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Suggested solution for 2017 Exam in Quantum Mechanics II

NOTE: The solutions below are meant as guidelines for how the problems may be solved and do not necessarily contain all the detailed steps of the calculations.

- **Problem 1**: When $c_n\sqrt{n} = \alpha c_{n-1}$ where α is a constant, we are guaranteed that $a|\alpha\rangle \propto |\alpha\rangle$. This equation is solved to give that generally $c_n = c_0\alpha^n/\sqrt{n!}$ where c_0 is a constant which should be determined so that $\langle\alpha|\alpha\rangle = 1$. Since

$$\langle\alpha| = c_0^* \sum_{n=0}^{\infty} \frac{(\alpha^*)^n}{\sqrt{n!}}\langle n|, \tag{1}$$

it follows that

$$|c_0|^2 = \frac{1}{\sum_{n=0}^{\infty}\frac{(\alpha^*\alpha)^n}{n!}}. \tag{2}$$

This determines how we must choose c_0.

- **Problem 2**: The detailed derivation is shown in the eBook for this course on page 21 and the result is

$$\lambda|\psi_n^{(1)}\rangle = \sum_{m\neq n}\frac{\langle\psi_m^{(0)}|\lambda\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^0 - E_n^0}|\psi_m^{(0)}\rangle. \tag{3}$$

The trick with the normalization condition is that it shows that $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = 0$ if one includes terms up to order λ in the normalization condition $\langle\psi_n|\psi_n\rangle = 1$, which is why the $m = n$ term does not contribute in the summation above.

- **Problem 3:**

  - The main idea behind the WKB approximation is that if the potential $V(x)$ which a particle moves in is sufficiently slowly varying, then a reasonable ansatz for the wavefunction is

$$\psi(x) = e^{iS(x)/\hbar} \tag{4}$$

where $S(x)$ is a slowly varying function. For a constant potential $V(x) = V_0$, this is indeed an exact solution with $S(x) = \pm\sqrt{2m(E-V_0)}x$. Inserting the above ansatz into the SE, one obtains a differential equation that determines $S(x)$. The validity of the approach relies on the second derivative of S is small in this differential equation compared to the main term, so that one can treat it as a perturbation, i.e.

$$|i\hbar S''| \ll |p^2|. \tag{5}$$

One can derive (the student is not expected to have accomplished this) that this effectively means that the change in wavelength λ of the particle over a distance λ should be small compared to λ itself.

  - Just as one assumed in the WKB-treatment that the potential varies slowly in space, in the adiabatic approximation one assumes that the potential varies slowly in time. The perturbation in $\hat{H}$ need not be small in magnitude. If this is satisfied, one can expect the approximate solutions of the time-dependent SE to be obtained in terms of the eigenfunctions $\psi_k(t)$ of the "instantaneous" Hamiltonian $H(t)$:

$$H(t)\psi_k(t) = E_k(t)\psi_k(t) \tag{6}$$

at any given time t, so that the total wavefunction Ψ satisfying the time-dependent SE can be expanded generally as:

$$\Psi(t) = \sum_k c_k(t)\psi_k(t)\mathrm{e}^{-\mathrm{i}\int_{t_0}^{t} E_k(t')dt'/\hbar}. \tag{7}$$

For a full score, the candidate should also discuss how to obtain a quantitative condition required for this method to be valid (i.e. a constraint on the time derivative of H as shown in the eBook).

– The expectation value of a Hamiltonian $\hat{H}$ in any state f will always be greater or equal to E_0, where E_0 is the lowest eigenvalue. In effect,

$$E[f] = \frac{\langle f|\hat{H}|f\rangle}{\langle f|f\rangle} \geq E_0. \tag{8}$$

The student should be able to derive this equation following the procedure of the lecture notes. The result obtained for $E[f]$ will be closer to E_0 the more similar f is to the true ground-state. Symmetry may be used as a guideline to identify a suitable trial function f. In practice, the variational method is only suited to estimate the ground-state energy and becomes of little use for excited states.

- **Problem 4**: We consider free electrons, neglecting spin for now, and show that for a constant $\mathbf{B}$, the SE can be solved exactly. In the derivation below, we may set $k_z = 0$ since we consider motion only in the xy-plane. We use a Landau-gauge $\mathbf{A} = (-By, 0, 0)$ so that the Hamiltonian for $q = -e$ becomes:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{\mathrm{i}e\hbar B}{m}y\partial_x + \frac{e^2B^2}{2m}y^2. \tag{9}$$

This $\hat{H}$ commutes with $\hat{p}_x$ and $\hat{p}_z$ and thus admits common eigenstates with these operators. The general solution should then have the form $\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}k_x x + \mathrm{i}k_z z}\phi(y)$. Inserted into $\hat{H}\psi = E\psi$, we obtain the following equation for ϕ:

$$-\frac{\hbar^2}{2m}\phi'' + \Big[\frac{\hbar^2 k_x^2}{2m} - \frac{\hbar e B k_x}{m}y + \frac{e^2B^2}{2m}y^2\Big]\phi + \frac{\hbar^2 k_z^2}{2m}\phi = E\phi. \tag{10}$$

This can be written in a more compact manner:

$$-\frac{\hbar^2}{2m}\phi'' + \frac{1}{2}m\omega_c^2(y-y_0)^2\phi = \tilde{E}\phi. \tag{11}$$

where $E = \tilde{E} + \hbar^2 k_z^2/2m$, $y_0 = \hbar k_x/eB$, and $\omega_c = eB/m$. We see that ω_c is the cyclotron frequencey: classical angular frequency for the circular motion of an electron in a $\mathbf{B}$ field. Now, Eq. (11) has a familiar form: a harmonic oscillator centered around y_0. We immediately know what the eigenvalues are according to our detailed previous treatment of such a system:

$$\tilde{E} = (n+1/2)\hbar\omega_c \rightarrow E = (n+1/2)\hbar\omega_c + \hbar^2 k_z^2/2m \ (n = 0, 1, 2, \ldots). \tag{12}$$

The belonging eigenfunctions are:

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}k_x x + \mathrm{i}k_z z}\phi_n(y - y_0) \tag{13}$$

where ϕ_n is the n-th harmonic oscillator function. The energy E for our particle thus has two parts: free particle motion along the $\mathbf{B}$ field (z-axis) and quantized motion perpendicularly to $\mathbf{B}$ (xy-plane).

- **Problem 5**: No, we cannot do so if the field-free region encloses an area where $B \neq 0$ since otherwise the line-integral of $\mathbf{A}$ around a contour that encloses that area gives zero whereas it should give the magnetic flux (via Stoke's theorem). This is crucial for the Aharonov-Bohm effect.

- **Problem 6**: A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonians spectrum.

- **Problem 7**: Due to the wavelike nature of particles in QM, the particle is affected by the entire surface area of the sphere at low energies rather than just its cross-section (as would be the case if the particle was a hard sphere itself). The surface area is 4 times larger than the maximum cross section, and hence the extra factor of 4.

- **Problem 8**: In order to get scattering, we have to weaken the incident beam (i.e. the propagation in the forward-direction $\theta = 0$). Therefore, it its reasonable that we should be able to say something about σ from the $\theta = 0$ contribution to the scattering amplitude, i.e. how much it has changed from the incident plane-wave. More specifically, we need destructive interference to weaken the incident beam. This means that we are looking for a contribution to f which is out-of-phase with the incident plane-wave part of the wavefunction. This is quantified by the imaginary part of f: if f is purely real, there is no phase-shift in the outgoing wave compared to the incident plane-wave and hence no interference effect has taken place.

- **Problem 9**: The method of partial waves excels for low-energy scattering where only a few of the lowest partial waves are expected to contribute. The basic idea is to expand the scattering amplitude in waves with increasing angular momentum quantum number and then say that at low energies, only the smallest values of angular momentum should contribute. The key quantity in the method of partial waves is the scattering phase δ_l which is the QM phase picked up by the wavefunction due to the potential scattering. The cross section σ is dictated by δ_l.

- **Problem 10**: The Born-approximation is expected to be good for weak potentials and/or high-energy scattering. For finite-ranged, finite-sized potentials, the Born-approximation is always good for sufficiently high energies. The scattering amplitude f in the Born-approximation (performing one iteration of the recursive equation determining ψ) is inconsistent with the optical theorem because this procedure does not take into account interference between the incoming and scattered wave. Whereas this interference is less important away from $\theta = 0$, it is crucial at $\theta = 0$ as the optical theorem shows, because it describes the weakening of the incident beam. The Born-approximation cannot capture such destructive interference and thus is inconsistent with the optical theorem.

- **Problem 11**: The candidate is expected to know (or be able to show from gauge-invariance) that $\mathbf{E} = -\partial_t \mathbf{A}$. Using this, one finds that (dropping the mode index $\mathbf{k}, \lambda$ for brevity of notation)

$$\langle \alpha | \mathbf{E}^2 | \alpha \rangle = -\frac{\hbar \omega_k}{2\varepsilon_0 V} \langle \alpha | a^2 \mathrm{e}^{2i\mathbf{k}\cdot\mathbf{r} - 2i\omega_k t} - aa^\dagger - a^\dagger a + (a^\dagger)^2 \mathrm{e}^{-2i\mathbf{k}\cdot\mathbf{r} + 2i\omega_k t} | \alpha \rangle. \tag{14}$$

  Now, we can use that $[a, a^\dagger] = 1$ and $\langle \alpha | (a^\dagger)^2 | \alpha \rangle = \langle \alpha | a^2 | \alpha \rangle^*$ so that

$$\begin{aligned} \langle \alpha | \mathbf{E}^2 | \alpha \rangle &= -\frac{\hbar \omega_k}{2\varepsilon_0 V} \langle \alpha | a^2 \mathrm{e}^{2i\mathbf{k}\cdot\mathbf{r} - 2i\omega_k t} - 2a^\dagger a - 1 + (a^\dagger)^2 \mathrm{e}^{-2i\mathbf{k}\cdot\mathbf{r} + 2i\omega_k t} | \alpha \rangle \\ &= -\frac{\hbar \omega_k}{2\varepsilon_0 V} (\alpha^2 \mathrm{e}^{2i\mathbf{k}\cdot\mathbf{r} - 2i\omega_k t} - 2\alpha^* \alpha - 1 + (\alpha^*)^2 \mathrm{e}^{-2i\mathbf{k}\cdot\mathbf{r} + 2i\omega_k t}) \\ &= [\langle \alpha | \mathbf{E} | \alpha \rangle]^2 + \frac{\hbar \omega_k}{2\varepsilon_0 V}. \end{aligned} \tag{15}$$

  It follows that

$$\Delta E = \sqrt{\frac{\hbar \omega_k}{2\varepsilon_0 V}} \tag{16}$$

  which is thus independent on the amplitude α of the coherent state.

- **Problem 12**: The difference is that for stimulated emission, there is a photon present in the initial state of the system whereas for spontaneous emission there is no photon present in the initial state of the system. In the stimulated emission state, the emitted photon gains some of the properties of the photon that was present initially, which is the crucial principle behind how a laser works.

- **Problem 13**: A mixed QM state represents a system which we have incomplete information about: there is a statistical mixture of different states, i.e. 50% of the particles are in one QM state whereas the other half are in a different state. In contrast, a superposition of states is still one well-defined quantum mechanical state. If N particles are in the same superposition of states $\psi = 0.5\psi_1 + 0.5\psi_2$, it is an experimentally different system than if half of the N particles are in state ψ_1 and the other half is in state ψ_2. Mathematically, mixed states and a superposition of states are differentiated by the fact that a superposition of states (a pure state) has $\mathrm{Tr}(\rho^2) = 1$ whereas a mixed state has $\mathrm{Tr}(\rho^2) \leq 1$. On the other hand, $\mathrm{Tr}(\rho) = 1$ is always satisfied.

- **Problem 14**: The resistivity is zero, because scattering comes about from defects in the lattice structure or scattering on phonons at finite temperatures. At zero temperature, the electron move as modulated plane-waves (Bloch states) through

the crystal and do not scatter. The Kronig-Penney model describes the lattice as a set of periodically placed δ-function wells. By solving the SE for this potential, one finds a condition on the eigenvalues which is an inequality. Therefore, in regions where this inequality is not satisfied, there are no available energy eigenvalues. These are gaps in the energy band structure. When the Fermi level is position inside a band (so that it is partially filled), the material is a metal. When it is inside an energy gap, it is a semiconductor or insulator. The size of the gaps determines whether it is a semiconductor or insulator.