

- $E_n = \left(n + \frac{1}{2}\right) \hbar \omega$
- $a^\dagger \psi_n = \sqrt{n+1} \psi_{n+1} \quad a \psi_n = \sqrt{n} \psi_{n-1}$
- $\psi_n = \frac{1}{\sqrt{n!}} (a^\dagger)^n \psi_0$
- $a = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right)$
- $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a)$

4 The Free Particle

- $V(x) = 0$ everywhere
- Wave packet: $\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$
- $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dx$
- $k \equiv \pm \frac{\sqrt{2mE}}{\hbar}, \quad \text{with } \begin{cases} k > 0 & \Rightarrow \text{traveling to the right} \\ k < 0 & \Rightarrow \text{traveling to the left} \end{cases}$
- Group velocity: $v_{group} = \frac{d\omega}{dk}$
- Phase velocity: $v_{phase} = \frac{\omega}{k}$

5 The Hydrogen Atom

- $E_n = \frac{-13.6 \text{ eV}}{n^2}$
- $\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \quad a = 0.53 \times 10^{-10} \text{ m}$
- Selection rules for transitions:
 - $\Delta l = \pm 1, \quad \Delta m = \pm 1, 0$

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Quantum Mechanical/Molecular Mechanical Approaches for the Investigation of Chemical Systems - Recent Developments and Advanced Applications Thomas S. Hofer, Sam P. de Visser, 2018-11-28 The QM MM method short for quantum mechanical molecular mechanical is a highly versatile approach for the study of chemical phenomena combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system Originally conceived in the 1970s by the influential work of the the Nobel laureates Martin Karplus Michael Levitt and Arieh Warshel QM MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods Whereas the first applications have been focused on studies of organic and biomolecular systems a large variety of QM MM implementations have been developed over the last decades extending the range of applicability to address research questions relevant for both solution and solid state chemistry as well Despite approaching their 50th anniversary in 2022 the formulation of improved QM MM methods is still an active field of research with the aim to i extend the applicability to address an even broader range of research questions in chemistry and related disciplines and ii further push the accuracy achieved in the QM MM description beyond that of established formulations While being a highly successful approach on its own the combination of the QM MM strategy with other established theoretical techniques greatly extends the capabilities of the computational approaches For instance the integration of a suitable QM MM technique into the highly successful Monte Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum mechanical basis This eBook presents the contributions of a recent Research Topic published in Frontiers in Chemistry that highlight novel approaches as well as advanced applications of QM MM method to a broad variety of targets In total 2 review articles and 10 original research contributions from 48 authors are presented covering 12 different countries on four continents The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM MM method and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources it can be expected that the impact of QM MM methods in chemical sciences will be further increased already in the near future

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