in terms of anti-commutators can be derived.*]

(d) Show that the second order term in $\tilde{H}$, which is proportional to $|M_{\mathbf{q}}|^2$, has terms where the operator is of the form

$$\hat{a}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}'-\mathbf{q}} \hat{a}_{\mathbf{k}'}.$$

What is the interpretation? [3]

4 Consider a system of three distinguishable spin-1/2 particles, which we denote with $+/-$ for up/down projections along the z-axis. Denote the Hilbert space as $\mathcal{H}$.

(a) Write down a basis for $\mathcal{H}$. [2]

(b) Give the expression for the entanglement S of a density operator ρ. Why is S zero for a pure state? [3]

(c) Write down an *entangled* state of these three spin-1/2 particles in which particles 2 and 3 are entangled, but the pair (2,3) is not entangled with particle 1. [5]

(d) Consider another entangled state,

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|++-\rangle - |--+\rangle).$$

What is the reduced density operator ρ_2 obtained from tracing out the third particle staring from the pure state $|\Psi\rangle$? Is ρ_2 describing a pure or a mixed state? What is the probability that the first two particles are entangled? [7]

(e) A variation on the so-called W-state that occurs in quantum computing is the V-state given as,

$$|\Phi\rangle = \frac{1}{\sqrt{3}}(|++-\rangle + |+-+\rangle + |-++\rangle).$$

What is the reduced density operator $\tilde{\rho}_2$ for *any* two particles obtained from tracing out the third. Describe $\tilde{\rho}_2$. Is it a pure or a mixed state? What is the probability to find two remaining particles in an entangled state? [8]