StudentID:

PHYS 452 Quantum Mechanics II (Fall 2018) Instructor: Sergiy Bubin Final Exam

Instructions:

- All problems are worth the same number of points (although some might be more difficult than the others). The problem for which you get the lowest score will be dropped. Hence, even if you do not solve one of the problems you can still get the maximum score for the exam.
- This is a closed book exam. No notes, books, phones, tablets, calculators, etc. are allowed. Some information and formulae that might be useful are provided in the appendix. Please look through this appendix *before* you begin working on the problems.
- No communication with classmates is allowed during the exam.
- Show all your work, explain your reasoning. Answers without explanations will receive no credit (not even partial one).
- Write legibly. If I cannot read and understand it then I will not be able to grade it.
- Make sure pages are stapled together before submitting your work.

Problem 1.

- (a) Prove that $\langle \varphi | H | \varphi \rangle \geq E_0$ for any normalized (and properly behaved) trial wave function φ , where E_0 is the ground state energy of the system with Hamiltonian H.
- (b) Prove that there is always at least one bound state for an attractive potential in 1D. Here we define an attractive potential as follows: V(x) ≤ 0 for any x, and V(x) → 0 when x → ±∞. Hint: use some relevant trial function with a variational parameter that defines its spatial extent and then play with that parameter.

Problem 2. Consider a quantum rigid rotor (in 3D) in a magnetic field. The Hamiltonian of this system can be written as

$$H_0 = \alpha \mathbf{L}^2 + \beta L_z \,,$$

where **L** is the angular momentum operator, L_z is the projection of the angular momentum on the z-axis, and α and β are some positive constants. The system is subjected to an additional perturbation in the form $V = \gamma L_y$, where γ is a positive constant such that $\gamma \ll \beta$.

- (a) What are the energies and eigenstates of H_0 ?
- (b) Using the perturbation theory find correction to the energies to lowest nonvanishing order in V.

Hint: using ladder operators might make calculations easier

Problem 3. Consider a two-level system with the Hamiltonian

$$H = \begin{pmatrix} +E & h(t) \\ h(t) & -E \end{pmatrix},$$

where h(t) is a real function such that $\int_{-\infty}^{+\infty} |h(t)| dt$ is finite and E is a constant. Let us label the states as

$$|1\rangle = \begin{pmatrix} 1\\ 0 \end{pmatrix}$$
, and $|2\rangle = \begin{pmatrix} 0\\ 1 \end{pmatrix}$.

- (a) At time $t = -\infty$ the system is in the state $|2\rangle$. Use time-dependent perturbation theory to determine the probability that at $t = +\infty$ the system undergoes a transition to state $|1\rangle$, to lowest order in h.
- (b) If E = 0, the probability of a transition from $|2\rangle$ to $|1\rangle$ can be computed *exactly*. Do that and compare it with the result obtained from time-dependent perturbation theory. What is the condition that the perturbative result is a good approximation to the exact result?

Problem 4. The Lippmann-Schwinger formalism can be used for solving scattering problems in 1D. The Green's function in 1D, i.e. the solution of the nonhomogeneous Helmholtz equation

$$\left[\frac{d^2}{dx^2} + k^2\right]G(x, x') = \delta(x - x'), \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

can be evaluated in a similar way as we did in lecture for 3D (you do not need to do this). For the outward wave the result is $G(x, x') = -\frac{i}{2k}e^{ik|x-x'|}$. Now, consider the case of scattering of a particle of mass m and energy E from an attractive δ -potential:

$$V(x) = -\alpha\delta(x),$$

where α is a positive constant. Solve the Lippmann-Schwinger equation and obtain the transmission and reflection amplitudes and probabilities.

Problem 5. Consider a two-level system with the following time-dependent Hamiltonian

$$H = \varepsilon \begin{pmatrix} 0 & a(t) \\ a(t) & 1 \end{pmatrix}$$

where ε is some constant that has units of energy and a(t) is given by:

$$a(t) = \begin{cases} \sqrt{2} e^{t/T}, & t < 0\\ 0, & t > 0 \end{cases}$$

Here T is some characteristic time. At $t = -\infty$ the system begins in its ground state and then evolves adiabatically.

- (a) What is the condition on T under which the adiabaticity is well maintained until t = 0? Be specific, do not just say T must be small or big.
- (b) What is the probability that the system will be found in the excited state at $t = +\infty$?

Problem 6.

- (a) Compute the geometric phase change when an infinite square well expands adiabatically from $[0, a_1]$ to $[0, a_2]$.
- (b) Do the same for the dynamic phase change, assuming that the rate of change is constant, i.e. $\frac{da}{dt} = C$.

Schrödinger equation

Time-dependent: $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$ Stationary: $\hat{H}\psi_n = E_n\psi_n$

De Broglie relations

 $\lambda=h/p, \ \nu=E/h \quad {\rm or} \quad {\bf p}=\hbar {\bf k}, \ E=\hbar \omega$

Heisenberg uncertainty principle

Position-momentum: $\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$ Energy-time: $\Delta E \, \Delta t \geq \frac{\hbar}{2}$ General: $\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$

Probability current

1D: $j(x,t) = \frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right)$ 3D: $j(\mathbf{r},t) = \frac{i\hbar}{2m} \left(\psi \nabla \psi^* - \psi^* \nabla \psi \right)$

Time-evolution of the expectation value of an observable Q (generalized Ehrenfest theorem)

 $\frac{d}{dt}\langle\hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle$

Infinite square well $(0 \le x \le a)$

Energy levels: $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, n = 1, 2, ..., \infty$ Eigenfunctions: $\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad (0 \le x \le a)$ Matrix elements of the position: $\int_0^a \phi_n^*(x) x \phi_k(x) dx = \begin{cases} a/2, & n = k \\ 0, & n \ne k; n \pm k \text{ is even} \\ -\frac{8nka}{\pi^2(n^2 - k^2)^2}, & n \ne k; n \pm k \text{ is odd} \end{cases}$

Quantum harmonic oscillator

The few first wave functions $(\alpha = \frac{m\omega}{\hbar})$: $\phi_0(x) = \frac{\alpha^{1/4}}{\pi^{1/4}} e^{-\alpha x^2/2}, \quad \phi_1(x) = \sqrt{2} \frac{\alpha^{3/4}}{\pi^{1/4}} x e^{-\alpha x^2/2}, \quad \phi_2(x) = \frac{1}{\sqrt{2}} \frac{\alpha^{1/4}}{\pi^{1/4}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$ Matrix elements of the position: $\langle \phi_n | \hat{x} | \phi_k \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{k} \, \delta_{n,k-1} + \sqrt{n} \, \delta_{k,n-1} \right)$ $\langle \phi_n | \hat{x}^2 | \phi_k \rangle = \frac{\hbar}{2m\omega} \left(\sqrt{k(k-1)} \, \delta_{n,k-2} + \sqrt{(k+1)(k+2)} \, \delta_{n,k+2} + (2k+1) \, \delta_{nk} \right)$ Matrix elements of the momentum: $\langle \phi_n | \hat{p} | \phi_k \rangle = i \sqrt{\frac{m\hbar\omega}{2}} \left(\sqrt{k} \, \delta_{n,k-1} - \sqrt{n} \, \delta_{k,n-1} \right)$

Creation and annihilation operators for harmonic oscillator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \,\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}} \,\hat{p} \qquad \qquad \hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2}\right) \qquad \qquad \hat{N} = \hat{a}^{\dagger}\hat{a} \qquad \qquad [\hat{a}, \hat{a}^{\dagger}] = 1 \\ \hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} \,\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}} \,\hat{p} \qquad \qquad \hat{a} \left|n\right\rangle = \sqrt{n} \left|n-1\right\rangle \qquad \qquad \hat{a}^{\dagger} \left|n\right\rangle = \sqrt{n+1} \left|n+1\right\rangle$$

Equation for the radial component of the wave function of a particle moving in a spherically symmetric potential V(r)

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R_{nl}}{\partial r} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]R_{nl} = E_{nl}R_{nl}$$

Energy levels of the hydrogen atom

$$E_n = -\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2},$$

The few first radial wave functions R_{nl} for the hydrogen atom $(a = \frac{4\pi\epsilon_0\hbar^2}{mZe^2})$

$$R_{10} = 2a^{-3/2} e^{-\frac{r}{a}} \qquad R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2}\frac{r}{a}\right) e^{-\frac{r}{2a}} \qquad R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-\frac{r}{2a}}$$

The few first spherical harmonics

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r} \qquad Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{\pm i\phi} = \mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$$

Operators of the square of the orbital angular momentum and its projection on the z-axis in spherical coordinates

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \qquad \hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$$

Fundamental commutation relations for the components of angular momentum

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \qquad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x \qquad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

Raising and lowering operators for the z-projection of the angular momentum

$$\hat{J}_{\pm} = \hat{J}_x \pm i \hat{J}_y$$
 Action: $\hat{J}_{\pm} | j, m \rangle = \hbar \sqrt{j(j+1) - m(m\pm 1)} | j, m \pm 1 \rangle$

Relation between coupled and uncoupled representations of states formed by two subsystems with angular momenta j_1 and j_2

$$|J M j_1 j_2\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle j_1 m_1 j_2 m_2 | J M j_1 j_2 \rangle | j_1 m_1 \rangle | j_2 m_2 \rangle \qquad m_1 + m_2 = M$$

$$|j_1 m_1\rangle | j_2 m_2\rangle = \sum_{J=|j_1-j_2|}^{j_1+j_2} \langle J M j_1 j_2 | j_1 m_1 j_2 m_2 \rangle | J M j_1 j_2 \rangle \qquad M = m_1 + m_2$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Matrix form of angular momentum operators for l = 1

$$L_x = \frac{1}{\sqrt{2}}\hbar \begin{pmatrix} 0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0 \end{pmatrix} \qquad \qquad L_y = \frac{1}{\sqrt{2}}\hbar \begin{pmatrix} 0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0 \end{pmatrix} \qquad \qquad L_z = \hbar \begin{pmatrix} 1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1 \end{pmatrix}$$

Electron in a magnetic field

Hamiltonian: $H = -\boldsymbol{\mu} \cdot \mathbf{B} = -\gamma \mathbf{B} \cdot \mathbf{S} = \frac{e}{m} \mathbf{B} \cdot \mathbf{S} = \mu_{\mathrm{B}} \mathbf{B} \cdot \boldsymbol{\sigma}$ here e > 0 is the magnitude of the electron electric charge and $\mu_{\mathrm{B}} = \frac{e\hbar}{2m}$

Bloch theorem for periodic potentials V(x+a) = V(x)

 $\psi(x) = e^{ikx}u(x)$, where u(x+a) = u(x) Equivalent form: $\psi(x+a) = e^{ika}\psi(x)$

Density matrix $\hat{\rho}$

$$\begin{split} \hat{\rho} &= \sum_{i} p_{i} |\psi_{i}\rangle \langle \psi_{i}|, \quad \text{where } \sum_{i} p_{i} = 1 \\ \text{Expectation value of some observable } A: \quad \langle \hat{A} \rangle &= \sum_{i} p_{i} \langle \psi_{i} | \hat{A} | \psi_{i} \rangle = \operatorname{tr}(\hat{\rho} \hat{A}), \text{ where } \operatorname{tr}(\hat{\rho}) = 1 \end{split}$$

Time evolution operator

 $\hat{U}(t_f, t_i) = \hat{\mathcal{T}} \exp\left[-\frac{i}{\hbar} \int_{t_i}^{t_f} \hat{H}(t) dt\right] = 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \dots \int_{t_i}^{t_{n-1}} dt_n \hat{H}(t_1) \hat{H}(t_2) \dots \hat{H}(t_n)$ In particular, $\hat{U}(t_f, t_i) = \exp\left[-\frac{i}{\hbar} \hat{H}(t_f - t_i)\right]$ when $\hat{H} \neq \hat{H}(t)$

Schrödinger, Heisenberg and interaction pictures

$$\begin{split} \psi_{H} &= \hat{U}^{-1}\psi_{S}, \ \psi_{H} = \psi_{S}(t=0), \ \hat{A}_{H} = \hat{U}^{-1}\hat{A}_{S}\hat{U}, \ i\hbar\frac{\hat{A}_{H}}{dt} = [\hat{A}_{H},\hat{H}] + i\hbar\frac{\partial\hat{A}_{H}}{\partial t}, \ \frac{\partial\hat{A}_{H}}{\partial t} \equiv \hat{U}^{-1}\frac{\partial\hat{A}_{S}}{\partial t}\hat{U} \\ \text{If} \ \hat{H} &= \hat{H}_{0} + \hat{V}(t), \ \text{then} \\ \psi_{I} &= \hat{U}_{0}^{-1}\psi_{S}, \ \hat{U}_{0} = \exp\left[-\frac{i}{\hbar}\hat{H}_{0}t\right], \ \hat{A}_{I} = \hat{U}_{0}^{-1}\hat{A}_{S}\hat{U}_{0}, \ i\hbar\frac{\partial\hat{\psi}_{I}}{\partial t} = \hat{V}_{I}\psi_{I} \\ \psi_{I}(t) &= \psi_{I}(0) + \frac{1}{i\hbar}\int_{0}^{t}\hat{V}_{I}(t')\psi_{I}(t')dt' \end{split}$$

Rayleigh-Ritz variational method

$$\psi_{\text{trial}} = \sum_{i=1}^{n} c_i \phi_i \quad Hc = \epsilon Sc, \quad \text{where } c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \quad \text{and} \quad \begin{array}{c} H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle \\ S_{ij} = \langle \phi_i | \phi_j \rangle \end{array}$$

Stationary perturbation theory formulae

$$H = H^{0} + \lambda H', \qquad E_{n} = E_{n}^{(0)} + \lambda E_{n}^{(1)} + \lambda^{2} E_{n}^{(2)} + \dots, \qquad \psi_{n} = \psi_{n}^{(0)} + \lambda \psi_{n}^{(1)} + \lambda^{2} \psi_{n}^{(2)} + \dots$$

$$E_{n}^{(1)} = H'_{nn}$$

$$\psi_{n}^{(1)} = \sum_{m} c_{nm} \psi_{m}^{(0)}, \quad c_{nm} = \begin{cases} \frac{H'_{mn}}{E_{n}^{(0)} - E_{m}^{(0)}}, & n \neq m \\ 0, & n = m \end{cases}$$

$$E_{n}^{(2)} = \sum_{m \neq n} \frac{|H'_{mn}|^{2}}{E_{n}^{(0)} - E_{m}^{(0)}}$$

$$\psi_{n}^{(2)} = \sum_{m} d_{nm} \psi_{m}^{(0)}, \quad d_{nm} = \begin{cases} \frac{1}{E_{n}^{(0)} - E_{m}^{(0)}} \left(\sum_{k \neq n} \frac{H'_{mk} H'_{kn}}{E_{n}^{(0)} - E_{k}^{(0)}}\right) - \frac{H'_{nn} H'_{mn}}{(E_{n}^{(0)} - E_{m}^{(0)})^{2}}, & n \neq m \\ 0, & n = m \end{cases}$$

Bohr-Sommerfeld quantization rules

 $\int_{a}^{b} p(x)dx = (n - \frac{1}{2})\pi\hbar$ - the potential has no vertical walls at *a* or *b* $\int_{a}^{b} p(x)dx = (n - \frac{1}{4})\pi\hbar$ - only one wall of the potential is vertical $\int_{a}^{b} p(x)dx = n\pi\hbar$ - both walls of the potential are vertical Here *a* and *b* are classical turning points and *n* = 1, 2, 3, ...

Semiclassical barrier tunneling

$$T \sim \exp\left[-2\int_{a}^{b}\kappa(x)dx\right] \qquad \kappa(x) = \frac{1}{\hbar}\sqrt{2m(V(x)-E)}$$

General time-dependence of the wave function (TDSE in matrix form)

$$H(\mathbf{r},t) = H^{0}(\mathbf{r}) + \lambda H'(\mathbf{r},t), \qquad H^{0}\varphi_{n} = E_{n}^{(0)}\varphi_{n}, \qquad \psi(\mathbf{r},t) = \sum_{n} c_{n}(t)\varphi_{n}(\mathbf{r})e^{\frac{-iE_{n}^{(0)}t}{\hbar}},$$
$$i\hbar\frac{dc_{n}(t)}{dt} = \lambda \sum_{k} H'_{nk}e^{i\omega_{nk}t}c_{k}(t), \qquad H'_{nk} = \langle \phi_{n}|H'|\phi_{k}\rangle, \qquad \omega_{nk} = \frac{E_{n}^{(0)}-E_{k}^{(0)}}{\hbar}$$

Time-dependent perturbation theory formulae

 $H(\mathbf{r},t) = H^{0}(\mathbf{r}) + \lambda H'(\mathbf{r},t), \qquad H^{0}\varphi_{n} = E_{n}^{(0)}\varphi_{n}, \qquad \lambda H' \text{ is small}$ $\psi(\mathbf{r},t) = \sum_{n} c_{n}(t)\varphi_{n}(\mathbf{r})e^{\frac{-iE_{n}^{(0)}t}{\hbar}}, \qquad c_{n}(t) = c_{n}^{(0)} + \lambda c_{n}^{(1)} + \lambda^{2}c_{n}^{(2)} + \dots$ If $c_{n}(t_{0}) = \delta_{nm}$ then at time $t > t_{0}$

$$c_n^{(0)} = \delta_{nm},$$

$$c_n^{(1)}(t) = \frac{1}{i\hbar} \int_{t_0}^t H'_{nm}(t') e^{i\omega_{nm}t'} dt',$$

$$c_n^{(2)}(t) = \left(\frac{1}{i\hbar}\right)^2 \sum_k \int_{t_0}^t dt' \int_{t_0}^{t'} H'_{nk}(t') H'_{km}(t'') e^{i\omega_{nk}t'} e^{i\omega_{km}t''} dt'', \dots$$

Fermi's golden rule

Transition probability: $P_{i \to f}(t) = \frac{2\pi t}{\hbar} |\mathcal{H}'_{fi}|^2 g(E_f)$, Transition rate: $\Gamma_{i \to f} = \frac{2\pi}{\hbar} |\mathcal{H}'_{fi}|^2 g(E_f)$ where $\mathcal{H}'_{fi} = \langle \varphi_f | \mathcal{H}'(\mathbf{r}) | \varphi_i \rangle$ and g(E) is the density of states

Stationary quantum scattering

Wave function at $r \to \infty$: $\psi(r, \theta, \phi) \approx A \left[e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \right], \quad k = \frac{\sqrt{2mE}}{\hbar}$ Differential cross section: $\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$ Total cross section: $\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega$

Partial wave analysis

For a spherically symmetric potential $\psi(r,\theta) = A \left[e^{ikz} + k \sum_{l=0}^{\infty} i^{l+1} (2l+1) a_l h_l^{(1)}(kr) P_l(\cos \theta) \right]$ $f(\theta) = \sum_{l=0}^{\infty} (2l+1) a_l P_l(\cos \theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin \delta_l P_l(\cos \theta)$ $\sigma_{\text{tot}} = 4\pi \sum_{l=0}^{\infty} (2l+1) |a_l|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$ Relation between partial wave amplitudes and phase shifts: $a_l = \frac{1}{k} e^{i\delta_l} \sin \delta_l$ Rayleigh formula for a plane wave expansion: $e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos \theta)$

Lippmann-Schwinger equation

 $\psi(\mathbf{r}) = \varphi(\mathbf{r}) + \frac{2m}{\hbar^2} \int G(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}',$ where $\varphi(\mathbf{r})$ is a free-particle solution (incident wave) and $G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$ is Green's function **Born approximation**

$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2} \int e^{i\mathbf{q}\cdot\mathbf{r}'} V(\mathbf{r}') d\mathbf{r}', \quad \mathbf{q} = \mathbf{k}' - \mathbf{k}, \quad q = 2k \sin\frac{\theta}{2}, \quad \mathbf{k} = k\mathbf{\hat{r}}, \quad \mathbf{k}' = k\mathbf{\hat{z}}$ For spherically symmetric potentials $f(\theta) = -\frac{2m}{\hbar^2 q} \int_{0}^{\infty} rV(r) \sin(qr) dr$

Adiabatic evolution of a particle that starts in the k-th state of a time-dependent Hamiltonian $\hat{H}(t)$

$$\Psi_{k}(\mathbf{r},t) = e^{i\theta_{k}(t)}e^{i\gamma_{k}(t)}\psi_{k}(\mathbf{r},t), \quad \hat{H}(t)\psi_{k}(\mathbf{r},t) = E_{k}(t)\psi_{k}(\mathbf{r},t), \quad \theta_{k}(t) = -\frac{1}{\hbar}\int_{0}^{t}E_{k}(t')dt',$$

$$\gamma_{k}(t) = i\int_{0}^{t}\langle\psi_{k}(\mathbf{r},t')|\frac{\partial}{\partial t'}\psi_{k}(\mathbf{r},t')\rangle dt' = i\int_{\mathbf{R}(0)}^{\mathbf{R}(t)}\langle\psi_{k}|\nabla_{\mathbf{R}}\psi_{k}\rangle \cdot d\mathbf{R}, \quad \mathbf{R}(t) = (R_{1}(t), R_{2}(t), \dots, R_{N}(t)),$$

$$R_{i}(t), \ i = 1, \dots, N \text{ are parameters in the Hamiltinian that change with time}$$

Dirac delta function

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx = f(x_0) \qquad \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}dk \qquad \delta(-x) = \delta(x) \qquad \delta(cx) = \frac{1}{|c|}\delta(x)$$

Fourier transform conventions

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)e^{-ikx}dx \qquad \qquad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{f}(k)e^{ikx}dk$$

or, in terms of $p = \hbar k$ $\tilde{f}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} f(x)e^{-ipx/\hbar} dx$ $f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{f}(p)e^{ipx/\hbar} dp$

Useful integrals

$$\begin{split} \int \sqrt{a^2 - x^2} \, dx &= \frac{1}{2} \left(x \sqrt{a^2 - x^2} + a^2 \arctan\left[\frac{x}{\sqrt{a^2 - x^2}}\right] \right) \\ &\int_{0}^{\infty} x^{2k} e^{-\beta x^2} \, dx = \sqrt{\pi} \frac{(2k)!}{k! 2^{2k+1} \beta^{k+1/2}} \quad (\text{Re }\beta > 0, \, k = 0, 1, 2, ...) \\ &\int_{0}^{\infty} x^{2k+1} e^{-\beta x^2} \, dx = \frac{1}{2} \frac{k!}{\beta^{k+1}} \quad (\text{Re }\beta > 0, \, k = 0, 1, 2, ...) \\ &\int_{0}^{\infty} x^k e^{-\gamma x} \, dx = \frac{k!}{\gamma^{k+1}} \quad (\text{Re }\gamma > 0, \, k = 0, 1, 2, ...) \\ &\int_{-\infty}^{\infty} e^{-\beta x^2} e^{iqx} \, dx = \sqrt{\frac{\pi}{\beta}} e^{-\frac{q^2}{4\beta}} \quad (\text{Re }\beta > 0) \\ &\int_{0}^{\pi} \sin^{2k} x \, dx = \pi \frac{(2k-1)!!}{2^k k!} \quad (k = 0, 1, 2, ...) \\ &\int_{0}^{\pi} \sin^{2k+1} x \, dx = \frac{2^{k+1} k!}{(2k+1)!!} \quad (k = 0, 1, 2, ...) \\ &\int_{0}^{2\pi} \cos m\phi \, e^{in\phi} \, dx = \pi (\delta_{m,n} + \delta_{m,-n}) \quad (m, n = 0, \pm 1, \pm 2, ...) \end{split}$$

Useful trigonometric identities

 $\sin(\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta \qquad \cos(\alpha \pm \beta) = \cos \alpha \cos \beta \mp \sin \alpha \sin \beta$ $\sin \alpha \sin \beta = \frac{1}{2} [\cos(\alpha - \beta) - \cos(\alpha + \beta)] \qquad \cos \alpha \cos \beta = \frac{1}{2} [\cos(\alpha - \beta) + \cos(\alpha + \beta)]$ $\sin \alpha \cos \beta = \frac{1}{2} [\sin(\alpha + \beta) + \sin(\alpha - \beta)] \qquad \cos \alpha \sin \beta = \frac{1}{2} [\sin(\alpha + \beta) - \sin(\alpha - \beta)]$

Useful identities for hyperbolic functions

 $\cosh^2 x - \sinh^2 x = 1$ $\tanh^2 x + \operatorname{sech}^2 x = 1$ $\operatorname{coth}^2 x - \operatorname{csch}^2 x = 1$