Lent Term 1996 — Mathematical Tripos Part II — I.T. Drummond

Applications of Quantum Mechanics

Problem Set I

1. A particle of mass m and charge e is contained within a cubical box of side a. Initially the particle is in the stationary state of energy $3\pi^2\hbar^2/2ma^2$. At time $t=0$, a uniform electric field strength E is switched on parallel to one of the edges of the cube. Obtain an expression to the second order in e for the probability of finding the particle of energy $3\pi^2\hbar^2/ma^2$ at time t.

2. The Hamiltonian for a quantum mechanical system is $H_0+V(t)$, where H_0 has no explicit time dependence. At $t=0$ the system is in the state $|a\rangle$. Show that the probability that at a latter time t it is in the state $|a'\rangle$, where both $|a\rangle$ and $|a'\rangle$ are eigenstates of H_0, is

$$|\langle a'|T(t)|a\rangle|^2\,,$$

where $T(t)$ satisfies the integral equation

$$T(t)=1-\frac{i}{\hbar}\int_0^t \widetilde{V}(t')T(t')dt'\,,$$

and

$$\widetilde{V}(t)=e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}\,.$$

A system has only two independent states $|1\rangle$ and $|2\rangle$, and, with respect to these, the Hamiltonian has a time-independent matrix representation

$$\begin{pmatrix} E & V \\ V & E \end{pmatrix}.$$

Show that, to lowest order in V, the probability of a transition from state $|1\rangle$ to state $|2\rangle$ in the time interval t is $V^2t^2/\hbar^2$. By comparing this with the exact result, state the conditions for such an approximation to be good.

3. A particle of mass m in 3-dimensional space lies in a rectangular box of sides L_1, L_2 and L_3. Its wave function, $\psi(\mathbf{x})$, is subject to the periodic boundary conditions

$$\psi(\mathbf{x}+L_i\mathbf{e}_i)=\psi(\mathbf{x})\qquad (i=1,2,3)\,,$$

where $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ are the three mutually orthogonal unit vectors parallel to the sides of the box. Show that the allowed momenta of the particle are of the form

$$\mathbf{p}=2\pi\hbar\left(\frac{n_1}{L_1}\mathbf{e}_1+\frac{n_2}{L_2}\mathbf{e}_2+\frac{n_3}{L_3}\mathbf{e}_3\right)\,,$$

where $\{n_1,n_2,n_3\}$ are integers. Show that, in a limit in which the sides of the box become very large, the sum over states $\sum_{\{n_1,n_2,n_3\}} f(\mathbf{p})$, where $f(\mathbf{p})$ is a smooth function of $\mathbf{p}$, can be expressed as

$$\frac{V}{(2\pi\hbar)^3}\int d^3\mathbf{p}\,f(\mathbf{p}),$$

where $V=L_1L_2L_3$ is the volume of the box. Note that this is result is independent of the ratios $L_1:L_2:L_3$.

If only L_1 and L_2 become large, what form does the sum over states take?

4. Calculate the Born approximation to the differential cross-section for the following potentials:

$$-V_0e^{-\lambda^2r^2},\qquad V_0r^{-2},\qquad V_0\delta(r-a)\,,\qquad V(r)=\begin{cases}V_0 & (r<a)\\ 0 & (r>a)\end{cases}.$$

5. An atom of atomic number Z is represented by the charge distribution

$$\rho(\mathbf{r})=Ze\left(\delta(\mathbf{r})-\frac{\lambda^3}{8\pi}e^{-\lambda r}\right).$$

Calculate the differential cross-section in the Born approximation. Identify the form factor of the charge distribution and comment on which range of momentum transfer is most sensitive to (a) the nucleus and (b) the electron cloud.

6. Calculate, in Born approximation, the differential cross-section $d\sigma/d\Omega$ for a particle of mass m scattering on a potential $V(r)=\lambda\exp(-\mu r)/r$ as a function of the momentum transfer. Express this as a function of energy E and scattering angle θ, and show that, for large E, $d\sigma/d\Omega$ is proportional to E^{-2} at fixed $\theta\neq 0$, that $d\sigma/d\Omega$ is independent of E at $\theta=0$, and that the total cross-section σ is proportional to E^{-1}.

7. Show that the p-wave phase shift for a three-dimensional square well potential of depth $\hbar^2K^2/2m$ and radius a, at low k, is given by

$$\frac{1}{3}k^3a^3\frac{(1-\gamma a)}{(2+\gamma a)}\,,$$

where the incident momentum is $\hbar\mathbf{k}$ and $\gamma=Kj_1'(Ka)/j_1(Ka)$.

8. Show that the phase shifts for the potential $-\frac{\hbar^2}{2m}\lambda\delta(r-a)$ are given by

$$\tan\delta_l=\frac{k\lambda a^2[j_l(ka)]^2}{1+k\lambda a^2 j_l(ka)n_l(ka)}\,.$$

9. A particle of mass m and energy $\frac{\hbar^2k^2}{2m}$ scatters on a hard sphere of radius a. Show that the phase shifts δ_l obey

$$e^{2i\delta_l}=-\frac{j_l(ka)-in_l(ka)}{j_l(ka)+in_l(ka)}\,.$$

10. A beam of particles of energy $E=\frac{\hbar^2k^2}{2m}$ is incident along the z-axis and suffers scattering by a spherically symmetric central potential $V(r)=\hbar^2U(r)/2m$ of finite range r_0 (*i.e.* $V(r)=0$, $r>r_0$). Show that the wave function $\psi_k(\mathbf{r})$, which behaves at infinity like

$$e^{ikz}+\frac{e^{ikr}}{r}f_k(\theta,\phi)\,,$$

satisfies the equation

$$\psi_k(\mathbf{r})=e^{ikz}-\int U(\mathbf{r})G_k(\mathbf{r},\mathbf{r}')\psi_k(\mathbf{r}')d^3\mathbf{r}'\,,$$

where

$$G_k(\mathbf{r}, \mathbf{r}') = \frac{e^{ikR}}{4\pi R}, \qquad R = |\mathbf{r} - \mathbf{r}'|,$$

and write down an expression, in terms of $\psi_0(\mathbf{r})$, for the scattering length a, which is defined by

$$a = \lim_{k\to 0} f_k(\theta).$$

In the case of $U(r) = U_0\delta(r - c)$, assume $\psi_0(\mathbf{r}) = \psi_0(r)$, solve the above the equation for $\psi_0(c)$, and hence show that

$$a = -\frac{c^2 U_0}{1 + cU_0}.$$

Why does a become infinite for $U_0 = -c^{-1}$?

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Applications of Quantum Mechanics

Problem Set II

1. The basis vectors for the basic cell of the Bravais lattice of a crystal are $\{\mathbf{a}_1,\ \mathbf{a}_2,\ \mathbf{a}_3\}$. Define the reciprocal vectors and the reciprocal lattice for the crystal. A beam of particles incident on the crystal has a wave vector $\mathbf{k}$ and is scattered into a state with wave vector $\mathbf{k}'$. Show that substantial scattering only occurs when $\mathbf{k}'-\mathbf{k}$ is an element of the reciprocal lattice.

Let $\mathbf{n}$ be the unit normal to the planes in the crystal parallel to $\{\mathbf{a}_1,\ \mathbf{a}_2\}$ and let d be the distance of separation of these planes. Show that one of the reciprocal vectors is $\mathbf{b}_3 = \frac{1}{d}\mathbf{n}$. Verify that the above condition for substantial scattering is satisfied by the specular reflection in this plane, of waves incident at an angle θ to the normal $\mathbf{n}$ where

$$2d\cos\theta = r\lambda, \qquad r = 1,\ 2,\ 3,\ \ldots$$

where λ is the wavelength of the incident beam. This is the standard Bragg condition for scattering on a crystal.

2. A one-dimensional crystal comprises a chain of atoms of mass m equally spaced by a distance a when in equilibrium. The forces between the atoms are such that the effective spring constants are alternately λ and $\alpha\lambda$. Show that the dispersion relation for phonons has the form

$$\omega_\pm^2 = \frac{\lambda}{m}\left[(1+\alpha) \pm (1 + 2\alpha\cos 2ka + \alpha^2)^{\frac{1}{2}}\right] ,$$

where the wave number k satisfies $-\pi/2a \leq k \leq \pi/2a$. What is the velocity of sound? What is the limiting value, at small wavenumber, of the optical band frequency?

3. For the model of the previous problem determine the 2-component polarisation vectors $\epsilon_\pm(k)$ corresponding to $\omega_\pm(k)$ describing normal mode oscillations in each unit cell. Quantise this system and express the displacements of the atoms and the Hamiltonian in terms of phonon annihilation and creation operators.

4. A square lattice crystal in two dimensions has atoms of mass M at the sites $a(r,s)$ where r and s are integers, joined by springs of equal force constant C and natural length $b(< a)$ to their four nearest neighbours $(r\pm 1, s)$ and $(r, s\pm 1)$. Let (ξ_{rs}, η_{rs}) be the displacement of the atom at $a(r,s)$. Show that the potential energy of the spring from $a(r,s)$ to $a(r+1,s)$ increases during the lattice vibration by

$$C(a-b)X + \tfrac{1}{2}CX^2 + \tfrac{1}{2}C\left(1-\frac{b}{a}\right)Y^2 ,$$

where $X = \xi_{r+1\,s} - \xi_{rs}$, $Y = \eta_{r+1\,s} - \eta_{rs}$ (the potential energy of a spring with force constant C is $\frac{1}{2}C\alpha^2$, where α is the extension from natural length).

Verify that the linear terms disappear on summing over all the springs. Setting $C' = C(1-b/a)$ derive the equations of motion

$$M\ddot{\xi}_{rs} = C(\xi_{r+1\,s} - 2\xi_{rs} + \xi_{r-1\,s}) + C'(\xi_{rs+1} - 2\xi_{rs} + \xi_{rs-1}) .$$

Show that this has a solution

$$\xi_{rs} = Q\exp i(rKa + sLa) ,$$

where $\ddot{Q} + \omega^2 Q = 0$, if $M\omega^2 = 2C(1-\cos Ka) + 2C'(1-\cos La)$.

This describes a ξ wave with the displacements all in the x-direction. For the same wave number (K, L) show that there is also an η-wave with displacements in the y-direction with frequency $\omega(L, K)$.

Show that for wave number $(K, 0)$ the ξ wave is longitudinal with velocity $v_\ell = (Ca^2/M)^{\frac{1}{2}} + \mathrm{O}(\mathrm{K}^2)$, while the η wave is transverse with velocity $v_t = (C'a^2/M)^{\frac{1}{2}} + \mathrm{O}(\mathrm{K}^2)$, and conversely for wave number $(0, L)$.

5. A neutron of momentum $\hbar\mathbf{K}$ is scattered elastically by a crystal, so that its final momentum is $\hbar\mathbf{K}'$ with $|\mathbf{K}'| = |\mathbf{K}|$. The crystal has N equivalent atoms of mass M and is in its ground state $|0\rangle$ before and after the scattering. The lattice potential is

$$V(\mathbf{r}) = C \sum_{\mathbf{a}} \delta(\mathbf{r} - \mathbf{a} - \mathbf{u_a}) ,$$

where $\mathbf{u_a}$ is the displacement of the atom whose equilibrium position is $\mathbf{a}$. In terms of phonon variables,

$$\mathbf{u_a} = \sum_{\mathbf{k},\alpha} \left(\frac{\hbar}{2MN\omega_{\mathbf{k}}} \right)^{\frac{1}{2}} \left(a_{\mathbf{k}\alpha}\, \mathbf{e}_\alpha(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{a}} + (a_{\mathbf{k}\alpha})^\dagger\, \mathbf{e}^*_\alpha(\mathbf{k})\, e^{-i\mathbf{k}\cdot\mathbf{a}} \right) ,$$

where $\mathbf{e}_\alpha(\mathbf{k})$, $\alpha = 1, 2, 3$ are the polarisation vectors for a phonon of wave number $\mathbf{k}$.

In the Born approximation, the scattering is described by the matrix element

$$\mathcal{M} = \int d^3r\, \langle 0| e^{-i\mathbf{K}'\cdot\mathbf{r}} V(\mathbf{r})\, e^{i\mathbf{K}\cdot\mathbf{r}} |0\rangle ,$$

where $|0\rangle$ is the ground state of the crystal. Show that $\mathcal{M} = e^{-W} \mathcal{M}_o$, where $\mathcal{M}_o$ is the matrix element for scattering by a rigid lattice, and give an expression for W.

$$[e^{\lambda a + \mu a^\dagger} = e^{\frac{1}{2}\lambda\mu}\, e^{\mu a^\dagger}\, e^{\lambda a}.]$$

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Applications of Quantum Mechanics

Problem Set III

The starred question is an optional but instructive example

1. A particle of mass m moves in 1-dimension under the influence of a potential

$$V(x) = -\frac{\hbar^2\lambda}{2m}\delta(x) \ .$$

Show that there is a bound state with energy $-\hbar^2\lambda^2/8m$.

Now suppose the potential becomes

$$V(x) = -\frac{\hbar^2\lambda}{2m}\sum_{\ell=-\infty}^{\infty}\delta(x-\ell a)$$

Show that in this case there is a band of allowed energies, corresponding to Bloch wave functions $\psi_k(x)$,

$$-\frac{\hbar^2}{2m}\beta_L^2 \le E \le -\frac{\hbar^2}{2m}\beta_U^2$$

where

$$1 = \cosh\beta_L a - \frac{\lambda}{2\beta_L}\sinh\beta_L a$$

and β_U satisfies a similar equation. Show that when $a \to \infty$ the band narrows down to the bound state energy.

2. Show how, for a general one-dimensional periodic potential

$$V(x) = \sum_{n=1}^{\infty}\alpha_n(e^{i2\pi nx/a} + e^{-i2\pi nx/a}) \ ,$$

the nearly-free electron model leads to a band structure for the energy levels. Determine, in this approximation, the energy gap between adjacent energy bands.

Verify that the approximate result is identical, for large energies, with the exact result obtained when $\alpha_n = \hbar^2\lambda/m$, for all n.

[You may assume $\sum_{-\infty}^{\infty} e^{int} = 2\pi\sum_{-\infty}^{\infty}\delta(t-2\pi n)$.]

3. The Hamiltonian for a particle moving in one dimension subject to a periodic potential is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \ , \quad \text{where} \quad V(x+a) = V(x) \ .$$

Explain carefully why the wave functions for states of definite energy $E_n(k)$ have the form

$$\psi_n(k,x) = e^{ikx}u_n(k,x)$$

where

$$u_n(k,x+a) = u_n(k,x) \ ,$$

and $n = 0, 1, \ldots$ is an index specifying the particular energy band. Discuss clearly the restrictions on the allowed values of k.

Show that $u_n(k,x)$ satisfies

$$H(k)u_n(k,x) = \epsilon_n(k)u_n(k,x) \ ,$$

$$H(k) = H + H_I \ , \quad H_I = \frac{\hbar k}{m}\left(-i\hbar\frac{d}{dx}\right) \ , \quad \epsilon_n(k) = E_n(k) - \frac{\hbar^2k^2}{2m} \ .$$

Verify that $H(k)$ is Hermitian and deduce that, for fixed k, the set $u_n(k,x)$ is an orthonormal basis for the space of wave functions $\{\psi(x)\}$ on the range $0 \le x \le a$ with periodic boundary conditions.

When k is small, H_I above may be treated as a perturbation. Show that, assuming that $u_n(0,x)$ are not degenerate,

$$E_n(k) \approx E_n(0) + \frac{\hbar k}{m}b_{nn} + \frac{\hbar^2k^2}{2m}\left[1 + \frac{2}{m}\sum_{m\neq n}\frac{|b_{mn}|^2}{[E_n(0) - E_m(0)]}\right]$$

where

$$b_{mn} = \int_0^a dx\, u_m^*(0,x)\left(-i\hbar\frac{d}{dx}\right)u_n(0,x) \ .$$

Using nearly free electron model wave functions for $u_{2n}(0,x)$ and $u_{2n-1}(0,x)$

$$\sqrt{\frac{2}{a}}\cos ngx \ , \quad \sqrt{\frac{2}{a}}\sin ngx \ , \quad g = \frac{2\pi}{a} \ ,$$

with $E_{2n}(0) \approx \mathcal{E}(ng) + \lambda$, $E_{2n-1}(0) \approx \mathcal{E}(ng) - \lambda$, where $\mathcal{E}(k) = \hbar^2k^2/2m$ and assuming $\int_0^a dx\, V(x) = 0$ to give $\lambda = \langle u_{2n}|V|u_{2n}\rangle = -\langle u_{2n-1}|V|u_{2n-1}\rangle > 0$, evaluate b_{mn} and hence find $E_n(k)$.

4. Show that for a two-dimensional simple square lattice, with spacing a, the 'tight-binding' model leads to an approximate energy function of the form

$$E = E_o + E'(\cos k_1 a + \cos k_2 a) \ .$$

Plot the contours of constant energy for (k_1, k_2) in a Brillouin zone. What is the effective mass at the bottom of the band?

5*. Atoms of a simple square crystal are situated at lattice points $\ell = a(s, s')$ for integral s, s'. The corresponding reciprocal lattice vectors are $\mathbf{g} = \gamma(n, n')$ for integral n, n' and $\gamma = 2\pi/a$. The potential is

$$V = 2A(\cos\gamma x + \cos\gamma y) \equiv \sum_{\mathbf{g}} V_{\mathbf{g}}\, e^{i\mathbf{g}\cdot\mathbf{r}}\ ,\quad A > 0\ ,$$

with $V_{\mathbf{g}} = A$ for $\mathbf{g} = \pm(\gamma, 0),\ \pm(0, \gamma)$; $V_{\mathbf{g}} = 0$ otherwise.

Applying the nearly free electron model show that the energies at $(\frac{1}{2}\gamma, 0)$ on either side of the boundary $k_x = \frac{1}{2}\gamma$ of the first Brillouin zone are given by

$$E_{\pm}(\tfrac{1}{2}\gamma, 0) = \frac{\hbar^2\gamma^2}{8m} \pm A\ .$$

Within this model use degenerate perturbation theory with a basis of two dimensional plane wave states

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L}\sum_{\mathbf{g}} \alpha_{\mathbf{k}-\mathbf{g}} \exp i(\mathbf{k} - \mathbf{g})\cdot\mathbf{r}\ ,$$

where in the sum $\mathbf{g} = (0,0),\ (\gamma,0),\ (0,\gamma), (\gamma,\gamma)$, to show that the energies $E_{\pm\pm}$ at $(\frac{1}{2}\gamma \pm \xi\,,\ \frac{1}{2}\gamma \pm \eta)$, near where two boundaries of the zone intersect, obey

$$\begin{vmatrix} x & A & A & 0 \\ A & x & 0 & A \\ A & 0 & x & A \\ 0 & A & A & x \end{vmatrix} = 0\ ,$$

for $x = \hbar^2\gamma^2/4m - E + \mathrm{O}(\xi, \eta)$. Use the fact that the equation has roots $2A,\ 0,\ 0,\ -2A$ to show that

$$E_{++} = \frac{\hbar^2\gamma^2}{4m} + 2A,\quad E_{--} = \frac{\hbar^2\gamma^2}{4m} - 2A,\quad E_{+-} = E_{-+} = \frac{\hbar^2\gamma^2}{4m}\ .$$

Show that, if the atoms of the lattice are supposed to have valency two, it should be an insulator provided that

$$\frac{\hbar^2\gamma^2}{8m}\ <\ 3A\ .$$